

## 251st American Chemical Society National Meeting & Exposition

March 13 –17, 2016  
San Diego, CA

# Computers in Chemistry

[www.acs.org/SanDiego2016](http://www.acs.org/SanDiego2016)  
#acsSanDiego



Download the ACS San Diego Mobile App or access the Digital Meeting Program at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016) for up-to-date meeting information.



[www.acs.org/meetingapp](http://www.acs.org/meetingapp)



\*Online version is also available for internet enabled devices.

March 13 -17, 2016  
San Diego, California  
#acsSanDiego  
www.acs.org/SanDiego2016

## 251st American Chemical Society National Meeting & Exposition

# Computers in Chemistry

### **Satellite Registration/ Onsite Program Purchase & Pickup**

Printed copies of the Onsite Program Book will no longer be available for free. In support of the ACS's sustainability efforts, we encourage the use of the ACS San Diego mobile app and Digital Program for quick access to the meeting's full technical program, maps, and search features.

### **Prefer a Printed Onsite Program?**

The Onsite Program Book will now be available for the fee of \$20. Visit the below locations to purchase your copy. Limited quantities will be available.

### **Satellite Registration also available at these locations.**

Manchester Grand Hyatt, Coronado Ballroom Foyer  
Hilton Bayfront, Sapphire North/West Foyer  
Westin San Diego, Broadway Terrace

Saturday, 3 to 6 PM  
Sunday, 7:30 AM to 7:30 PM  
Monday, 7:30 AM to 9 PM  
Tuesday, 7:30 AM to 5 PM

### **Registration & Program Purchase & Pickup available at the San Diego Convention Center, Lobby D during the standard schedule.**

Learn more about the ACS National Meetings  
Sustainability Efforts at [www.acs.org/greenermeetings.com](http://www.acs.org/greenermeetings.com)

Please note that if you misplace your purchased Onsite Program,  
you will be charged \$20 for a replacement.



Questions?  
Contact [NationalMeetings@acs.org](mailto:NationalMeetings@acs.org)

# 251st American Chemical Society National Meeting & Exposition

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## ACS OPERATIONS OFFICES

- **San Diego Convention Center (Room 14B):** 619-525-6208
- **Hilton San Diego Bayfront Sapphire (410B):** 619-321-2893
- **Hilton Gaslamp Quarter (Coronado Room):** 619-702-8298
- **Manchester Grand Hyatt (Show Office 6):** 619-358-6870
- **Marriott Marquis San Diego Marina (Encinitas):** 619-645-6920
- **Omni San Diego Hotel (Boardroom 1):** 619-770-1720
- **Westin San Diego (Ivory Room):** 619-338-3652
- **US Grant (Chaffee Court):** 619-744-2092

## INFORMATION CONTACTS

- **Attendee Registration, San Diego Convention Center, Lobby D:**  
619-525-6219
- **Career Fair Information Center, San Diego Convention Center, Hall A:**  
619-525-6224
- **Exhibitor Registration, San Diego Convention Center, Lobby C:**  
619-525-6221
- **Finance Office, San Diego Convention Center, Box Office E:**  
619-525-6218
- **Host Local Section Booth, San Diego Convention Center, Lobby D:**  
619-525-6225
- **Member Services, San Diego Convention Center, Lobby D:** 619-525-6228
- **Press Center, San Diego Convention Center, Room 16B:** 619-525-6215
- **Shuttle Desk, San Diego Convention Center, Box Office A:** 619-525-6226
- **Society Program Office, Hilton San Diego Bayfront, Sapphire 410 A:**  
619-321 6543
- **Governance Office, Hilton San Diego Bayfront, Sapphire 400 A/B:**  
619-321-6541

## ACS OFFICERS

Donna J. Nelson, President  
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Diane Grob-Schmidt, Immediate Past President  
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## American Chemical Society

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Fax: 202-872-4615 E-mail: [help@acs.org](mailto:help@acs.org) Website: [www.acs.org](http://www.acs.org)

The American Chemical Society is a self-governed individual membership organization of members at all degree levels and in all fields of chemistry. The Society provides a broad range of opportunities for peer interaction and career development, regardless of professional or scientific interests. The programs and activities conducted by ACS today are the products of a tradition of excellence in meeting member needs that dates from the Society's founding in 1876.

This On-site Meeting Program is published by the American Chemical Society as a service to its attendees. Information contained herein is subject to change without notice. While every effort is made to ensure accuracy, ACS makes no warranties, expressed or implied, related to the information. For the official technical program for the 251st National Meeting & Exposition, refer to [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016). All San Diego photos in this program are courtesy of the San Diego Convention and Visitors Bureau and Shutterstock.



**ACS**  
Chemistry for Life®

# ACS NO RECORDING POLICY

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from the ACS.

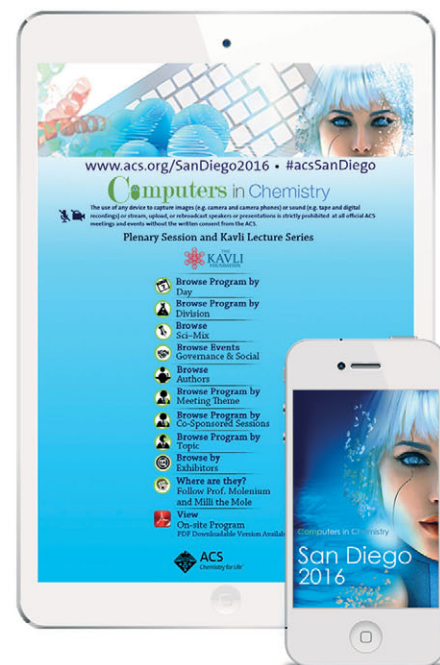
## EMBRACING SUSTAINABILITY PRACTICES

The American Chemical Society continues to be a sustainability leader within the meeting and events community with most recently being the recipient of the 2014 Trade Show Executive's Gold 100 Award as the show with the Most Commendable Green Initiatives. ACS and the Greener Meetings Program have also been showcased in Convene Magazine's August 2015 annual Best in Show issue for the "Best CSR Initiatives" and awarded the 2011 and 2012 PCMA Capital Chapter Green Leader Award.

Efforts of our sustainability practices are briefly noted below. These changes not only support a greener meeting but also improve your meeting experience.

- Condensed Onsite Program book with enhancing the mobile application and digital options
- Decreased print-run of the Onsite Program book due to digital and mobile applications
- Moved to using recycled paper for the Onsite Program Book
- Reformatted National Meeting website based on viewer analytics
- Free WiFi inside public areas at the Convention Center and many contracted hotels
- Established partnership with American Forests to offset carbon missions
- Audited contracted hotels on their sustainability efforts
- Partnered with Convention Center to source local foods for designated events
- Increased usage of digital signage
- Partnered with vendors that engaged in sustainability practices
- Increased attendee engagement through the Greener Meetings Challenge
- Adjusted meeting room temperature to 70° F for energy conservation

Thank you for your support in making ACS a leader in sustainability. Further information can be found at: [www.acs.org/greenermeetings](http://www.acs.org/greenermeetings). There you will find the ACS 2015 Sustainability Report including information on how to join the Greener Meetings Challenge.





251st American Chemical Society National Meeting & Exposition

# Where to Find Meeting Information

## San Diego, CA

March 13 - 17, 2016

[www.acs.org/SanDiego2016](http://www.acs.org/SanDiego2016)

### Official Meeting Website

[www.acs.org/SanDiego2016](http://www.acs.org/SanDiego2016)

### Announcements & Changes

[www.acs.org/meetingupdates](http://www.acs.org/meetingupdates)

### Digital Meeting Program

[www.acs.org/SanDiego2016](http://www.acs.org/SanDiego2016)



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[www.facebook.com/  
americanchemicalsociety](http://www.facebook.com/americanchemicalsociety)



[http://communities.acs.org/  
community/science/meetings](http://communities.acs.org/community/science/meetings)



Download the free mobile app  
at [www.acs.org/meetingapp](http://www.acs.org/meetingapp)

# Computers in Chemistry

Text your question to 754.227.2012

*(Standard text rates apply)*

## Welcome to San Diego and the 251st ACS National Meeting

**T**wenty-nine technical divisions and five committees are hosting original programming based on the meeting theme of Computers in Chemistry. More than 12,000 papers will be presented, and nearly 5,000 poster presentations will take place at the meeting. As well, there are a number of special events planned throughout the meeting. The ACS Board of Directors Regular Meeting will be an opportunity to hear Amy Harmon, New York Times National Correspondent, talk about 'Telling Science Stories: Dispatch from a Conflict Zone.' Please join your colleagues from noon to 1:00 p.m. in Room 20D of the San Diego Convention Center.

The presidential programming promises excellent science as well as opportunities to become involved in discussions and community efforts to address member concerns. On Sunday afternoon, "Discussions with the President's Task Force on Employment" will present speakers from academe, government, and industry reporting the results of last year's efforts on topics pertinent to unemployment in the chemical sciences.

Representatives from publishers of comprehensive undergraduate organic chemistry textbooks will speak Monday morning addressing the question "Is there a Crisis in Organic Chemistry? They will discuss changes in organic chemistry prerequisites, current teaching methods, and responses of organic chemistry programs, professors, and requirements. Monday afternoon, researchers will present their demographic data, disaggregated by race and gender, on various sectors of the chemical sciences in a symposium titled "Diversity—Quantification—Success." In order to encourage community efforts to address member concerns in each of these three areas, there will be corresponding contributed Presidential posters sessions on Sunday evening, and on Monday evening during Sci-Mix.

All of the above programming was designed to respond to the concerns of ACS members. Therefore, members now have the opportunity to address these community concerns by attending and participating in the discussions.



Donna J. Nelson  
ACS President

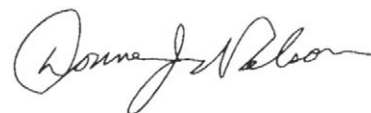
PHOTO: DAVID MOORESE

"How to Foster Diversity in the Chemical Sciences: Lessons Learned and Taught from the Stories of Recipients of the Stanley C. Israel Award" promises ideas and inspiration for increasing diversity in our communities. Finally, the Dreyfus Award Symposium will honor its most recent recipient of this award, Krzysztof Matyjaszewski, by focusing on "Making Molecules and Materials." Details of these symposia can be found at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016).

On Monday afternoon, Dr. Rommie Amaro, Associate Professor of Chemistry and Biochemistry at the University of California, San

Diego will deliver The Kavli Foundation Emerging Leader in Chemistry Lecture on 'Computing Cures: Enabling Chemical Discovery through the Lens of a Computational Microscope.' Dr. Emily Carter, Founding Director of the Andlinger Center for Energy and the Environment at Princeton University then will give The Fred Kavli Innovations in Chemistry Lecture (San Diego Convention Center, Ballroom 20 A-C) on 'Quantum Solutions for a Sustainable Energy Future.'

A range of professional development classes will be available; ACS Short Courses have a separate registration and fee. Job seekers can meet and interview with potential employers at the ACS Career Fair, find one-on-one career assistance, and pick among more than 20 career workshops. The exposition will feature more than 250 companies that will showcase services, instruments, books, lab equipment, and much more in more than 400 booths. I express thanks to members of the San Diego Local Section, the Committee on Meetings and Expositions, the divisional program and symposium chairs who organized the technical sessions, ACS staff, and thanks to all of you for attending.



Donna J. Nelson  
ACS President

## Welcome Message from Kenneth Merz, Jr., San Diego Thematic Program Chair

The 251st ACS National Meeting, (San Diego, March 13-17), will showcase the impact and role of Computers in Chemistry. Computers have had a transformative effect on the chemical sciences impacting areas from data acquisition and storage to the design of novel materials. With the ever-increasing performance of computers in terms of networking, central processing unit (CPU) performance to data storage capabilities the role of computers and computation in our common field of Chemistry will continue to grow in the coming years. Through MPPG organized symposia and collaborative sessions with a broad range of ACS Divisions the impact of computers in the chemical sciences, both in the past and in the future, will be highlighted.

The plenary session, on Sunday afternoon, March 13, will inaugurate the theme with four invited lectures: Prof. Sharon Hammes-Schiffer (UIUC) will discuss her studies on proton-coupled electron transfer in catalysis and energy conversion; Prof. Bill Jorgensen (Yale, University) will present an overview of challenges and future opportunities in computer-aided drug design and discovery; Prof. David Baker (University of Washington) will discuss his lab's innovative computational and experimental work on designing proteins with specific structures and functions; and Prof. George Schatz will describe his computational work focused on the use of self-assembly to design functional materials. The afternoon of Monday, March 14 the Fred Kavli Innovations in Chemistry Lecture will be delivered by Prof. Emily Carter (Princeton University) "Quantum Solutions for a Sustainable Energy Future" and will be coupled with the Kavli Foundation Emerging Leader in Chemistry Lecture, "Computing Cures: Enabling Chemical Discovery through the Lens of a Computational Microscope" which will be delivered by Prof. Rommie Amaro.

Coupled with the exceptional technical program constructed by the ACS divisions that includes both topical sessions and sym-



**Kenneth Merz, Jr.**  
San Diego Thematic  
Program Chair

posia honoring the winners of ACS awards, MPPG and partner divisions will add multiple half and full day symposia focused on the role of Computers in Chemistry. The choice of possible session topics was immense, but MPPG will focus on five contemporary areas where computation is having a broad impact: Computer-aided Drug Design will discuss the current and future impact of computation on drug discovery and design; Big Data Science will explore the role of computation in dealing with the explosion of data available to chemical and allied fields; Computational Materials and Nanoscience will examine the role of computation in understanding the structure and function of novel materials as

well as the design of novel materials with unique functions; Multiscales Chemistry will explore the theoretical challenges involved in moving from molecular to macroscopic assemblies; and last, but not least, the session on Preparing for the Real World: Challenges Faced by Young Investigators will provide timely advice and insights to young investigators (both in computational and experimental fields) as they transition from the Ph.D. to the postdoc to the first permanent job. The session chairs for each of these topics are listed as well and without their tireless help the sessions organized under the MPPG banner would not of been possible. Along with these five MPPG sponsored sessions there are a broad range of joint session between MPPG and a number of divisions that will further highlight Computers in Chemistry.

- Computer-aided Drug Design: Prof. Rommie Amaro (UCSD), Dr. Kate Holloway (Merck) and Dr. Hanneke Jansen (Novartis).
- Big Data Science: Prof. Alex Tropsha (UNC) and Prof. Brian Shoichet (UCSF).

## Welcome Message from Kenneth Merz, Jr., San Diego Thematic Program Chair

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CONTINUED FROM PAGE 5

- Computational Materials and Nanoscience: Theory Meets Experiment: Prof. Alan Aspuru-Guzik (Harvard), Dr. Sergei Tretiak (Los Alamos National Laboratory) and Prof. Oleg Prezhdo (USC).
- Multiscales Chemistry: Prof. Sharon Hammes-Schiffer (UIUC) and Prof. Rigoberto Hernandez (Georgia Tech).
- Preparing for the Real World: Challenges Faced by Young Investigators: Prof. Sereina Riniker (ETH), Prof. Ben Levine (MSU), Prof. Dominika Zgid (UM) and Dr. Whitney Kellett (Oxford).
- The program for the meeting and other information is available online at the website for the San Diego ACS meeting.

I am very grateful to the Chairs of the themed sessions for their efforts, the program chairs of a broad range of divisions, and the ACS staff for their unstinting aid in helping to develop the Computers in Chemistry theme for this meeting. I look forward to meeting you in San Diego.



Kenneth M. Merz, Jr.  
Thematic Program Chair





## OFFICE OF THE GOVERNOR

March 13, 2016

### *American Chemical Society*

On behalf of the State of California, I am pleased to welcome you to the 251st American Chemical Society (ACS) National Meeting & Exposition.

Since 1876, ACS has been a leader in the advancement of the fields of science. With a commitment to sharing professional work via public outreach programs and supporting future chemists with free educational resources, ACS has improved the lives of many through the transforming power of chemistry. Science is a high calling and I hope this event provides you the opportunity to visit with friends, make new acquaintances and share your experiences from the field.

Best wishes for a memorable and productive meeting.

Sincerely,

  
EDMUND G. BROWN JR.



March 13-17, 2016

On behalf of the citizens of San Diego, welcome to America's Finest City!  
Thank you for choosing San Diego for the 251st American Chemical Society  
National Meeting & Exposition.

We are delighted that you have made your way to San Diego. Our city  
boasts a relaxed atmosphere filled with friendly people and a thriving  
tourism industry. It's no surprise that San Diego is so often chosen as the  
host city of several large conventions and events.

With nearly perfect weather every day, no attraction is off limits. Each  
community in San Diego has something different to offer! Our vibrant,  
multicultural city is home to relaxing beaches, luxurious shops in beautiful  
La Jolla, authentic Mexican food in Old Town, a vibrant nightlife in the  
Gaslamp Quarter, historic Balboa Park, the San Diego Zoo and so  
much more.

I am confident you will enjoy your time in San Diego, and thank you  
for choosing to visit our great city. I extend my warmest wishes for an  
enjoyable and successful event in San Diego.

Sincerely,

Kevin L. Faulconer  
Mayor, City of San Diego

# Computers in Nanoscience & Nanotechnology

## Symposium at the Spring 2016 ACS National Meeting

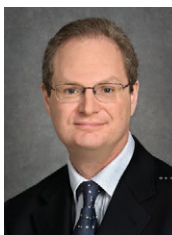
**Monday, March 14 | 1:00 PM – 3:40 PM**

**San Diego Convention Center | Room 5A**

Join the Editors of *ACS Nano* and *Nano Letters* for the next semi-annual joint session in conjunction with the ACS National Meeting. The 2016 spring symposium is specially designed for the National Meeting theme with world-renowned speakers from the nanoscience and nanotechnology community presenting their ground-breaking research.



**PAUL WEISS**  
EDITOR-IN-CHIEF, ACS NANO



**PAUL ALIVISATOS**  
CO-EDITOR, NANO LETTERS

### GUEST SPEAKERS & PRESENTATIONS

**Kenneth Merz**, Editor-in-Chief, *Journal of Chemical Information & Modeling*, Michigan State University

*Thermodynamics of Virus Capsid Assembly*

**Carlton Willson**, University of Texas at Austin

*Polymers for Microelectronics: A View of the Future*

**Philip Kim**, Harvard University

*Electron Transport across the van der Waals Interfaces*

**Julia Greer**, California Institute of Technology

*Fractal Arrangement of Atomic Structures in Metallic Glasses*

**Paul Weiss**, University of California, Los Angeles

*New approaches to multimodal nanoscale imaging and analyses*



251st ACS National Meeting  
San Diego, CA  
March 13-17, 2016  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## PRESIDENTIAL SYMPOSIA AND EVENTS

Photo: David McNeese



**Donna J. Nelson, Ph.D.**  
ACS President

*Sponsored by the ACS President*

### Saturday, March 12, 2016

1:00 PM-4:00 PM

#### **Presidential Outreach Event: Exploring Our World Through Chemistry**

(Cosponsored by CCA and ACS Member Communities)  
Central Library  
(330 Park Boulevard San Diego, CA 92101)

### Monday, March 14, 2016

8:30 AM-12:00 PM

#### **How to Foster Diversity in the Chemical Sciences: Lessons Learned and Taught from the Stories of Recipients of the Stanley C. Israel Award**

(Cosponsored by CMA & PROF)  
San Diego Convention Center, Room 5A  
(Upper Level)

### Tuesday, March 15, 2016

9:00 AM-4:30 PM

#### **Dreyfus Award Symposium**

San Diego Convention Center, Room 2  
(Upper Level)

*Organized by the ACS President in response to ACS members' concerns. Attend – participate – discuss! Please help our community!!*

### Sunday, March 13, 2016

1:30 PM-4:00 PM

#### **Discussions with the President's Task Force on Employment**

(Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB & WCC)

San Diego Convention Center, Room 2  
(Upper Level)

8:00 PM-10:00 PM

(Poster Sessions)

San Diego Convention Center, Hall D  
(Ground Level)

- **My Comments to the President's Task Force on Employment**  
(Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB & WCC)
- **My Experience with and Advice for Improving Diversity in Chemistry**  
(Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF & WCC)
- **My Experiences in and Advice for Organic Chemistry Courses**  
(Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY & PROF)

### Monday, March 14, 2016

9:15 AM-11:30 AM

#### **Is There a Crisis in Organic Chemistry Education?**

(Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY & PROF)

San Diego Convention Center, Room 3  
(Upper Level)

1:30 PM-4:00 PM

#### **Diversity - Quantification - Success?**

(Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF & WCC)

San Diego Convention Center, Room 3  
(Upper Level)

8:00 PM-10:00 PM (Sci-Mix)

(Poster Sessions)

San Diego Convention Center, Halls D/E, (Ground Level)

- **My Comments to the President's Task Force on Employment**
- **My Experience with and Advice for Improving Diversity in Chemistry**
- **My Experiences in and Advice for Organic Chemistry Courses**



American Chemical Society



WE'VE BEEN WORKING  
TOGETHER ALL ALONG

IT'S TIME WE MET

We're the scientists, technologists and business leaders behind *Chemical Abstracts* and solutions such as **SciFinder®** and **STN®**.

While we've been contributing to scientific breakthroughs for more than a century, it's the future that motivates us. We're always pursuing new knowledge.

Together, we will do great things.

**Discover CAS | Visit CAS at the ACS Booth**



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REGULAR SESSION**



Guest Speaker: **Amy Harmon**  
National Correspondent  
*The New York Times*

Sunday, March 13, 2016  
Noon – 1:00 PM  
Room 20D (Upper Level)  
San Diego Convention Center

***“Telling Science Stories: Dispatch from a Conflict Zone”***

Amy Harmon, a reporter for the New York Times, covers the social implications of science and technology. Harmon has won two Pulitzer Prizes, one in 2008 for her series, “The DNA Age,” the other as part of a team in 2001. She received a Guggenheim Fellowship in science writing in 2013. In 2014, her articles on genetically engineered crops were awarded a prize for in-depth reporting from the Society of Environmental Journalists and the Science in Society award from the National Association of Science Writers. Autism has long been an interest of Harmon’s. Her article, “Autistic and Seeking a Place in an Adult World” won the 2012 Casey Medal for excellence in reporting on children and families, and the Times published a version of her story, “Asperger Love,” as an e-book. In 2011, her series about the clinical testing of a new cancer drug received the National Academies of Science award for print journalism. Harmon has also written about her adventures on a treadmill-desk and the search for wildness on a family vacation in Costa Rica.

Her career began at The Michigan Daily, the student newspaper at the University of Michigan, where she earned a B.A. in American culture. She lives in New York City with her husband and 11-year-old daughter.

**Doors Open at 11:45 a.m.**

***Sandwiches and soft drinks will be available to the first 200 attendees.***



# Research Opportunities for Future Energy Technologies

Sunday, March 13, 2016 • 1:30 pm – 5:10 pm  
San Diego Convention Center, Room 4 • (Upper Level)

*Sponsored by ACS Division of Energy & Fuels (ENFL), ACS Publications Division, Chemical Abstracts Service (CAS) & ACS Immediate Past President Diane Grob Schmidt*

Michelle Buchanan, Symposium Co-organizer and Presider  
Oak Ridge National Laboratory

Photo: Peter Cutts Photography



**Diane Grob Schmidt, Ph.D.**  
Symposium Co-organizer  
ACS Immediate Past President



- |                   |   |
|-------------------|---|
| 1:30 pm – 1:40 pm | Introductory Remarks  |
| 1:40 pm – 2:10 pm | The Honorable Franklin (Lynn) M. Orr<br>Under Secretary for Science and Energy<br>U.S. Department of Energy<br><i>The Quadrennial Technology Review: Creating a Clean Energy Future</i> |
| 2:10 pm – 2:40 pm | Donald J. DePaolo<br>Lawrence Berkeley National Laboratory<br><i>Basic Research for Carbon Capture and Storage</i>  |
| 2:40 pm – 3:10 pm | Krishan L. Luthra<br>General Electric<br><i>Structural Materials Needs for Energy Technologies</i>  |
| 3:10 pm – 3:40 pm | Jeremy T. Busby<br>Oak Ridge National Laboratory<br><i>Modern Materials and Chemical Science: Enabling Nuclear Power into the Future</i>  |
| 3:40 pm – 4:10 pm | Peter D. Olmsted<br>Georgetown University<br><i>Basic Science Challenges in Additive Manufacturing</i>  |
| 4:10 pm – 4:40 pm | Tom F. Jaramillo<br>Stanford University<br><i>Hydrogen Generation and Fuel Cells: Current Status, Research Challenges, and Future Prospects</i>   |
| 4:40 pm – 5:10 pm | George W. Crabtree<br>Argonne National Laboratory<br><i>Energy Storage for Transportation and the Electricity Grid: Challenges and Opportunities</i>                                    |
|                   | Closing Remarks   |

# GENERAL MEETING INFORMATION

**YOUR MEETING REGISTRATION** entitles you to a wide range of programming, including more than 12,000 scientific sessions, invited symposia, poster sessions, special lectures and events, award presentations, workshops, and the exposition. Interact with chemical scientists from around the world by participating in social events, networking opportunities, exhibitor sessions, and educational activities, with many events offered at no additional charge. Certain workshops, short courses, and ticketed events require a separate entry fee, as indicated in this program.

## REGISTRATION

**ALL ATTENDEES**, including speakers and poster presenters, must register for the meeting to participate in the technical sessions. Sponsored speakers should contact their symposium organizer or division program chair to clarify the terms of their invitation and to determine who will complete the speaker's registration. Attendees must display their badge at all times for admission to all official ACS sessions and events.

**Early Registration.** Attendees within the U.S. who registered prior to January 24 received their badge credentials by mail before the meeting. International registrants must pick up their badge credentials at ACS Attendee Registration (this includes Canada and Mexico).

**Standard & On-Site Registration.** Attendees who registered after January 24 must pick up their badge credentials on-site at Attendee Registration.

### MEETING INFO ON THE WEB

Registration, housing, technical programming, special events, participating exhibitors, and other meeting details are available at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016).

**Registration Changes.** Attendees can modify their existing registration or generate a receipt from the registration website by following the instructions in their confirmation message. Bring your confirmation and/or badge credentials with you to the meeting for faster processing.

**Registration Methods.** All registrants received confirmation via the original method of registration.

**Internet.** Register online at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016) until March 17. A valid credit card is required to register online, and online registrations are real-time transactions.

**Telephone.** Call the ACS National Meeting Registration Center by March 17 at (800) 251-8629 (U.S./Canada only) or (508) 743-0192 (international), Monday through Friday, 9:00 AM to 5:00 PM ET.

**Fax/Mail.** Submit the registration form by fax, (508) 743-9604, or mail, ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532. Mailed registrations will be accepted until March 17.

**On-site.** Register during the meeting at ACS Attendee Registration at standard registration rates. ACS Attendee Registration will be open at the San Diego Convention Center, Lobby D, on Saturday, 3:00 to 6:00 PM; Sunday, 7:30 AM to 7:30 PM; Monday, 7:30 AM to 9:00 PM; Tuesday, 7:30 AM to 5:00 PM; Wednesday, 7:30 AM to 4:00 PM; and Thursday, 7:30 AM to 1:00 PM.

**REGISTRATION PAYMENTS.** Registration fees can be paid by check, money order, credit card (American Express, Discover, MasterCard, or VISA), or bank wire transfer. Make checks payable in U.S. dollars to the American Chemical Society, and include a completed registration form with each payment. Registration fees should not be combined with any other payment (such as membership dues). Purchase orders and training requests are not accepted. For wire transfer payments, contact the ACS Finance Department at (202) 872-6106 or e-mail [bankwires@acs.org](mailto:bankwires@acs.org). **Registration forms received without payment will not be processed.**

**REGISTRATION ASSISTANCE.** The ACS National Meeting Registration Center will be available from 9:00 AM to 5:00 PM ET by telephone, fax, mail, or e-mail. Ser-

## BADGES

All attendees are required to wear their badges for all technical sessions, poster sessions, and other official meeting events. Our badge holders are recyclable and biodegradable. Please discard appropriately.

REGISTRATION CATEGORY	FEE	
	EARLY BY JAN. 24	STANDARD JAN. 25
<b>MEMBERS</b>		
ACS member or society affiliate	\$415	\$500
Postdoctoral member	415	500
Emeritus or retired member	210	255
50-year member	No fee	No fee
Unemployed member (Dues waiver required)	No fee	No fee
Precollege teacher	105	105
Graduate student	210	210
Undergraduate	105	105
One-day registrant	210	255
<b>NONMEMBERS</b>		
Chemical scientist	\$730	\$880
Postdoctoral scientist	730	880
Visitor: Nonchemical scientist or chemical technician	415	500
Precollege teacher	105	105
Graduate student	415	415
Undergraduate	210	210
One-day registrant	415	500
Guest of registrant <sup>a</sup>	45	45
<b>EXPOSITION-ONLY VISITORS</b>		
Adult, exposition only	\$50	\$50
Student, exposition only	25	25

<sup>a</sup> Registration is restricted to a spouse or family member of registered attendee having no affiliation with the field of chemical science and who is not eligible to become an ACS member. Only one guest registration is allowed per registering attendee, and the guest registration must be completed and paid by the registering attendee at time of original registration.

### ACS BADGE REPRINT POLICY

**1st badge reprint:** no charge, upon proper identification and confirmation of registration payment, a duplicate badge is issued.

**2nd badge reprint:** attendee completes a duplicate badge request, shows identification (which we copy), a charge of \$25 is paid (cash/credit card), a duplicate badge is issued.

**3rd badge reprint:** attendee completes a duplicate badge request, shows identification (which we copy), a charge of \$50 is paid (cash/credit card), a duplicate badge is issued.

**For any badge beyond the 3rd:** attendee completes a duplicate badge request, shows identification (which we copy), a charge of \$100 is paid (cash/credit card), a duplicate badge is issued.



## GENERAL INFORMATION

vice representatives can be reached at (800) 251-8629 (U.S./Canada only) or (508) 743-0192 (international), by fax, (508) 743-9604, e-mail, [acs@xpress-reg.net](mailto:acs@xpress-reg.net), or mail, ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532.

### Registration Cancellations/Refunds.

The deadline for refund requests was February 8. Refund requests made after February 8 will not be honored. Your registration badge credentials and a copy of your registration confirmation must be attached to your request. All refunds will be issued via the original payment method, and refunds will be processed within 30 days after the meeting. Send your request to ACS Registration Cancellation, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532, or fax to (508) 743-9604 (save your fax confirmation sheet).

**Social Event Ticket Cancellations/Refunds.** Social event cancellations received by February 8 entitle the registrant to a full refund. Refund requests made after February 8 will not be hon-

ored. Event tickets and a copy of your registration confirmation must be attached to your request.

### Abstract Cancellations/Refunds.

Abstract USB flash drives (thumb drives) and their shipping costs are nonrefundable.

**MEMBER REGISTRATION.** You must enter a valid ACS membership number during registration to register as a member and receive your ACS member discount on registration fees. Your registration options will automatically appear in accordance with your current membership status in the ACS membership database. Your ACS membership number can be found on your ACS membership card or your Chemical & Engineering News address label. Address questions about your membership status to ACS Member Services at (800) 333-9511 (U.S./Canada only), (614) 447-3776 (international), [service@acs.org](mailto:service@acs.org).

**NONMEMBER REGISTRATION.** Save money on registration fees by joining ACS. You can join ACS now through the online ACS membership application at [www.acs.org/join](http://www.acs.org/join) or by contacting ACS Member Services and then registering for the meeting at your member rate. To receive your meeting discount, you must join the society before you register for the meeting. New memberships or questions about membership status should be handled through ACS Member Services at (800) 333-9511 (U.S./Canada only), (614) 447-3776 (international), or [service@acs.org](mailto:service@acs.org).

**PRESS/MEDIA REGISTRATION.** Press registration is complimentary for credentialed members of the news media (restricted to reporters and editors working full-time for print or broadcast news) who are approved by the ACS Office of Communications. Press badges may be picked up with valid media credentials from the Press Room at the San Diego Convention Center. For more information, visit [www.acs.org/pressroom](http://www.acs.org/pressroom).

**EXPO-ONLY ADMISSION.** All meeting attendees with a valid badge receive complimentary admittance into the exposition as part of their registration. Individuals who want to visit the exposition without registering for the meeting's technical sessions can register for an expo-only adult badge for \$50 or \$25 for students with school identification. Reg-

ister online or in person at ACS Attendee Registration.

**EXHIBITOR REGISTRATION.** Exhibitor registration is handled exclusively through ACS National Expositions at [www.acs.org/expositions](http://www.acs.org/expositions).

**CAREER FAIR EMPLOYER REGISTRATION.** ACS Career Fair Employer registration is handled exclusively through ACS Careers at [www.acs.org/careers](http://www.acs.org/careers).

## ACCOMMODATIONS

ConferenceDirect is the official housing bureau for the ACS National Meeting in San Diego. ACS does not endorse booking hotel reservations through any other sources. All attendees who made their reservations through ConferenceDirect will receive complimentary internet access in their sleeping rooms and will be automatically entered in the ACS Housing Drawing.

**On-Site Housing.** An on-site housing desk will be available during the meeting in the registration area of the San Diego Convention Center to assist with last-minute housing changes or needs.

**RESERVATION.** All registrants will receive confirmation for reservations made directly through ConferenceDirect. Each confirmation contains a unique number that is proof of your reservation through ConferenceDirect.

Published ACS rates apply to hotel stays between March 5 and March 22. To extend your stay beyond these dates, you must reserve additional nights directly through the hotel.

**KEEP YOUR MEETING COSTS AFFORDABLE.** Attendee support of the official hotels allows ACS to use meeting space at a discount and to keep registration fees to a minimum. Stay in an official hotel whenever possible, and reserve your hotel room through ConferenceDirect at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## ACS GREENER MEETINGS

**THE AMERICAN CHEMICAL SOCIETY** Department of Meetings & Expositions Services and the Committee on Meetings & Expositions are committed to greener meetings. For each national meeting, we collaborate with the destination city, convention center, and our

### ONSITE PROGRAM BOOK NO LONGER FREE

Printed copies of the Onsite Program Book will no longer be available for free. The Onsite Program Book will now be available at the advance fee of \$10 until Jan. 24 and at the standard/on-site fee of \$20 after Jan. 24. Orders can be made during registration and on-site at several locations. Limited quantities will be available on-site.

Please note that if you misplace your purchased Onsite Program, you will be charged \$20 for a replacement.

In support of ACS's sustainability efforts, we encourage our meeting attendees to download the ACS San Diego mobile app in early March or access the Digital Meeting Program in mid-March at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016). The ACS San Diego mobile app and Digital Meeting Program will provide quick access to the full technical program along with special features so you can easily build your schedule. Learn more about ACS national meetings sustainability efforts at [www.acs.org/greenermeetings](http://www.acs.org/greenermeetings).

# Make the greener meetings Pledge

[www.acs.org/greenermeetings](http://www.acs.org/greenermeetings)

Each year, ACS holds two National Meetings, attracting over 25,000 chemistry professionals and students to different regions in the US. Through our ACS Greener Meetings Program, we strive to reduce the environmental impacts of our meetings and expositions while enhancing the positive impacts on communities locally and globally.

To accomplish this, we focus on three key initiatives:



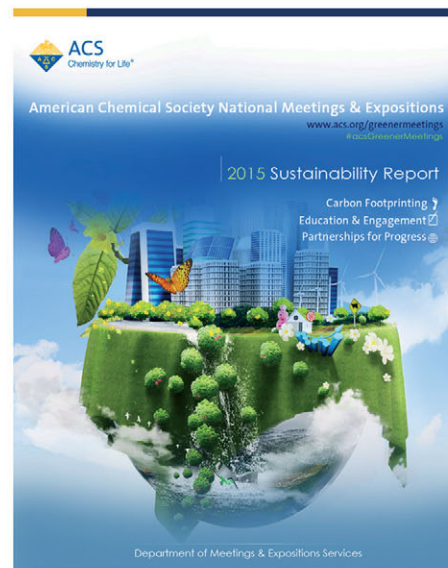
- Calculating and offsetting our event carbon footprint  
(In 2015, over 7,700 trees planted with American Forests)



- Collaborating with convention centers, hotels and other event partners to raise the bar for sustainable practices



- Engage with our attendees—that's YOU!  
(Over 5000 attendees have made the Greener Meetings Pledge. Join them today!)



Learn more and access the  
2015 ACS Sustainability Report  
<http://www.acs.org/greenermeetings>

The ACS Department of Meetings & Expositions Services was awarded the **2014 Trade Show Executive's Gold 100 Award** for Show with the Most Commendable Green Initiatives. ACS and the Greener Meetings Program have also been showcased in **Convene Magazine's August 2015** annual Best in Show issue for "Best CSR Initiatives" and awarded the 2011 and 2012 PCMA Capital Chapter Green Leader Award.

# Greener meetings & Mobile App Lounge

A place to relax and learn more about ACS Greener Meetings & the ACS San Diego Mobile App. Daily prizes, contests, photo opps, and refreshments will be available.

San Diego Convention Center, Lobby C/D

Saturday	2 – 6 PM
Sunday	8AM – 3 PM
Monday	8AM – 3 PM
Tuesday	8AM – 3 PM
Wednesday	8AM – 12 PM

**Download the Free ACS San Diego Mobile App Today!**

- Access the full and up-to-date program
- Build and sync your schedule
- Take notes and share via email
- Connect with social media



#ACSGreenerMeetings  
[www.acs.org/greenermeetings](http://www.acs.org/greenermeetings)  
E-mail - [greenermeetings@acs.org](mailto:greenermeetings@acs.org)



## GENERAL INFORMATION

hotel and vendor partners to reduce our environmental footprint and raise the bar with regard to industry sustainability practices.

Interested in learning more about how we're leading the way? Go to [www.acs.org/greenermeetings](http://www.acs.org/greenermeetings) to read about our greener meeting initiatives and access our annual Event Sustainability Report.

For our efforts, ACS has been recognized as a sustainable event leader and received the 2014 Trade Show Executive's Gold 100 Award for the Show with the Most Commendable Green Initiatives and was highlighted in **Convene** magazine's Best in Show edition for corporate social responsibility initiatives. Here are a few reasons why:

- ACS partners with conservation non-profit American Forests to indirectly offset emissions (staff travel, staff and attendee accommodations, show management freight, and venue energy) through regional tree-planting efforts. In 2015, ACS and its attendees planted 7,739 trees (totaling 9,086 trees since the beginning of the program in 2014).
- ACS's offset partners, along with attendees who opted to offset their footprint by donating \$1.00 to the tree-planting program, reached total indirect offsets for 2015 equal to 3,788 metric tons of carbon dioxide (equivalent to not driving 14,514,750 km in an average passenger vehicle).
- ACS performed on-site walkthroughs for 58% of our hotel room block properties in 2015, nearly 100% of hotels recycle and 50% of hotels participate in food composting programs.
- ACS designates Sci-Mix as a "zero waste" event to raise awareness around responsible waste generation and disposal.

### MAKE THE GREENER MEETING PLEDGE TO SUPPORT OUR EFFORTS!

#### I pledge to

1. Take advantage of linen reuse initiatives at my hotel, decline delivery of unread newspapers, and turn off the lights when away from your hotel room.
2. Responsibly dispose of recyclable materials (paper, plastic, glass, aluminum) in the convention center and hotels.

3. Use the meeting mobile app and digital program instead of the printed on-site program.
4. Use the ACS carbon-offset shuttle service when walking isn't an option.
5. Bring a reusable water bottle to avoid the cost and waste associated with disposable, petroleum-based plastic water bottles.

If you did not pledge during the registration process, you can log into your attendee registration account using your badge number and pledge today. At the end of the meeting, you will have an opportunity to submit your personal sustainability story. Greener Meeting All-stars are eligible to win fun prizes for going above and beyond. Don't forget to stop by the Greener Meetings & Mobile App Lounge in Lobby C/D Saturday (2:00 to 6:00 PM), Sunday (8:00 AM to 3:00 PM), Monday (8:00 AM to 3:00 PM), Tuesday (8:00 AM to 3:00 PM), and Wednesday (8 AM to noon). Prize giveaways, such as water bottles, T-shirts, and edible cups from Loliware will happen daily.

Come take your picture in our photo booth lounge. The best social media posts using the hashtag #ACSGreenerMeetings will win additional prizes.

Got feedback? Please e-mail your suggestions to [greenermeetings@acs.org](mailto:greenermeetings@acs.org).

## TRAVEL & TRANSPORTATION

### AIRPORT GROUND TRANSPORTATION

**Taxis.** Many companies provide taxicab service at San Diego International Airport. If you need a taxi, simply follow the signs leading to the transportation plazas. A transportation coordinator will place you with the first available taxi unless you specify a particular taxicab company. Base fare and rates are displayed on the meter and include a flag drop charge plus a per-mile and/or a per-hour charge. If you are traveling from the airport, they will also add \$1.50 to your final total. Visit <http://goo.gl/ujXue8> for more information on taxi rates in San Diego.

**SuperShuttle.** SuperShuttle service to and from the hotel can be arranged at [www.supershuttle.com/default.aspx?GC=MFPQQ](http://www.supershuttle.com/default.aspx?GC=MFPQQ). The shared ride shuttle discount is \$1.00 one way, \$2.00

round trip. You can also book sedans. To reserve by phone, call (800) blue-van (258-3826) and use the discount code MFPQQ.

### AIRLINES:

#### Delta

(800) 328-1111  
Discount code: NMMMMK

#### United Airlines

(800) 426-1122  
Discount code: ZWFB960724

#### Southwest Airlines

[swabiz.com](http://swabiz.com) (online only)  
Discount code: 99331750

### TRAIN:

#### Amtrak

[amtrak.com](http://amtrak.com); (800) 872-7245  
Discount code: X03V-918

### RENTAL CARS

#### Avis

(800) 331-1600  
Discount code: B923099

#### Hertz

(800) 654-2240  
Discount code: CV# 02UZ0015

### TRAVELING TO MEETING VENUES

The San Diego Convention Center is located at 111 West Harbor Dr., San Diego, CA 92101.

**ACS Shuttle.** Complimentary shuttle service will be provided between the San Diego Convention Center and official ACS hotels, with the exception of hotels within walking distance.

## ACS MEMBER SERVICES

**ACS MEMBER SERVICES.** ACS staff assist you on-site with joining ACS, renewing memberships, completing adjustments to member records, and answering general membership questions. ACS members receive discounted rates when registering for the meeting.

ACS Member Services is located in Lobby D near registration in the San Diego Convention Center and is open Saturday, March 12, 3:00 to 6:00 PM; Sunday, March 13, 7:30 AM to 7:30 PM; Monday, March 14, 7:30 AM to 9:00 PM; Tuesday, March 15, 7:30 AM to 5:00 PM; Wednesday, March 16, 7:30 AM to 4:00 PM; and Thursday, March 17, 7:30 AM to 1:00 PM.

## GENERAL INFORMATION

### ONLINE SOCIAL NETWORKING TOOLS.

Start discussions and connect with other attendees on the ACS Network and the ACS Facebook page. Follow ACS national meetings on Twitter.

### ATTENDEE NATIONAL MEETING

**E-NEWSLETTER.** Receive official updates on ACS national meetings, including locations, registration and accommodation dates, information and discounts, resources, and event details. You can sign up and manage your subscriptions with your free ACS ID. Subscribe at [www.emailpref.acs.org](http://www.emailpref.acs.org).

**BUSINESS CENTER.** The FedEx store, located in Hall D, offers in-store and online printing, notary services, document finishing, packing and shipping, and a variety of other services tailored to help you make the best of the convention.

**MEMBER INSURANCE PROGRAM.** Inside the Exposition at booth 427, the ACS Member Insurance Program offers coverage and policies for every stage of life, from college student to young professional, from raising a family to enjoying retired life and everything in between. Stop by the Member Insurance Booth to learn how you can sign up for Life & International Life Insurance, Auto & Homeowners, Disability Income, Long-Term Care, Medicare Supplement, Medical Discount Cards, Pet Insurance, and Professional Liability.

Also learn more about our newest policy available to ACS educators: Chemical Educators Legal Liability Insurance. Visit the booth for a complimentary 15-minute consultation, and learn how this policy provides the unique coverage necessary for chemistry educators. To learn more about the insurance plans available to you, visit [www.acs.org/insurance](http://www.acs.org/insurance).

## ON-SITE MEETING ARRANGEMENTS

**ADA-COMPLIANT MEETING.** The San Diego Convention Center provides service ramps to entrances and elevated areas, braille instructions and directions throughout the building, and pay phones on each level of the facility with (TDD) hearing-impaired functions. More information is available at [visitsandiego.com](http://visitsandiego.com).

ACS is dedicated to ensuring that no

individual with a disability is excluded, denied services, segregated, or otherwise treated differently because of the absence of auxiliary aids and services identified in the Americans with Disabilities Act. If you require special accommodations to participate in the meeting, communicate your needs to ACS Meeting Services by e-mail: [nationalmeetings@acs.org](mailto:nationalmeetings@acs.org); fax: (202) 872-6128; or phone: (202) 872-6111 by January 28 to allow enough time to fulfill your request. Keep in mind that ACS may not be able to accommodate last-minute requests.

If you have an emergency or need immediate assistance during the meeting, contact any ACS Operations Office.

**ASSISTANCE.** Our information clerks will be positioned throughout the convention center and can help you navigate the On-site Program, find a particular session or room, and answer questions. Lost-and-found items at the convention center should be directed to the ACS Operations Office located in Room 14B. Messages left at the ACS Operations Office will be conveyed to attendees via the Meeting Mail system, but ACS cannot accept responsibility for the delivery of any messages, mail, or packages.

**ATTENDEE BADGES.** Attendees and guests must be registered and display their badges at all times to be admitted to all official ACS sessions and events.

### ATTENDEE MESSAGING/MEETING

**MAIL.** After registering for the meeting, you will be assigned a temporary electronic mailbox to exchange personal messages with other registered attendees via Meeting Mail. Meeting Mail will be available before, during, and after the meeting at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016). Use the Meeting Mail terminals located in the San Diego Convention Center. Telephone messages left at the ACS Information Booth will be conveyed to attendees via the electronic message center, but ACS cannot accept responsibility for the delivery of any messages. No one will be paged in meeting rooms.

### AUDIOTAPING, PHOTOGRAPHY &

**VIDEOTAPING.** The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital rebroadcast) of speakers or presentations is strictly prohibited at

## TIPS FOR A SAFE STAY IN SAN DIEGO

- Attendees should be aware of their surroundings at all times.
- Don't wear your meeting badge outside the convention center or hotels.
- Don't wear fancy jewelry or carry expensive technology in plain sight.
- Carry your briefcase, tote bag, purse, or laptop carrier close to your body.
- Don't leave valuables in your hotel room. Get a hotel safe deposit box.
- Walk in open and in well-lit areas at night.
- Travel in groups. Don't be a loner, particularly in the evening.
- Use common sense. If someone or someplace looks suspicious, report it and/or avoid it.
- If an emergency occurs during a meeting event, refer to detailed instructions placed by ACS staff inside each meeting room to follow in case of emergencies. Report emergencies to the nearest security guard or to any ACS Operations Office during the meeting.
- If an emergency occurs outside an ACS event, contact police or emergency assistance by dialing 911 or seeking assistance from the facility where the emergency occurs.
- Should a catastrophic event occur while the meeting is underway, follow safety and security instructions issued by the facility where you are located at the time of the event.

all ACS meetings and events without express written consent from ACS.

**CHILD CARE.** Camp ACS will be available to all meeting attendees free of charge from 7:00 AM to 6:00 PM on Sunday, March 13, through Thursday, March 17. At Camp ACS, children two (and potty-trained) to 16 years of age can participate in age-appropriate activities, including arts and crafts and active games, while you enjoy the meeting. To ensure your child's participation, register online by February 26 at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016). For your child's safety, the location of Camp ACS will not be communicated until your registration is confirmed. On-site reg-

## GENERAL INFORMATION

istration will be accepted on a space-available basis.

**LUGGAGE & COAT CHECK.** A luggage and coat check station will be available during registration hours from Sunday through Thursday at the San Diego Convention Center, Lobby D. Items left beyond published hours of operation will be turned over to building security at the end of each day.

**ELECTRONIC DEVICES.** As a courtesy to other meeting attendees, electronic devices must be operated in silent/vibrate mode in technical or educational sessions. Cell phone conversations are not permitted in meeting rooms.

**EMERGENCIES DURING ACS MEETING EVENTS.** ACS will place detailed instructions inside each meeting room to be used if an emergency occurs during an ACS meeting event. These instructions will revolve around following the established emergency guidelines of the facility where the emergency occurs. Report emergencies to the nearest security guard or to any ACS Operations Office during the meeting. Should a catastrophic event occur, attendees should follow safety and security instructions issued by the facility where they are located at the time of the event.

**HOST LOCAL SECTION.** ACS gratefully acknowledges the cooperation and assistance of the ACS San Diego local section and its members in handling local arrangements. Volunteers have planned many interesting activities; the Host Local Section booth will be located in the San Diego Convention Center, Lobby D.

**INTERNATIONAL REGISTRANTS.** Many international visitors are required to hold a visa to be admitted to the U.S. All visa applicants are advised to apply for their

visa in their home country as soon as possible. Detailed information for international attendees can be found at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016).

**INTERNET & COMPUTER SERVICES.** Use our electronic communication services before, during, and after the meeting. Once you get to the meeting, you can access your e-mail and the Internet as well as your personal Meeting Mail mailbox from Meeting Mail terminals, which will be located throughout the San Diego Convention Center.

**LITERATURE & PRODUCT DISTRIBUTION.** Promotions, posters, and literature distribution by attendees, exhibitors, or other groups during the meeting must be done within their own contracted meeting space or exhibit booth and not in public meeting space, with the exception of designated marketing opportunities. No one except the ACS Operations Office is authorized to place any promotional items in public meeting space at a given location. Items left in violation of this policy will be removed and discarded. Literature distribution at specific division tables is under the control of that division, and permission must be secured from the division before placing any items on their table.

**MEETING OFFICES.** The following ACS offices will be located in the San Diego Convention Center:

**Attendee Registration:** Lobby D

**Career Fair:** Hall A

**Exhibitor Registration:** Lobby C

**Exposition:** Halls B–C

**Finance Office:** Box Office E

**Host Local Section:** Lobby D

**Member Services:** Lobby D

**Press Center:** Room 16B

**Shuttle Desk:** Box Office A

### THANK YOU

The society thanks the many volunteers of the San Diego local section who are contributing to the 251st ACS National Meeting & Exposition by participating as division officers or program chairs, symposium organizers, session or award presiders, oral and poster presenters, short course or workshop instructors, career consultants, and society governance members.

The following offices are located at the identified properties:

**Operations Offices:** San Diego Convention Center, Hilton San Diego Bayfront, Hilton San Diego Gaslamp Quarter, Manchester Grand Hyatt San Diego, Omni San Diego Hotel, Marriott Marquis San Diego Marina, U.S. Grant Hotel, Westin San Diego, Wyndham San Diego Bayside

**Governance Office:** Hilton San Diego Bayfront

**Society Programs:** Hilton San Diego Bayfront

**MOTHERS ROOM.** For your convenience and privacy, ACS will provide a room for nursing mothers at the San Diego Convention Center. Please see the Operations Office in Room 14B for access to the room.

**SMOKING.** ACS policy prohibits smoking in all rooms during ACS functions at the convention center and official hotels. Additionally, the convention center and many of the official hotels are designated as smoke-free environments at all times.

Exhibiting companies will also host FREE educational sessions for attendees that will:

Introduce new products and services

Highlight innovative applications for existing instrumentation

Build skills with specific tools and techniques

Please visit [www.acs.org/SanDiego2016](http://www.acs.org/SanDiego2016) to register for exhibitor workshops.

## Sunday, March 13

### Flow Chemistry Seminar

Sponsor: ThalesNano Nanotechnology Inc., 3:30 PM - 6:00 PM  
SDCC, Room 12

## Monday, March 14

### McGraw-Hill Technology Workshops

Sponsor: McGraw-Hill Education, 9:30 AM - 12:00 PM  
SDCC, Room 15B

### Waters Technical Workshops

Sponsor: Waters, 9:30 AM - 12:00 PM  
SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2

### ACS on Campus

Sponsor: ACS Store, 12:30 PM - 3:00 PM  
SDCC, Room 15B

### CAS Solutions

Sponsor: CAS, 9:30 AM - 3:00 PM  
SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 1

### Solutions for Innovation: From Composition to Structure

Sponsor: JEOL USA, Inc., 12:30 PM - 3:00 PM  
SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2

### Seamless Integration of 2D and 3D SAR to Guide

#### Multi-Parameter Optimization

Sponsor: Optibrium Ltd., 3:30 PM - 6:00 PM  
SDCC, Room 15B

## Tuesday, March 15

### Spinsolve Benchtop NMR for Industry and Academia

Sponsor: Magritek Inc., 10:00 AM - 12:00 PM  
SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2

### McGraw-Hill Technology Workshops

Sponsor: McGraw-Hill Education, 9:30 AM - 12:00 PM  
SDCC, Room 15B

### WebAssign 101: Getting Started with WebAssign

Sponsor: Webassign, 3:30 PM - 6:00 PM  
SDCC, Room 12

### Introduction to Protein and Peptide HPLC & State-of-the-Art Protein and Peptide Reversed-Phase Separations by UHPLC

Sponsor: MilliporeSigma (Sigma-Aldrich), 9:30 AM - 12:00 PM  
SDCC, Room 12

### CAS Solutions

Sponsor: CAS, 9:30 AM - 3:00 PM  
SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 1

### Reverse Engineering of Materials and Polymers Using Infrared and Raman Spectroscopy

Sponsor: Bruker, 12:30 PM - 3:00 PM  
SDCC, Room 15B

### Part I: A New and Exciting Line of High Pressure Ion Chromatography (HPIC) Instruments. Part 2: Advances in UHPLC Instrumentation

Sponsor: Thermo Scientific, 12:30 PM - 3:00 PM  
SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2

### Characterizing Structure and Chemistry of Functional Nanomaterials by advanced Electron Microscopy

Sponsor: FEI, Company, 12:30 PM - 3:00 PM  
SDCC, Room 12

### Exploiting Matched Molecular Pairs in Drug Discovery

Sponsor: Simulations Plus, Inc., 3:30 PM - 6:00 PM  
SDCC, Room 15B

## Wednesday, March 16

### Inhibitor Design Using MOE Structure-Based Drug Design Applications

Sponsor: Chemical Computing Group, 3:30 PM - 6:00 PM  
SDCC, Room 15B

Visit the ACS Exposition  
Meet Over 250 Exhibitors  
San Diego Convention Center, Exhibit Halls B&C  
Sunday, 6 - 8:30 PM • Monday & Tuesday, 9:00 AM - 5:00 PM  
Attendee Welcome Reception - Sunday, 6:00 - 8:30 PM  
Relax and visit the Expo on Tuesday for an afternoon break from 3:00 - 5:00 PM.

# 251st American Chemical Society National Meeting & Exposition

March 13 –17, 2016  
San Diego, California

## Kavli Foundation Lecture Series

The Kavli Foundation Lecture Series promotes groundbreaking discovery and public understanding of the world's mounting challenges and how chemistry can provide solutions.

## The Kavli Foundation Emerging Leader in Chemistry Lecture



San Diego Convention Center, Ballroom 20 A – C

Monday, March 14, 2016

4:00 – 5:10 PM

Dr. Rommie E. Amaro

Director, National Biomedical Computation Resource, Senior Editor Chemical Biology & Drug Design, Co-Director Drug Design Data Resource, Associate Professor of Chemistry and Biochemistry, University of California, San Diego

### ***Computing Cures: Enabling Chemical Discovery***

The potential of chemistry to help in solving societal problems has probably never been greater. Its enthusiasm for doing so is substantially less. How might it expand its ambitions, and change its structure, to broaden its role in attacking these large-scale problems?

***The Kavli Foundation Emerging Leader in Chemistry Lecture is awarded to an outstanding chemical scientist who is less than 10 years past receipt of his/her PhD and is under 40 years of age.***

***The candidate is a distinguished younger scientist who is highly regarded by his or her peers for significant contributions to an area of chemistry or related multidisciplinary area of chemistry.***

## The Fred Kavli Innovations in Chemistry Lecture



San Diego Convention Center, Ballroom 20 A – C

Monday, March 14, 2016

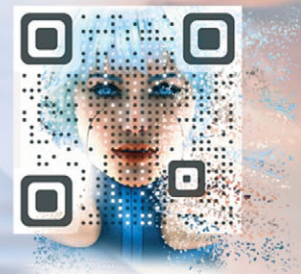
5:15 – 6:30 PM

Dr. Emily Carter

Founding Director, Andlinger Center for Energy and the Environment  
Gerhard R. Andlinger Professor in Energy and the Environment,  
Professor of Mechanical Engineering, and Applied and Computational Mathematics  
Princeton University

### ***Quantum Solutions for a Sustainable Energy Future***

The current energy landscape is unsustainable; the burning of fossil fuels is causing tremendous harm to the planet, threatening the survivability of civilization as we know it. Using quantum mechanical computational methods, we explore the viability of alternative clean energy strategies for conversion of sunlight to electricity and fuels, clean and efficient combustion of biodiesel, and optimization of robust materials for fusion reactor walls.





# GOVERNANCE & BUSINESS MEETINGS

**MANY MEMBERS PARTICIPATE** in meetings concerning the business of the Society, technical divisions, and governance committees in conjunction with the meeting. On the following pages, you will find a listing of the open meetings scheduled for San Diego. ACS encourages its members to get active in governance at all levels in order to contribute their vision to the direction of the Society. You can share ideas and insights into the Society and the chemical profession, network with peers, and catch up with friends through these volunteer connections. With nearly thirty national governance committees and leadership opportunities in technical divisions and local sections to choose from, there are many opportunities for

members to become actively involved in ACS at the national level. If you are an ACS member interested in volunteering for a governance committee, contact the Office of the Secretary by email at [secretary@acs.org](mailto:secretary@acs.org) or by phone 202-872-4461. Someone will put you

in contact with the ACS Committee on Committees to discuss your desire to volunteer for a committee assignment. If you wish to volunteer with a specific technical division or local section, contact the officers listed at [www.acs.org](http://www.acs.org) to explore your specific interests.

## ACS COUNCIL

The ACS Council meeting will begin at 8:00 AM, Wednesday, March 16, at the Hilton San Diego Bayfront. The meeting will be preceded by a continental breakfast for councilors beginning at 7:00 AM. Councilors are asked to check in beginning at 7:00 AM and proceed to the breakfast area, keeping in mind that the meeting starts promptly at 8:00 AM. Space will be available for ACS members and nonmembers to observe the council in action. We hope that many will take advantage of this opportunity to learn firsthand of the society's operation. Alternate councilors and division and local section officers are particularly urged to attend.



The Gaslamp Quarter in San Diego from San Diego convention center. SHUTTERSTOCK

## GOVERNANCE MEETINGS

### BOARD & COUNCIL MEETINGS

**ACS BOARD OF DIRECTORS.** The ACS Board of Directors meeting, open to members who wish to participate, will be held in the San Diego Convention Center, Room 20D from noon to 1:00 PM on Sunday, March 13.

**ACS COUNCIL.** The ACS Council meeting will begin at 8:00 AM, Wednesday, March 16, at the San Diego Hilton Bayfront. The meeting will be preceded by a continental breakfast for councilors beginning at 7:00 AM. Councilors are asked to check in beginning at 7:00 AM and proceed to the breakfast area, keeping in mind that the meeting starts promptly at 8:00 AM. Space will be available for ACS members and nonmembers to observe the council in action. We hope that many will take advantage of this opportunity to learn firsthand of the society's operation. Alternate councilors and division and local section officers are particularly urged to attend.

### COUNCILOR CAUCUS MEETINGS

#### District I Councilor Caucus

Tuesday, March 15, 5:30 – 7:00 PM  
Hilton San Diego Bayfront, Indigo 202A

#### District II Councilor Caucus

Sunday, March 13, 6:00 – 7:00 PM  
Hilton San Diego Bayfront, Indigo 202B

#### Middle Atlantic (District III) Councilor Caucus

Sunday, March 13, 6:00 – 7:00 PM  
Hilton San Diego Bayfront, Indigo 202A

#### District IV Councilor Caucus

Sunday, March 13, 6:00 – 7:00 PM  
Hilton San Diego Bayfront, Indigo 204A

#### District V Councilor Caucus

Sunday, March 13, 6:00 – 7:00 PM  
Hilton San Diego Bayfront, Indigo 204B

#### District VI Councilor Caucus

Sunday, March 13, 6:00 – 7:00 PM  
Hilton San Diego Bayfront, Indigo 206

#### Division Officers/Councilors Caucus

Tuesday, March 15, 4:00 – 6:00 PM San Diego Convention Center Room 24A

### COMMITTEE AGENDA

**THE COMMITTEE ON COMMITTEES** has clarified three types of committee meetings:

**OPEN.** May be attended by any ACS member. At these sessions, members are encouraged to voice concerns, issue compliments, offer suggestions, express interest in, or raise questions about matters over which the committee has purview. The assumption is that participation is welcomed and will be orderly and courteous. Only committee members can vote.

**EXECUTIVE.** Attendance and participation are limited to officially appointed/elected committee members, associates, advisers, consultants, staff liaisons, and the appointed Committee on Committees liaison. Liaisons from other groups and both ex officio and elected councilors may attend; active participation by these groups would be at the invitation of the chair. Only committee members can vote.

**CLOSED.** The committee chair must declare any EXECUTIVE session CLOSED when confidential or sensitive personnel, financial, or legal matters of the society are discussed. At that point, only officially appointed/elected committee members, associates, consultants, staff liaisons, and the appointed Committee on Committees liaison shall remain in the session. Others may stay in the session at the discretion of the chair. Once these discussions have been completed, the committee should return to EXECUTIVE mode.

During the open and executive committee meetings, ACS members are given a chance to express their views on issues under consideration before these issues are acted on by the board or the council, or to bring up other subjects that

### COUNCIL POLICY COMMITTEE

The Council Policy Committee will open the floor during its meeting at 11:00 AM on Tuesday, March 15, to councilors who would like to raise issues of concern that affect them and/or their local sections or divisions. For further information, contact Alan M. Ehrlich, vice chair of CPC, at [cpc@acs.org](mailto:cpc@acs.org).

deserve attention. Members are urged to examine the agenda and make known any opinions or ideas they may have. If you cannot attend the particular sessions involved, write to the officers listed or ask someone attending the session to speak on your behalf. For further information, contact the officers listed.

### BUDGET & FINANCE

*Kristen M. Omberg, chair; [b\\_feedback@acs.org](mailto:b_feedback@acs.org)*

#### Open Meeting

Saturday, March 12, 8:00 AM to noon  
Hilton San Diego Bayfront, Sapphire E/F

1. Report of the Chair
2. Report of the Treasurer & CFO:
  - a. Budgetary Performance Report for the Year Ended December 31, 2015
3. Reports from the Subcommittees:
  - a. Financial Impact of Constitution & Bylaw Changes
  - b. Communications
  - c. Program Funding Requests
  - d. Program Review

### CHEMICAL SAFETY

*Elizabeth M. Howson, chair; [safety@acs.org](mailto:safety@acs.org)*

#### Open Executive Session

Monday, March 14, 8:30 to 11:30 AM  
Hilton San Diego Bayfront, Sapphire Ballroom E/F

1. Reports of the chair and staff liaison
2. Reports from the subcommittees and task forces
3. Reports of the committee liaisons
4. Old and new business

### CHEMISTRY & PUBLIC AFFAIRS

*Susan B. Butts, chair; [sbuttsdc@gmail.com](mailto:sbuttsdc@gmail.com)*

#### Open Meeting

Saturday, March 12, 3:00 to 4:00 PM  
Hilton San Diego Bayfront, Sapphire Ballroom A/B

1. Reports from the Subcommittees:
  - a. Public Policy
  - b. Fellowships
  - c. Member Advocacy
2. Committee Liaison Reports
3. Public Comment
4. Closing Comments

### CHEMISTS WITH DISABILITIES

*John J. Johnston, chair; USDA-FSIS, Fort Collins, CO 80526-8116*

#### Combined Open and Executive Meeting

Sunday, March 13, 8:30 AM to 4:30 PM  
Hilton San Diego Bayfront, Indigo Ballroom H

1. Welcome
2. Chair Report
  - a. Update of CWD Activities/Events, and Collaborative Opportunities
  - b. Diversity & Inclusion Advisory Group Report
  - c. Minutes from (Boston 2015)
3. Strategic Planning Group Updates
4. CWD 35th Anniversary/ADA 25th Anniversary Celebration Recap

# GOVERNANCE & BUSINESS MEETINGS

5. Update Ratification of the UN Human Rights for Persons with Disabilities Treaty
6. Collaboration with CWD: ACS Standardized Exams Update
7. Collaboration with CWD: Creating Equitable Chemistry Classrooms Update
8. Staff Report
9. Future Event and Programming Planning
10. Subcommittee Progress Reports
11. Reports of Liaisons to/from other committees
12. Ongoing Business
13. New Business

## COMMITTEES

Wayne E. Jones Jr., chair; Department of Chemistry, Binghamton University, SUNY, Vestal Pkwy. East, Binghamton, NY 13902-6000

### Open Session

Monday, March 14, 1:30 to 2:00 PM Hilton San Diego Bayfront, Aqua Salon C

1. Welcome
2. Minutes of August 17-19, 2015
3. Reports of chair/staff liaison
4. Report of Subcommittees and Task Forces:
  - a. Diversity
  - b. Leadership Development
  - c. Committee Performance Review Process
  - d. Society Committee Bylaws
5. Topics from floor

## COMMUNITY ACTIVITIES

Michael B. McGinnis, chair;  
mmcginni@norwich.edu

### Open Executive Session

Sunday, March 13, 7:45 AM to noon

Hilton San Diego Bayfront, Indigo Ballroom C/G

1. Chair's welcome and comments
2. Reports from liaisons
3. Reports from subcommittees on:
  - a. Program Development and Promotion
  - b. Tools & Training
  - c. Volunteer Engagement and Recognition
4. New business

Hilton San Diego Bayfront

### CCA/LSAC Joint Open Meeting

Tuesday, March 15, 2:00 to 3:30 PM Hilton San Diego Bayfront, Indigo Ballroom C/G

## CONSTITUTION & BYLAWS

James C. Carver, chair; Carver Law Firm, Baton Rouge, LA; bylaws@acs.org

### Open Meeting

Sunday, March 13, 1:15 to 1:45 PM

Hilton San Diego Bayfront, Aqua Salon A/B

Open forum to discuss bylaws, petitions, and other issues that may arise

### Executive Sessions (Closed)

Sunday, March 13, 9:00 AM to noon and 1:45 to 4:30 PM

Hilton San Diego Bayfront, Aqua Salon A/B

1. Status of unit bylaws
2. Charter bylaws
3. Petition to Extend the Unemployed Members' Dues Waiver
4. Draft petitions under consideration by others
5. Reports from liaisons from other committees
6. FAQ for bylaws
7. Bulletin 5 review
8. Open discussion

## CORPORATION ASSOCIATES

Diane Grob Schmidt, chair, d.schmidt@acs.org

### Open Meeting

Monday, March 14, 8:00 AM to noon

Hilton San Diego Bayfront, Aqua Salon D

1. Chair's Report
2. Staff Report
3. Strategic Investment and Awards Subcommittee
4. Public Policy Subcommittee
5. CA Relations Subcommittee
6. Industry Insights Subcommittee
7. CA Member Benefits Subcommittee
8. New Business

## COUNCIL POLICY

Alan M. Ehrlich, vice chair; cpc@acs.org

### Open Meeting

Tuesday, March 15, 9:30 AM to noon

Hilton San Diego Bayfront, Indigo Ballroom B/F

1. Committee and Officer Reports
2. Report of CPC vice chair
3. Reports of Subcommittees on:
  - a. Petitions, Constitution & Bylaws
  - b. Long Range Planning
4. Report of the Task Force on Councilor and member duties and conduct
5. Schedule of business sessions, fall 2016
6. Review of Council agenda
7. Open forum
8. Old and new business

## DIVISIONAL ACTIVITIES

Rodney Bennett, chair;  
rodbennett@acs.org

### Open Session

Sunday, March 13, 8:00 AM to noon

Hilton San Diego Bayfront, Aqua Salon C

1. Welcome
2. Review San Diego agenda
3. Minutes from 250th ACS National Meeting in Boston, MA
4. DAC Chair Report
5. Subcommittee Reports

## ECONOMIC & PROFESSIONAL AFFAIRS

Rick Ewing, chair; william.ewing@bms.com

### Executive Session

Saturday, March 12, 8:00 AM to 3:00 PM

San Diego Convention Center, Room 6D

1. Opening Remarks
2. Subcommittee Meetings
3. Invited Guest Reports
4. Staff Reports

### Open Session

Saturday, March 12, 3:00 to 5:30 PM

San Diego Convention Center, Room 6D

1. Subcommittee Reports
  - a. Public Policy
  - b. Events, Volunteers and Employment Services
  - c. Marketing and Research
  - d. Standards and Ethics
2. Reports from Liaisons to and from CEPA
3. Ongoing Business / New Business

## EDUCATION

Diane Krone, chair; kroned@alumni.stevens.edu

### Executive Session

Friday, March 11, 1:00 to 5:30 PM

San Diego Convention Center, Room 4

1. K-12 science topics, including ChemCom, ChemMatters, the American Association of Chemistry Teachers, High School Chemistry Clubs, Chemistry Olympiad, ACS Science Coaches, ACS-Hach programs, and teacher professional development
2. College/university topics, including undergraduate programs, graduate and postdoctoral education, Chemistry in Context, and faculty development

Items 1-2 open to all Councilors with prior approval of the Chair

### Open Meeting

Monday, March 14, 3:00 to 4:00 PM Hilton San Diego Bayfront, Room 4

Review of meeting, as below, plus items from the floor.

## ENVIRONMENTAL IMPROVEMENT

Anthony M. Noce, chair; anoce@haleyaldrich.com

### Open Session

Monday, March 14, 7:45 to 9:00 AM

Manchester Grand Hyatt, Coronado E

1. Review of the Saturday-Sunday CEI Executive Session
2. Preview of CEI activities in San Diego
3. Preview of 2016 policy statement development (climate, regulatory decision making)
4. Open discussion period

## ETHICS

Keith Vitense, chair; Cameron University, Physical Science Department, 2800 West Gore Blvd., Lawton, OK 73505-6320

### Open Executive Session

Sunday, March 13, 9:00 AM to 4:30 PM

Hilton San Diego Bayfront, Indigo Ballroom H

1. Welcome & Introductions
2. Approval of Minutes from San Francisco Meeting
3. Review of Committee on Ethics Charge
4. Chair/Staff Liaison Reports
5. Liaison Reports
6. Subcommittee Progress Reports
  - a. Communications and Awareness
  - b. Education and Materials
  - c. Programming and Screening
7. Committee Discussion
8. Subcommittee Working Sessions
9. Old Business /New Business/ Action Items

## INTERNATIONAL ACTIVITIES

Ellen T. Contis, chair; c/o ACS Office of International Activities, 1155-16th St., N.W., Washington, DC 20036

### Open Meeting

Saturday, March 12, 1:00 to 3:00 PM

Hilton San Diego Bayfront, Sapphire Ballroom E/F

1. Welcome
2. Minutes of previous meeting
3. Reports of Chair/Staff Liaison
4. Report of Subcommittees:
  - a. Subcommittee on Africa and the Americas
  - b. Subcommittee on Europe and the Middle East
  - c. Subcommittee on Asia / Pacific Rim
5. New Business

# GOVERNANCE & BUSINESS MEETINGS

## LOCAL SECTION ACTIVITIES

Martin Rudd, chair; martin.rudd@uwc.edu

### LSAC/CCA Joint Open Meeting

Tuesday, March 15, 2:00 to 3:30 PM

Hilton San Diego Bayfront, Indigo Ballroom C/G

1. Report from the LSAC and CCA Executive Sessions
2. Interactive session: questions, answers and best practices

### Open Executive Session

Sunday, March 13, 8:00 AM to noon

Hilton San Diego Bayfront, Sapphire Ballroom I/J

1. Report of chair, subcommittee chairs, staff liaison
2. Review of petitions for Council consideration
3. Reports of committee liaisons

## MEETINGS & EXPOSITIONS

John Pochan, chair; johnpochan@gt.org

### Open Executive Session

Sunday, March 13, 7:00 AM to noon

San Diego Convention Center, Room 5A

1. Welcome
2. Minutes from Boston National Meeting
3. Chair's report
4. Subcommittee reports
5. Finance/Staff Liaison Report
6. New Business

## MEMBERSHIP AFFAIRS

James M. Landis Jr., chair; jim.landis@gt.org

### Open Session

Monday, March 14, 1:00 to 2:00 PM

Hilton San Diego Bayfront, Aqua 310B

1. Welcome
2. Minutes of August 16, 2015
3. Reports of Chair/Staff Liaison
4. Reports of Subcommittees
  - a. Categories & Dues
  - b. Retention, Benefits & Services
  - c. Recruitment & Admissions
5. Petition to Extend the Unemployed Member Dues Waiver (For Consideration)
6. International Chapter Recruiting Trial Extension
7. Two Year Academic Program Member Services
8. Topics from floor

## MINORITY AFFAIRS

Madeleine Jacobs, chair;

madeleine.s.jacobs@gmail.com

### Closed Executive Session

Sunday, March 13, 8:00 AM to 12:30 PM

Hilton San Diego Bayfront, Sapphire Ballroom A/B

1. Opening Remarks
2. Staff Report
3. Spring Meeting Minutes
4. Subcommittee Meetings

### Open Session

Sunday, March 13, 12:30 to 2:00 PM

Hilton San Diego Bayfront, Sapphire Ballroom A/B

1. Subcommittee Reports
2. Old Business
4. New Business

5. Open Discussion with Dr. Willie E. May, Director of the National Institute of Standards and Technology (NIST).

## NOMENCLATURE, TERMINOLOGY & SYMBOLS

Michael Mosher, chair; Professor and Chair, Department of Chemistry & Biochemistry, Ross Hall 3480, Campus Box 98, University of Northern Colorado, Greeley, CO 806395

### Executive Session

Monday, March 14, 2:00 to 5:00 PM

Hilton San Diego Bayfront, Aqua 300 A/B

1. Review Boston minutes, August national meeting
2. Chair/Staff Liaison reports
3. Subcommittee Reports
  - a. Communication/Outreach
  - b. Education
  - c. Liaison
  - d. Long Range Planning
4. IUPAC Reports
5. Update to Kilogram, Amount of Substance and Mole issues
6. Chemical Ontology Update
7. San Diego Exposition Booth for Outreach
8. Planning for Philadelphia Meeting

## NOMINATIONS & ELECTIONS

D. Richard Cobb, chair; nomelect@acs.org

### Open Executive Session

Monday, March 14, 11:30 AM to noon

Hilton San Diego Bayfront, Aqua Salon E

1. Report of the Executive Session
2. Topics from the floor

## PATENTS & RELATED MATTERS

Sadiq Shah, chair; sadiq@utpa.edu

### Open Meeting

Saturday, March 12, 9:00 AM to 5:00 PM

Hilton San Diego Bayfront, Sapphire K/L

1. Legislation & Regulation Subcommittee.
2. Education and Outreach Subcommittee.
3. Awards Subcommittee.
4. Executive Session

## PROFESSIONAL TRAINING

Thomas J. Wenzel, chair; cpt@acs.org

### Open Meeting

Sunday, March 13, 4:00 to 5:00 PM

Marriott Marquis, La Jolla

1. Evaluation of the Macromolecules/Materials Requirement
2. Online Instruction and Virtual Labs
3. Supplements to the ACS Guidelines
4. Planning for Graduate Work in the Chemical Sciences
5. PhD Recipient Survey Results
6. Topics from floor

## PROJECT SEED

Anna G. Cavinato, chair, Eastern Oregon University, Department of Chemistry, One University Blvd., LaGrande, OR 97850-2807

### Open Session

Sunday, March 13, 9:30 to 10:30 AM

Omni San Diego Hotel, Balboa 1

1. Report from executive session
2. Topics from the floor

## Executive Session

Saturday, March 12, 10:30 AM to 5:00 PM

Omni San Diego Hotel, Grand Ballroom E

1. Subcommittee meetings 10:30 AM to noon
2. Minutes of previous meeting
3. Reports of Chair/Staff Liaison
3. Report of Subcommittees
4. Old and new business

## PUBLICATIONS

Nicole S. Sampson, chair; nicole.sampson@stonybrook.edu

### Open Meeting

Friday, March 11, 4:30 to 5:00 PM

Hilton San Diego Bayfront, Cobalt 501 B/C

1. Updates from ACS Publications Division
2. Open Discussion

### Executive Session

Friday, March 11, 1:00 to 5:00 PM

(Closed Executive Session until 4:30 PM)

San Diego Hilton Bayfront, Cobalt 501 B/C

1. Report of C&EN Editorial Board
2. Reports of the Publications Division and of the Governing Board for Publishing
3. Reports from Other Committees
4. Discussion of Journal Monitoring Reports and Editor Appointments
5. Open Session:
  - a. Updates from ACS Publications Division
  - b. Open Discussion

## SCIENCE

Mark C. Cesa, chair; markcesa@comcast.net

### Open Meeting

Saturday, March 12, 8:00 AM to 4:30 PM

Hilton San Diego Bayfront, Sapphire Ballroom G/H

1. Welcome
2. Approval of Minutes
3. Reports of Chair/Staff Liaison
4. Report of Subcommittees:
  - a. Science and Technology,
  - b. Awards,
  - c. Public Policy and Communication
5. Subcommittee Breakouts
6. Subcommittee Reports from Breakouts

## SENIOR CHEMISTS

Thomas R. Beattie, chair; beattietr@aol.com

### Open Meeting

Monday, March 14, 8:00 AM to noon

Hilton San Diego Bayfront, Indigo Ballroom D/H

1. Welcome & Introductions
2. Discussion and approval of Boston Meeting Minutes
3. Reports of Chair & Staff Liaison
4. Subcommittee Reports
  - a. Newsletter – December 2015
  - b. Senior Activities in Local Sections
  - c. Consulting & Mentoring
    1. Undergraduate Speed Networking Event
  - d. Planning and Priorities
5. Old Business
  - a. Senior Chemists Breakfast
6. New Business
  - a. SCC Strategic Planning Retreat

### TECHNICIAN AFFAIRS

Kara Allen, chair; cta@acs.org

#### Closed Executive Session

Sunday, March 13, 8:30 AM to 12:30 PM

Hilton San Diego Bayfront, Indigo 202 A/B

1. Welcome
2. Minutes of Spring Meeting
3. Reports of Chair/Staff Liaison
4. Subcommittee breakout
5. Subcommittee reports
6. New business
7. Final comments/Feedback

#### Open Session

Sunday, March 13, Noon to 1:00 PM

Hilton San Diego Bayfront, Indigo 202 A/B

1. Welcome
2. Chair's Report
3. Subcommittee reports
4. Topics from the floor
5. Adjourn

### WOMEN CHEMISTS

Amber F. Charlebois, chair; afcharleb@gmail.com

#### Executive Session

Saturday, March 12, 8:00 AM to 5:00 PM

Hilton San Diego Bayfront, Sapphire Ballroom M/N

1. Welcome
2. Review of Action Items and Minutes
3. Reports of Chair and Staff Liaison
4. Subcommittee Meetings and Reports
5. Committee Liaison Reports
6. New Business & Special Discussion Topics

#### WCC Open Meeting & Just Cocktails Reception

Monday, March 14, 4:00 - 5:00 PM

### YOUNGER CHEMISTS

Natalie A. LaFranzo, chair; nlafranzo@gmail.com

#### Open Session

Sunday, March 13, 8:00 AM to noon

Hilton San Diego Bayfront, Sapphire Ballroom C/D

1. Welcome
2. Staff Report
3. Subcommittee Reports
  - a. Communications
  - b. Governance Interface and Outreach
  - c. Membership Engagement
4. Liaison Reports
5. Petitions (CLOSED)
6. New Business
7. Visitors
8. Adjourn

#### Executive Session

Sunday, March 13, noon to 1:00 PM

1. YCC Executive Session (CLOSED)



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# DIVISION MEETINGS & SOCIAL EVENTS

## Division of Agricultural & Food Chemistry— AGFD

AGFD Special Committee Meeting	12:00 PM–1:00 PM	Sunday, March 13	US Grant Hotel, Palm Court
AGFD Executive Committee Meeting	5:00 PM–8:00 PM	Sunday, March 13	US Grant Hotel, Palm Court
AGFD Future Programs Planning Meeting	12:00 PM–1:00 PM	Monday, March 14	US Grant Hotel, Crystal Blrm
Caribbean Cuisine Program	12:00 PM–5:00 PM	Tuesday, March 15	San Diego Wine & Culinary Center, 200 Harbor Drive #120, San Diego, CA
AGFD Poster Session	3:00 PM–5:00 PM	Tuesday, March 15	San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)
AGFD Business Meeting	12:00 PM–1:00 PM	Tuesday, March 15	US Grant Hotel, Crystal Blrm

## Division of Analytical Chemistry— ANYL

ANYL Poster Session	6:00 PM–8:00 PM	Sunday, March 13	San Diego Convention Center, Sails Pavillion
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## Division of Biological Chemistry— BIOL

BIOL Poster Session I	7:00 PM–9:00 PM	Sunday, March 13	San Diego Convention Center, Hall F
BIOL Poster Session II	7:00 PM–9:00 PM	Tuesday, March 15	San Diego Convention Center, Hall E

## Division of Biochemical Technology— BIOT

BIOT Recovery Board Meeting	7:00 AM–1:00 PM	Sunday, March 13	Westin San Diego, Diamond II
Lunch Seminars	12:30 PM–2:00 PM	Sunday, March 13	Westin San Diego, Topaz
BIOT Lunch Seminars	12:30 PM–2:00 PM	Monday, March 14	Westin San Diego, Topaz
BIOT Ex–Comm Meeting	7:00 PM–10:00 PM	Monday, March 14	Westin San Diego, Topaz
BIOT Future Programming Meeting	12:30 PM–2:00 PM	Tuesday, March 15	Westin San Diego, Crystal I
BIOT Lunch Seminars	12:30 PM–2:00 PM	Tuesday, March 15	Westin San Diego, Topaz
BIOT Program Chair Lunch	12:30 PM–2:00 PM	Wednesday, March 16	Westin San Diego, Pearl Room
BIOT Poster Session	6:00 PM–9:00 PM	Tuesday, March 15	San Diego Convention Center, Hall E
BIOT Lunch Seminars	12:30 PM–2:00 PM	Wednesday, March 16	Westin San Diego, Topaz
BIOT Networking Session	6:00 PM–8:00 PM	Wednesday, March 16	Westin San Diego, Topaz

## Division of Catalysis Science and Technology— CATL

CATL Poster Session	8:00 PM–10:00 PM	Tuesday, March 15	San Diego Convention Center, Hall D
CATL Business Meeting	5:30 PM–7:30 PM	Monday, March 14	Manchester Grand Hyatt San Diego, Pier

## Division of Carbohydrate Chemistry— CARB

CARB Executive Committee Meeting	5:30 PM–8:30 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Oceanside
CARB Division Award Dinner – Ticketed Event	6:30 PM–9:30 PM	Monday, March 14	Rocking Baja
CARB Poster Session	7:00 PM–9:00 PM	Tuesday, March 15	San Diego Convention Center, Hall D

## GOVERNANCE & BUSINESS MEETINGS

### Division of Cellulose and Renewable Materials— CELL

CELL Strategic Planning Meeting	5:00 PM–10:00 PM	Friday, March 11	San Diego Convention Center, Room 10
CELL Strategic Planning Meeting	8:00 AM–2:00 PM	Saturday, March 12	San Diego Convention Center, Room 10
CELL Executive Committee Meeting	5:00 PM–7:30 PM	Saturday, March 12	Marriott Marquis San Diego Marina, Point Loma
CELL Poster Session	6:00 PM–8:00 PM	Sunday, March 13	San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)
CELL Division Awards Banquet – Ticketed Event	6:30 PM–10:00 PM	Tuesday, March 15	Fogo de Chao
CELL Business Meeting/Program Planning Meeting	5:30 PM–7:30 PM	Wednesday, March 16	Marriott Marquis San Diego Marina, Leucadia

### Division of Chemistry and the Law— CHAL

CHAL Executive Committee Meeting	5:00 PM–8:00 PM	Sunday, March 13	San Diego Convention Center, Room 6D
CHAL Drug & Power Luncheon – Ticketed Event	12:00 PM–1:30 PM	Monday, March 14	San Diego Convention Center, Room 20D
CHAL Reception	6:00 PM–8:00 PM	Monday, March 14	San Diego Convention Center, Room 22

### Division of Chemical Health and Safety— CHAS

CHAS Lab Safety Workshop	7:30 AM–5:00 PM	Friday, March 11	San Diego Convention Center, Room 31A
CHAS Laboratory Waste Management Workshop	7:30 AM–5:00 PM	Friday, March 11	San Diego Convention Center, Room 31B
CHAS Meeting Chemical Safety Expectations in Instructional Laboratories	7:30 AM–5:00 PM	Saturday, March 12	San Diego Convention Center, Room 31A
CHAS Reactive Chemical Management for Laboratories & Pilot Plants	7:30 AM–5:00 PM	Saturday, March 12	San Diego Convention Center, Room 31B
CHAS How to be a More Effective Chemical Hygiene Officer	7:30 AM–5:00 PM	Saturday, March 12	San Diego Convention Center, Room 31C
CHAS Cannabis Extraction & Analysis	7:30 AM–5:00 PM	Saturday, March 12	San Diego Convention Center, Room 32A
CHAS Executive Committee	7:00 AM–12:00 PM	Sunday, March 13	Hilton Gaslamp Quarter, Santa Rosa

### Division of Chemical Education— CHED

DivCHED Fiduciary Workshop	5:30 PM–8:30 PM	Friday, March 11	San Diego Convention Center, Room 28A
ACS Exams Institute – Board of Trustees Meeting	7:30 AM–12:00 PM	Saturday, March 12	San Diego Convention Center, Room 29A
ACS Exams – General Chemistry Paired Questions 2017 Exam	8:00 AM–5:00 PM	Saturday, March 12	Embassy Suites San Diego Downtown Bay, Monterey I
ACS Exams – Diagnostic of Undergraduate Chemical Knowledge (DUCK) 2017 Exam	8:00 AM–5:00 PM	Saturday, March 12	Embassy Suites San Diego Downtown Bay, Monterey II
ACS Exams – Instrumental Analysis 2017 Exam	8:00 AM–5:00 PM	Saturday, March 12	Embassy Suites San Diego Downtown Bay, Santa Fe
ACS DivCHED JCE Board of Publication Meeting	8:00 AM–12:30 PM	Saturday, March 12	San Diego Convention Center, Room 28E
ACS Exams – Inorganic Chemistry Foundations 2016 Exam	8:00 AM–5:00 PM	Saturday, March 12	San Diego Convention Center, Room 28A
ACS Exams – General Chemistry 2nd Term 2017 Exam	8:00 AM–5:00 PM	Saturday, March 12	San Diego Convention Center, Room 28C
ACS Exams – Biochemistry 2017 Exam	8:30 AM–5:00 PM	Saturday, March 12	Embassy Suites San Diego Downtown Bay, Topeka
DivCHED Program Committee Meeting	10:30 AM–12:00 PM	Saturday, March 12	Manchester Grand Hyatt San Diego, Ocean Beach

## GOVERNANCE & BUSINESS MEETINGS

DivCHED Executive Committee Meeting	1:00 PM–5:30 PM	Saturday, March 12	San Diego Convention Center, Room 2
DivCHED Biennial Conference on Chemical Education	4:00 PM–6:00 PM	Saturday, March 12	San Diego Convention Center, Room 3
DivCHED Chemical Education Research Committee	7:00 AM–9:00 AM	Sunday, March 13	Manchester Grand Hyatt San Diego, Coronado E
ACS Exams – General Chemistry Paired Questions 2017 Exam	8:00 AM–5:00 PM	Sunday, March 13	Embassy Suites San Diego Downtown Bay, Atchison
ACS Exams – Organic Chemistry 2018 Exam	8:00 AM–5:00 PM	Sunday, March 13	Embassy Suites San Diego Downtown Bay, Monterey II
ACS Exams – Organic Chemistry 1st Term 2017 Exam	8:00 AM–5:00 PM	Sunday, March 13	Embassy Suites San Diego Downtown Bay, Santa Fe
ACS Exams – Instrumental Analysis 2017 Exam	8:00 AM–5:00 PM	Sunday, March 13	Embassy Suites San Diego Downtown Bay, U. Pacific
DivCHED International Activities Committee Meeting	8:00 AM–9:30 AM	Sunday, March 13	San Diego Convention Center, Room 12
ACS Exams – Biochemistry 2017 Exam	8:00 AM–5:00 PM	Sunday, March 13	The Westin San Diego Gaslamp Quarter, Plaza B
ACS Exams – Diagnostic of Undergraduate Chemical Knowledge (DUCK) 2017 Exam	8:00 AM–5:00 PM	Sunday, March 13	The Westin San Diego Gaslamp Quarter, Plaza C
ACS Exams – Workshop	9:00 AM–5:00 PM	Sunday, March 13	Embassy Suites San Diego Downtown Bay, Topeka
DivCHED Finance Committee Meeting	9:30 AM–11:30 AM	Sunday, March 13	Manchester Grand Hyatt San Diego, Coronado E
DivCHED Younger Chemists Committee Meeting	10:30 AM–12:30 PM	Sunday, March 13	San Diego Convention Center, Room 12
High School/College Interface Luncheon— Ticketed Event	12:00 PM–1:00 PM	Sunday, March 13	Manchester Grand Hyatt San Diego, Harbor Blrm A
DivCHED Regional Meetings Committee	12:00 PM–2:00 PM	Sunday, March 13	Manchester Grand Hyatt San Diego, Coronado E
DivCHED Long Range Planning Committee	2:30 PM–4:30 PM	Sunday, March 13	Manchester Grand Hyatt San Diego, Coronado E
DivCHED Safety Committee Meeting	4:00 PM–5:30 PM	Sunday, March 13	Embassy Suites San Diego Downtown Bay, Mariposa
DivCHED Social Reception	5:30 PM–7:00 PM	Sunday, March 13	Manchester Grand Hyatt San Diego, Coronado, Foyer
ACS Exams Workshop 2	9:00 AM–5:00 PM	Monday, March 14	Embassy Suites San Diego Downtown Bay, Mariposa
DivCHED Business Meeting	12:00 PM–12:30 PM	Monday, March 14	Manchester Grand Hyatt San Diego, Promenade A
CHED Undergraduate Research Posters	12:00 PM–2:00 PM	Monday, March 14	San Diego Convention Center, Hall D/E
DivCHED New Member Committee Meeting	12:30 PM–1:00 PM	Monday, March 14	Manchester Grand Hyatt San Diego, Promenade A
CHED Poster Session	7:00 PM–9:00 PM	Sunday, March 13	San Diego Convention Center, Hall D

### Division of Chemical Information— CINF

CINF Division Education Committee Meeting	1:00 PM–3:00 PM	Saturday, March 12	San Diego Convention Center, Room 32B
CINF Division Program Committee Meeting	1:00 PM–3:00 PM	Saturday, March 12	San Diego Convention Center, Room 33B
CINF Division Awards Committee Meeting	1:00 PM–3:00 PM	Saturday, March 12	San Diego Convention Center, Room 33C
CINF Division Executive Committee Meeting	3:00 PM–6:00 PM	Saturday, March 12	San Diego Convention Center, Room 33A
Chemical Structure Association Trust (CSAT) Meeting	12:00 PM–2:00 PM	Sunday, March 13	San Diego Convention Center, Room 6D
CINF Division Welcoming Reception and Poster Session	6:30 PM–8:30 PM	Sunday, March 13	San Diego Convention Center, Room 3
CINF Division Luncheon— Ticketed Event	12:00 PM–1:30 PM	Tuesday, March 15	San Diego Convention Center, Room 20D



## GOVERNANCE & BUSINESS MEETINGS

### Division of Colloid and Surface Chemistry— COLL

COLL Program/Executive Committee Meeting	5:00 PM–7:00 PM	Saturday, March 12	San Diego Convention Center, Room 30D
COLL Social Hour/Open Business Meeting/Poster Session	5:30 PM–8:00 PM	Sunday, March 13	San Diego Convention Center, Hall E
COLL Luncheon	12:00 PM–1:30 PM	Tuesday, March 15	San Diego Convention Center, Room 20B/C

### Division of Computers in Chemistry— COMP

COMP Executive Committee Meeting	3:00 PM–6:00 PM	Saturday, March 12	San Diego Convention Center, Room 29D
COMP Poster Session	6:00 PM–8:00 PM	Tuesday, March 15	San Diego Convention Center, Hall E

### Division of Energy and Fuels— ENFL

ENFL Program Meeting	12:00 PM–2:00 PM	Sunday, March 13	Wyndham San Diego Bayfront, Harborside
ENFL Executive Meeting	4:00 PM–7:00 PM	Sunday, March 13	Wyndham San Diego Bayfront, Harborside
ENFL Dinner— Ticketed Event	6:00 PM–10:00 PM	Tuesday, March 15	Prado, 1549 El Prado, San Diego, CA
ENFL Poster Session	2:00 PM–4:00 PM	Monday, March 14	San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)

### Division of Environmental Chemistry— ENVR

ENVR Program Planning Meeting	2:00 PM–3:00 PM	Sunday, March 13	Omni San Diego Hotel, Balboa 1
ENVR Long Range Planning Meeting	3:00 PM–5:00 PM	Sunday, March 13	Omni San Diego Hotel, Balboa 2
ENVR Executive Committee Meeting	7:00 PM–10:00 PM	Sunday, March 13	Omni San Diego Hotel, Gaslamp 4
ENVR Division Reception— Ticketed Event	6:30 PM–8:00 PM	Tuesday, March 15	Meze Greek, 345 6th Avenue, San Diego, CA
ENVR Poster Session	6:00 PM–8:00 PM	Wednesday, March 16	San Diego Convention Center, Hall D

### Division of Fluorine Chemistry— FLUO

FLUO Creative Work in Fluorine Chemistry Banquet	6:30 PM–9:30 PM	Monday, March 14	Off Site
FLUO Executive Committee Meeting	8:00 AM–12:00 PM	Tuesday, March 15	The Westin San Diego Gaslamp Quarter, Harbor B
FLUO Poster Session	6:00 PM–8:00 PM	Sunday, March 13	San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)

### Division of Geochemistry— GEOC

Executive Committee Meeting	6:00 PM–8:00 PM	Sunday, March 13	Omni San Diego Hotel, Balboa 1
Geochemistry Division Reception	5:30 PM–7:30 PM	Tuesday, March 15	Omni San Diego Hotel, Gallery 1/2
GEOC Poster Session	8:00 PM–10:00 PM	Wednesday, March 16	San Diego Convention Center, Hall D

### Division of Industrial and Engineering Chemistry— I&EC

I&EC Green Chemistry & Engineering Subdivision Business Meeting	12:00 PM–12:30 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Conf. Rm 1
I&EC Novel Chemistry in Action Subdivision Business Meeting	12:30 PM–1:00 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Conf. Rm 2
I&EC Applied Chemical Technicians Subdivision Business Meeting	1:00 PM–1:30 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Conf. Rm 1
I&EC Separation Science & Technology Subdivision Business Meeting	1:30 PM–2:30 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Conf. Rm 2

## GOVERNANCE & BUSINESS MEETINGS

I&EC Steering Committee Meeting	2:30 PM–4:00 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Carlsbad
I&EC Program Committee Meeting	4:00 PM–5:00 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Carlsbad
I&EC Realities of the Chemistry Industry: Career Opportunities & Paths Speaker Luncheon	11:30 AM–1:00 PM	Monday, March 14	Marriott Marquis San Diego Marina, Palomar Rm
I&EC Realities of the Chemistry Industry: Career Opportunities & Path Speaker Lunch	12:00 PM–1:30 PM	Tuesday, March 15	Marriott Marquis San Diego Marina, Carlsbad
I&EC Poster Session	5:00 PM–7:00 PM	Tuesday, March 15	San Diego Convention Center, Hall D

### Division of Inorganic Chemistry— INOR

INOR Poster Session I	6:00 PM–8:00 PM	Sunday, March 13	San Diego Convention Center, Hall D
INOR Poster Session II	6:00 PM–8:00 PM	Tuesday, March 15	San Diego Convention Center, Hall D

### Division of Medicinal Chemistry— MEDI

MEDI Executive Meeting	8:30 AM–1:00 PM	Sunday, March 13	San Diego Convention Center, Room 15B
MEDI Division Business Meeting	5:30 PM–6:30 PM	Sunday, March 13	San Diego Convention Center, Room 15B
MEDI Poster Session	7:00 PM–9:00 PM	Sunday, March 13	San Diego Convention Center, Hall F
MEDI Long Range Planning Committee Meeting	5:30 PM–10:00 PM	Monday, March 14	San Diego Convention Center, Room 5A
Joint MEDI/ORGN Poster Session	7:00 PM–10:00 PM	Wednesday, March 16	San Diego Convention Center, Hall F

### Division of Nuclear Chemistry and Technology— NUCL

NUCL Division Executive Committee Meeting	5:00 PM–7:00 PM	Sunday, March 13	San Diego Convention Center, Room 15A
NUCL Business Meeting	5:00 PM–6:00 PM	Tuesday, March 15	San Diego Convention Center, Room 10
NUCL Social Hour	6:00 PM–8:00 PM	Tuesday, March 15	San Diego Convention Center, Room 20D

### Division of Organic Chemistry— ORGN

ORGN Executive Committee Meeting	1:00 PM–5:30 PM	Sunday, March 13	San Diego Convention Center, Room 30A
ORGN Poster Session I	8:00 PM–10:00 PM	Sunday, March 13	San Diego Convention Center, Hall D
ORGN Poster Session II	8:00 PM–10:00 PM	Tuesday, March 15	San Diego Convention Center, Hall D
Joint MEDI/ORGN Poster Session	7:00 PM–10:00 PM	Wednesday, March 16	San Diego Convention Center, Hall D

### Division of Physical Chemistry— PHYS

PHYS Executive Committee Meeting	4:30 PM–7:30 PM	Sunday, March 13	San Diego Convention Center, Room 5A
PHYS Poster Session	6:00 PM–8:00 PM	Wednesday, March 16	San Diego Convention Center, Hall D

### Division of Polymeric Materials Science and Engineering— PMSE

PMSE Executive Committee Meeting	4:30 PM–7:00 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Coronado
PMSE Business Meeting and PMSE/POLY Coordination Meeting	5:00 PM–6:00 PM	Monday, March 14	Marriott Marquis San Diego Marina, Oceanside
Joint PMSE/POLY Poster Session	6:00 PM–8:00 PM	Tuesday, March 15	San Diego Convention Center, Hall F

## GOVERNANCE & BUSINESS MEETINGS

### Division of Polymer Chemistry— POLY

POLY Workshop Committee	11:00 PM–12:00 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Newport Bch
POLY Board Meeting	12:00 PM–2:00 PM	Sunday, March 13	Hilton San Diego Bayfront, Sapphire M/N
POLY Strategic/Long Range Planning	3:00 PM–4:00 PM	Sunday, March 13	Marriott Marquis San Diego Marina, Newport Bch
POLY International Committee Meeting	11:00 AM–12:00 PM	Monday, March 14	Marriott Marquis San Diego Marina, Newport Bch
POLY Financial/Executive Planning	12:00 PM–1:00 PM	Monday, March 14	Marriott Marquis San Diego Marina, Oceanside
POLYEd Meeting	7:30 AM–9:30 AM	Tuesday, March 15	Marriott Marquis San Diego Marina, Oceanside
POLY Industrial Advisory Board Meeting	7:30 AM–9:30 AM	Tuesday, March 15	Marriott Marquis San Diego Marina, Temecula 3&4
POLY IPEC Meeting	9:30 AM–12:00 PM	Tuesday, March 15	Marriott Marquis San Diego Marina, Malibu
POLY Programming Committee	12:00 PM–2:00 PM	Tuesday, March 15	Marriott Marquis San Diego Marina, Marina Sn E
POLY Membership Committee	2:00 PM–3:00 PM	Tuesday, March 15	Marriott Marquis San Diego Marina, Oceanside
Joint PMSE/POLY Poster Session	6:00 PM–8:00 PM	Tuesday, March 15	San Diego Convention Center, Hall F
PMSE/POLY Awards Lecture & Reception	5:30 PM–8:00 PM	Wednesday, March 16	Marriott Marquis San Diego Marina, SD Blrm B

### Division of Small Chemical Businesses— SCHB

SCHB Executive Committee	5:00 PM–10:00 PM	Saturday, March 12	Marriott Marquis San Diego Marina, Newport Bch
SCHB Poster Session	11:00 AM–1:00 PM	Monday, March 14	Marriott Marquis San Diego Marina, Santa Rosa
SCHB & PROF Luncheon	11:30 AM–1:30 PM	Monday, March 14	Marriott Marquis San Diego Marina, Vista
SCHB Business Meeting	12:00 PM–1:00 PM	Monday, March 14	Marriott Marquis San Diego Marina, Vista
SCHB & PROF Luncheon	11:30 AM–1:30 PM	Tuesday, March 15	Marriott Marquis San Diego Marina, Vista

# SOCIAL & EDUCATIONAL EVENTS

## PRESIDENTIAL EVENTS

### ACS PRESIDENT DONNA NELSON

welcomes attendees to the 251st ACS National Meeting. The presidential programming promises excellent science as well as opportunities to become involved in discussions and community efforts to address member concerns. This direct solicitation for member feedback is unprecedented in presidential programming, so please participate if you want to see it continued.

Three presidential sessions address ACS member concerns about employment in the chemical sciences, demographic data and their applications to diversity in chemistry, and changes in organic chemistry as a prerequisite. In order to facilitate members voicing their concerns, each symposium will be a panel discussion including participation by the audience. In addition to these three presidential sessions, there will be two traditional sessions featuring past Stanley C. Israel Award winners and the current Dreyfus Prize recipient.

The first presidential symposium, titled "Discussions with the President's Task Force on Employment," will take place on Sunday, March 13, from 1:30 to 4:00 PM. Speakers will be members of the president's task force, representing academe, government, and industry. Task force members were charged with examining (1) issues broadly related to employment of chemistry professionals in the U.S., (2) the plight of demographic subgroups and people at different education and experience levels, and (3) different sectors of employment reflecting the situation of all chemical professionals, not just ACS members. They will report the results of their first year of efforts on topics pertinent to unemployment in the chemical sciences, such as supply and demand in the chemical workforce, career opportunities for undergraduate professionals, professional certificates, preparing graduates for industrial jobs, challenges of unemployment, and global factors influencing employment.

The second session addressing member concerns is titled "Is There a Crisis in Organic Chemistry?" Representatives from publishers of comprehensive undergraduate organic chemistry textbooks will speak. Cengage, Elsevier, McGraw-Hill, Macmillan, Pearson, and Wiley will discuss changes in organic chemistry as a prerequisite, current teaching methods, and responses of organic chemistry programs, professors, and requirements. This symposium will take place Monday, March 14, from 9:00 to 11:30 AM.

The third session on member concerns, "Diversity—Quantification—Success," will address the use of data to drive activities diversifying the chemical sciences. Researchers will present their demographic data, disaggregated by race and gender, on various sectors of the chemical sciences. Madeleine Jacobs, Valerie Kuck, Sibrina Collins, Rigoberto Hernandez, and Dontarie Stallings will speak on Monday, March 14, from 1:30 to 4:00 PM.

A new method will be tried for encouraging community efforts to address member concerns in these three areas via contributed presidential poster sessions at this meeting. The topics will correspond to the oral sessions described above. View the posters Sunday, March 13, from 8:00 to 10:00 PM, and Monday evening during Sci-Mix. The panel discussions and contributed poster sessions are opportunities for ACS communities to grow together via teamwork and improve our Society. Please attend these trial activities and voice your ideas.

In addition, "How To Foster Diversity in the Chemical Sciences: Lessons Learned and Taught from the Stories of Recipients of the Stanley C. Israel Award" will be held Monday, March 14, from 8:30 AM to noon. Building on symposia of the same name at previous national meetings, this symposium promises ideas and inspiration for increasing diversity in our communities.

Finally, the Dreyfus Prize Symposium will honor the most recent recipient of this award, Krzysztof Matyjaszewski, by focusing its content on his area of research, "Making Molecules & Materials." Supporting talks will be delivered Tuesday, March 15, from 9:00 to 11:45 AM, and 2:00 to 4:30 PM.

Details of these presidential events and other recommended symposia can be found at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016).

## ACS 2016 NATIONAL AWARD WINNERS

**THE ACS NATIONAL** awards recognize individual or team accomplishments in diverse fields of the chemical sciences. Award recipients traditionally receive their national award in person during the ACS awards dinner and general meeting and deliver an award address on the scientific work that is being recognized to an appropriate division.

This year's event will be held on the evening of Tuesday, March 15, at the Manchester Grand Hyatt San Diego Hotel, Harbor Ballroom D-I. Dinner begins at 7:30 PM, and the general meeting begins at 8:30 PM.

Mostafa A. El-Sayed will deliver the Priestley Medal Address at the general meeting. See Ticketed Events on page 39 for ticket information.

Several awards, such as the Arthur C. Cope Scholar Awards and the Arthur C. Cope Award, will be presented at the Arthur C. Cope Symposium in conjunction with the 252nd ACS National Meeting in Philadelphia in August.

**ACS Award for Achievement in Research for the Teaching and Learning of Chemistry**, sponsored by Pearson Education, **Avi Hofstein**, Weizmann Institute of Science, Israel. Address to be presented before the Division of Chemical Education. March 14; Manchester Grand Hyatt San Diego; Mission Beach A/B; 11:55 AM.

**ACS Award for Affordable Green Chemistry**, sponsored by Dow Chemical and endowed by Rohm and Haas, **Martin D. Johnson and Joseph R. Martinelli**, Eli Lilly and Co., and **Shannon S. Stahl**, University of Wisconsin, Madison. Address to be presented before the Division of Organic Chemistry. March 14; San Diego Convention Center; Room 6B; 9:50 AM, 10:50 AM & 11:20 AM.

**ACS Award for Computers in Chemical & Pharmaceutical Research**, sponsored by the ACS Division of Computers in Chemistry, **Warren J. Hehre**, Wavefunction Inc. and the University of California, Irvine, (Emeritus). Address to be presented before the Division of Computers in Chemistry. March 15; San Diego Convention Center; Room 28A; 4:15 PM.

**ACS Award for Creative Advances in Environmental Science & Technology**, sponsored by the ACS Division of Environmental Chemistry and the ACS Publications journals *Environmental Science & Technology* and *Environmental Science & Technology Letters*, **Bruce E. Logan**, Penn State University. Address to be presented before the Division of Environmental Chemistry. March 16; Omni San Diego; Grand Ballroom E; 10:25 AM.

**ACS Award for Creative Invention**, sponsored by ACS Corporation Associates, **Antonio Facchetti** Polyera Corp. and Northwestern University. Address to be presented before the Division of Polymeric Materials: Science & Engineering. March 15; Marriott Marquis San Diego Marina; Point Loma; 4:25 PM.

**ACS Award for Creative Work in Fluorine Chemistry**, sponsored by the Juhua Group Technology Center (China), **Steven H. Strauss**, Colorado State University. Address to be presented before the Division of Fluorine Chemistry. March 14; The Westin San Diego Gaslamp Quarter; Harbor A/B; 6:00 PM.

**ACS Award for Creative Work in Synthetic Organic Chemistry**, sponsored by Aldrich Chemical Co. LLC, **Scott J. Miller**, Yale University. Address to be presented before the Division of Organic Chemistry. March 13; San Diego Convention Center; Room 6A; 4:10 PM

**ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry**, sponsored by Strem Chemicals, **Vincent L. Pecoraro**, University of Michigan, Ann Arbor. Address to be presented before the Division of Inorganic Chemistry. March 14; San Diego Convention Center; Room 20A-C; 8:45 AM.

**ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences**, sponsored by the Camille & Henry Dreyfus Foundation, **Luis A. Colón**, University at Buffalo, SUNY. Address to be presented before the Division of Analytical Chemistry at the fall ACS national meeting in Philadelphia.

**ACS Award for Encouraging Women into Careers in the Chemical Sciences**, sponsored by the Camille and Henry Dreyfus Foundation, **Carol A. Fierke**, University of Michigan, Ann Arbor. Address to be presented before the ACS Women Chemists Committee and the ACS Division of Bio-

logical Chemistry. March 15; Hilton San Diego Bayfront; Cobalt 520; 11:35 AM.

**ACS Award for Research at an Undergraduate Institution**, sponsored by Research Corporation for Science Advancement, **Thomas E. Goodwin**, Hendrix College. Address to be presented before the Division of Organic Chemistry. March 15; San Diego Convention Center; Room 6C; 11:00 AM.

**ACS Award for Team Innovation**, sponsored by ACS Corporation Associates, **Matthew F. Brown**, **Mark E. Flanagan** and **Chakrapani Subramanyam**, Pfizer Worldwide Medicinal Chemistry; **Paul S. Changelian**, Confluence Life Sciences; and **Michael John Munchhof**, Michael J. Munchhof, LLC. Address to be presented before the Division of Medicinal Chemistry. March 15; San Diego Convention Center; Room 6F; 9:40 AM.

**ACS Award in Analytical Chemistry**, sponsored by the Battelle Memorial Institute, **William R. Heineman**, University of Cincinnati. Address to be presented before the Division of Analytical Chemistry at the fall ACS national meeting in Philadelphia.

**ACS Award in Applied Polymer Science**, sponsored by Eastman Chemical, **Thomas P. Russell**, University of Massachusetts, Amherst and Lawrence Berkeley National Laboratory. Address to be presented before the Division of Polymeric Materials: Science & Engineering. March 14; Marriott Marquis San Diego Marina; San Diego Ballroom C; 4:00 PM.

**ACS Award in Chromatography**, sponsored by MilliporeSigma, **Harold M. McNair**, Virginia Polytechnic Institute & State University. Address to be presented before the Division of Analytical Chemistry at the fall ACS national meeting in Philadelphia.

**ACS Award in Colloid and Surface Chemistry**, sponsored by Colgate-Palmolive Co., **Nicholas L. Abbott**, University of Wisconsin, Madison. Address to be presented before the Division of Colloid & Surface Chemistry. March 15; San Diego Convention Center; Room 7A; 4:00 PM.

**ACS Award in Industrial Chemistry**, sponsored by the ACS Division of Industrial & Engineering Chemistry, **Ted C. Germroth**, Eastman Chemical. Address to be presented before the Division of Industrial & Engineering Chemistry.

March 15; Marriott Marquis San Diego Marina; Temecula 1&2; 11:05 AM.

**ACS Award in Inorganic Chemistry**, sponsored by Aldrich Chemical Co., LLC, **Mercouri G. Kanatzidis**, Northwestern University. Address to be presented before the Division of Inorganic Chemistry. March 14; San Diego Convention Center; Room 20A-C; 8:15 AM.

**ACS Award in Organometallic Chemistry**, sponsored by the Dow Chemical Co. Foundation, **Karen I. Goldberg**, University of Washington. Address to be presented before the Division of Inorganic Chemistry. March 14; San Diego Convention Center; Room 20A-C; 10:25 AM.

**ACS Award in Polymer Chemistry**, sponsored by ExxonMobil Chemical, **Edmund M. Carnahan**, Dow Chemical. Address to be presented before the Division of Polymer Chemistry. March 14; Marriott Marquis San Diego Marina; Torrey Pines 1&2; 4:00 PM.

**ACS Award in Pure Chemistry**, sponsored by Alpha Chi Sigma Fraternity and Alpha Chi Sigma Educational Foundation, **Jonathan S. Owen**, Columbia University. Address to be presented before the Division of Inorganic Chemistry. March 14; San Diego Convention Center; Room 20A-C; 11:25 AM.

**ACS Award in Separations Science & Technology**, sponsored by Waters Corp., **Steven M. Cramer**, Rensselaer Polytechnic Institute. Address to be presented before the Division of Industrial & Engineering Chemistry Separations Science and Technology Symposium. March 13; Marriott Marquis San Diego Marina; Temecula 3&4; 10:50 AM.

**ACS Award in the Chemistry of Materials**, sponsored by E. I. du Pont de Nemours & Co., **Jean-Luc E. Brédas**, King Abdullah University of Science & Technology, Thuwal, Saudi Arabia. Address to be presented before the Division of Physical Chemistry. March 15; San Diego Convention Center; Room 29A/B; 2:40 PM.

**ACS Award in Theoretical Chemistry**, sponsored by ACS, **Roberto Car**, Princeton University. Address to be presented before the Division of Physical Chemistry. March 15; San Diego Convention Center; Room 29A/B; 2:05 PM.

**Award for Volunteer Service to the American Chemical Society**, sponsored

by ACS, **H. N. Cheng**, U.S. Department of Agriculture and Agricultural Research Service. Address to be presented before the ACS ChemLuminary Awards at the ACS fall national meeting in Philadelphia.

**Alfred Bader Award in Bioinorganic or Bioorganic Chemistry**, sponsored by the Alfred R. Bader Fund, **Edward I. Solomon**, Stanford University and SLAC National Accelerator Laboratory. Address to be presented before the Division of Inorganic Chemistry. March 14; San Diego Convention Center; Room 20A-C; 11:55 AM.

**Earle B. Barnes Award for Leadership in Chemical Research Management**, sponsored by the Dow Chemical Co. Foundation, **Henry E. Bryndza**, DuPont. Address to be presented before the Division of Inorganic Chemistry. March 14; San Diego Convention Center; Room 20A-C; 9:45 AM.

**Ronald Breslow Award for Achievement in Biomimetic Chemistry**, sponsored by the Ronald Breslow Award Endowment, **Thomas W. Muir**, Princeton University. Address to be presented before the Division of Biological Chemistry at the ACS fall national meeting in Philadelphia.

**Herbert C. Brown Award for Creative Research in Synthetic Methods**, sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment, **Alois Fürstner**, Max-Planck-Institut für Kohlenforschung, Mülheim/Ruhr, Germany. Address to be presented before the Division of Organic Chemistry. March 15; San Diego Convention Center; Room 6A; 3:55 PM.

**James Bryant Conant Award in High School Chemistry Teaching**, sponsored by Thermo Fisher Scientific, **Julia Winter**, Alchemie Games and Detroit Country Day School, Beverly Hills, MI. Address to be presented before the Division of Organic Chemistry. March 15; San Diego Convention Center; Room 6C; 4:05 PM.

**Alfred Burger Award in Medicinal Chemistry**, sponsored by Gilead Sciences, Inc., **Richard DiMarchi**, Indiana University. Address to be presented before the Division of Medicinal Chemistry. March 15; San Diego Convention Center; Room 6F; 11:40 AM.

**Arthur C. Cope Award**, sponsored by the Arthur C. Cope Fund, **Eric N. Jacobsen**, Harvard University. Address to be presented before the Division of Organic

Chemistry at the ACS fall national meeting in Philadelphia.

**Arthur C. Cope Scholar Awards**, sponsored by the Arthur C. Cope Fund, **Takahiko Akiyama**, Gakushuin University, Japan; **Kristi S. Anseth**, University of Colorado, Boulder; **Geert-Jan Boons**, University of Georgia and Utrecht University, the Netherlands; **Luis M. Campos**, Columbia University; **Seth M. Cohen**, University of California, San Diego; **Matthew J. Gaunt**, University of Cambridge, England; **Marc M. Greenberg**, Johns Hopkins University; **Thomas J. Kodadek**, Scripps Research Institute, Florida; **Lawrence T. Scott**, Boston College and University of Nevada, Reno; **David A. Spiegel**, Yale University. Address to be presented before the Division of Organic Chemistry at the ACS fall national meeting in Philadelphia.

**Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator**, sponsored by the Pfizer Endowment Fund, **Phil S. Baran**, Scripps Research Institute, La Jolla. Address to be presented before the Division of Organic Chemistry. March 14; San Diego Convention Center; Room 6A; 10:40 AM.

**F. Albert Cotton Award in Synthetic Inorganic Chemistry**, sponsored by the F. Albert Cotton Endowment Fund, **François P. Gabbaï**, Texas A&M University. Address to be presented before the Division of Inorganic Chemistry. March 14; San Diego Convention Center; Room 20A-C; 10:55 AM.

**Peter Debye Award in Physical Chemistry**, sponsored by E. I. du Pont de Nemours & Co., **Mark A. Ratner**, Northwestern University. Address to be presented before the Division of Physical Chemistry. March 15; San Diego Convention Center; Room 29A/B; 1:30 PM.

**Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry**, sponsored by Waters Corp., **Albert John Roeland Heck**, Netherlands Proteomics Centre and Utrecht University, The Netherlands. Address to be presented before the Division of Analytical Chemistry. March 15; Wyndham San Diego Bayside; East Coast; 11:35 AM.

**Francis P. Garvan–John M. Olin Medal**, sponsored by the Francis P. Garvan–John M. Olin Medal Endowment, **Annie**

**B. Kersting**, Lawrence Livermore National Laboratory. Address to be presented before the Division of Nuclear Chemistry & Technology. March 14; San Diego Convention Center; Room 15A; 5:25 PM.

**James T. Grady–James H. Stack Award for Interpreting Chemistry for the Public**, sponsored by ACS, **Peter Atkins**, Lincoln College and University of Oxford, England. Address to be presented before the ACS Office of Public Affairs at the fall ACS national meeting in Philadelphia.

**Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator**, sponsored by the Gray Award Endowment, **Eric J. Schelter**, University of Pennsylvania. Address to be presented before the Division of Inorganic Chemistry. March 14; San Diego Convention Center; Room 20A-C; 9:15 AM.

**Ernest Guenther Award in the Chemistry of Natural Products**, sponsored by Givaudan, **Eric Block**, University at Albany, SUNY. Address to be presented before the Division of Organic Chemistry. March 14; San Diego Convention Center; Room 6A; 4:05 PM.

**Kathryn C. Hach Award for Entrepreneurial Success**, sponsored by the Kathryn C. Hach Award Fund, **Scott D. Allen and Anthony R. Eisenhut**, Novomer, Inc., and **Geoffrey W. Coates**, Cornell University. Address to be presented before the Division of Polymer Chemistry. March 13; Marriott Marquis San Diego Marina; Mission Hills; 3:45 PM.

**Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids**, sponsored by ExxonMobil Research and Engineering, **Kenneth S. Schweizer**, University of Illinois, Urbana-Champaign. Address to be presented before the Division of Physical Chemistry. March 15; San Diego Convention Center; Room 29A/B; 4:15 PM.

**Ralph F. Hirschmann Award in Peptide Chemistry**, sponsored by Merck Research Laboratories, **Ronald T. Raines**, University of Wisconsin, Madison. Address to be presented before the Division of Organic Chemistry. March 16; San Diego Convention Center; Room 6A; 4:00 PM.

**Ipatieff Prize**, sponsored by the Ipatieff Trust Fund, **Aditya Bhan**, University of Minnesota, Twin Cities. Address to be presented before the Division of Cataly-

sis Science & Technology. March 15; Manchester Grand Hyatt San Diego; Coronado A; 2:15 PM.

**Frederic Stanley Kipping Award in Silicon Chemistry**, sponsored by Dow Corning, **Michael A. Brook**, McMaster University, Ontario. Address to be presented before the U.S. Based Silicon Symposium, Portland, OR, and the Division of Polymer Chemistry, March 14; Marriott Marquis San Diego Marina; Rancho Sante Fe 1&2; 11:00 AM.

**Irving Langmuir Award in Chemical Physics**, sponsored by GE Global Research and the ACS Division of Physical Chemistry, **George C. Schatz**, Northwestern University. Address to be presented before the Division of Physical Chemistry. March 15; San Diego Convention Center; Room 29A/B; 3:15 PM.

**Josef Michl ACS Award in Photochemistry**, sponsored by the Josef Michl Award Endowment, **Frederick D. Lewis**, Northwestern University. Address to be presented before the Division of Organic Chemistry. March 15; San Diego Convention Center; Room 6A; 11:05 AM.

**E. V. Murphree Award in Industrial & Engineering Chemistry**, sponsored by ExxonMobil Research and Engineering, **Michael Thackeray**, Argonne National Laboratory. Address to be presented before the Division of Industrial & Engineering Chemistry at the ACS fall national meeting in Philadelphia, PA.

**Nobel Laureate Signature Award for Graduate Education in Chemistry**, sponsored by Avantor Performance Materials, **Matthew J. Polinski (student)**, Bloomsburg University of Pennsylvania, and **Thomas E. Albrecht-Schmitt (preceptor)**, Florida State University. Address to be presented before the Division of Nuclear Chemistry & Technology. March 13; San Diego Convention Center; Room 15A; 8:15 AM & 8:45 AM.

**James Flack Norris Award in Physical Organic Chemistry**, sponsored by the ACS Northeastern Section, **J. C. (Tito) Scaiano**, University of Ottawa, Ontario. Address to be presented before the Division of Catalysis Science & Technology. March 16; Manchester Grand Hyatt San Diego; Coronado A; 3:40 PM.

**George A. Olah Award in Hydrocarbon or Petroleum Chemistry**, sponsored by the George A. Olah Award Endowment, **Mieczyslaw M. Boduszynski**, Retired,

Chevron Energy Technology Co. Address to be presented before the Division of Energy & Fuels. March 16; Wyndham San Diego Bayside; Pacific B; 1:45 PM.

**George C. Pimentel Award in Chemical Education**, sponsored by Cengage Learning and the ACS Division of Chemical Education, **Richard S. Moog**, Franklin & Marshall College and The POGIL Project. Address to be presented before the Division of Chemical Education. March 15; Manchester Grand Hyatt San Diego; Harbor Ballroom A; 3:30 PM.

**Priestley Medal**, sponsored by ACS, **Mostafa A. El-Sayed**, Georgia Institute of Technology. Address to be presented at the ACS National Awards Banquet Ceremony & General Meeting of the Society at the spring national meeting in San Diego.

**Glenn T. Seaborg Award for Nuclear Chemistry**, sponsored by the ACS Division of Nuclear Chemistry & Technology, **E. (Earl) Philip Horwitz**, Eichrom Technologies, LLC. Address to be presented before the Division of Nuclear Chemistry & Technology at the ACS fall national meeting in Philadelphia, PA.

**Gabor A. Somorjai Award for Creative Research in Catalysis**, sponsored by the Gabor A. and Judith K. Somorjai Endowment Fund, **Donna G. Blackmond**, The Scripps Research Institute, La Jolla. Address to be presented before the Division of Organic Chemistry. March 16; San Diego Convention Center; Room 6A; 11:05 AM.

**George & Christine Sosnovsky Award for Cancer Research**, sponsored by the George & Christine Sosnovsky Endowment Fund, **Juswinder Singh**, Ankaa Therapeutics. Address to be presented before the Division of Medicinal Chemistry. March 15; San Diego Convention Center; Room 6F; 9:00 AM.

**E. Bright Wilson Award in Spectroscopy**, sponsored by the ACS Division of Physical Chemistry, **Robert G. Griffin**, Massachusetts Institute of Technology. Address to be presented before the Division of Physical Chemistry. March 15; San Diego Convention Center; Room 29A/B; 5:25 PM.

**Ahmed Zewail Award in Ultrafast Science & Technology**, sponsored by the Ahmed Zewail Endowment Fund established by the Newport Corp., **Andrei Tokmakoff**, The University of Chicago.

Address to be presented before the Division of Physical Chemistry. March 15; San Diego Convention Center; Room 29A/B; 4:50 PM.

**National Fresenius Award**, sponsored by Phi Lambda Upsilon, the National Chemistry Honor Society, **Douglas A. Mitchell**, University of Illinois, Urbana-Champaign. Address to be presented before the Division of Biological Chemistry at the ACS fall national meeting in Philadelphia, PA.

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### STUDENT & EDUCATOR ACTIVITIES

**EDUCATION-FOCUSED** programs and specialty activities are being held for undergraduate students, graduate students, high school teachers, faculty at two- and four-year colleges, and chemical professionals. Explore these opportunities in depth at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016).

**UNDERGRADUATE PROGRAM.** A vibrant program designed especially for undergraduate students has been planned by the Society Committee on Education's Undergraduate Programs Advisory Board. This educational and career-oriented program includes technical symposia and workshops on essential skills for employment in chemistry and success in graduate school. Eminent scientist Richard Zare from Stanford University will discuss his life with lasers.

**Sunday, March 13**

**Undergraduate Hospitality Center**  
8:00 AM to 5:00 PM

**Undergraduate Research Papers (Oral) (sponsored by CHED)**  
8:30 AM to 5:00 PM

**Two-Year Guidelines: What's New?**  
8:30 AM to noon

**Making the Most of Your First ACS Meeting**  
9:00 to 9:45 AM

**Graduate School Reality Check, Step I: Getting In (cosponsored by YCC)**  
10:00 to 11:15 AM

**Chem Demo Exchange**  
11:00 AM to 12:30 PM

## SOCIAL & EDUCATIONAL EVENTS

### **Graduate School Reality Check, Step II: You're In—Now What? (cosponsored by YCC)**

11:15 AM to 12:15 PM

### **Technical Symposium: Trends in Computational Chemistry (cosponsored by COMP)**

1:00 to 2:30 PM

### **Networking Social with Graduate School Recruiters**

1:00 to 5:00 PM

### **Workshop: Effective Chemistry Demos for Community Outreach**

2:45 to 4:00 PM

### **Workshop: Improving Scientific Communication Skills**

3:00 to 4:15 PM

### **Workshop: Networking 101 (cosponsored by PROF and YCC)**

4:15 to 5:45 PM

### **Student Chapter Awards Ceremony**

7:00 to 8:30 PM

### **Undergraduate Social**

8:30 to 11:00 PM

### **Monday, March 14**

### **Undergraduate Hospitality Center**

8:00 AM to 5:00 PM

### **Symposium: Realities of the Chemistry Industry: Career Opportunities & Paths (sponsored by I&EC)**

8:30 AM to 5:00 PM

### **Undergraduate Research Papers (Oral) (sponsored by CHED)**

8:30 AM to 5:00 PM

### **Technical Symposium: Advances in Chemical Imaging: Ultra-Resolution to Single Molecules (cosponsored by ANYL and PHYS)**

9:00 to 10:30 AM

### **Technical Symposium: Frontiers in Inorganic Chemistry (cosponsored by INOR)**

9:30 to 11:30 AM

### **Workshop: Chemists Celebrate Earth Day Outreach Ideas (sponsored by CCA)**

9:45 to 11:00 AM

### **Undergraduate Research Poster Session (sponsored by CHED)**

Noon to 2:00 PM

### **Eminent Scientist Lecture: "My Life with Lasers," with Richard Zare, Stanford University (cosponsored by ANYL and PHYS)**

2:30 to 3:30 PM

### **Student Speed Networking with Chemistry Professionals**

3:45 to 5:15 PM

### **Sci-Mix/Successful Student Chapter Posters**

8:00 to 10:00 PM

### **Tuesday, March 15**

### **Realities of the Chemical Industry: Career Paths and Opportunities (cosponsored by I&EC)**

8:30 AM to 5:00 PM

### **Chemistry & the Environment Film Series**

Noon to 2:00 PM

All events are sponsored or cosponsored by the Society Committee on Education's Undergraduate Programs Advisory Board. Chair: Michael R. Adams, Xavier University of Louisiana, New Orleans. Program Chair: Steven Emory, Western Washington University, Bellingham. For more information, go to [www.acs.org/undergrad](http://www.acs.org/undergrad) or contact the ACS Undergraduate Programs Office at (800) 227-5558 ext. 4480.

**GRADUATE & POSTDOCTORAL SCHOLARS OFFICE.** With support from the Graduate Education Advisory Board, this office provides and promotes programs and resources for graduate students and postdoctoral scholars. All events will take place at the San Diego Convention Center.

### **Sunday, March 13**

### **Faculty & Postdoc Afternoon Networking Coffee Break**

3:00 to 5:00 PM

### **Monday, March 14**

### **Student Speed Networking with Chemistry Professionals**

3:45 to 5:15 PM

### **Graduate & Postdoctoral Scholars Reception**

7:00 to 8:30 PM

### **Tuesday, March 15**

### **ChemIDP Workshop: A New Career Planning Tool**

10:00 AM to noon

For more information about this reception and other ACS programs offered to graduate students and postdocs, visit [www.acs.org/grad](http://www.acs.org/grad) or contact the ACS Graduate & Postdoctoral Scholars Office at [graded@acs.org](mailto:graded@acs.org).

### **HIGH SCHOOL TEACHERS PROGRAM.**

The Division of Chemical Education and the ACS Education Division are sponsoring the High School Teachers Program. It will include presentations and demonstrations on current pedagogies, resources, and activities that align with the meeting theme, "Computers in Chemistry." The High School/College Interface Luncheon will bring together educators from all grade levels with the goal of facilitating an exchange of ideas and networking among teachers.

High school teachers can register for the program directly through Attendee Registration; the special registration fee includes course materials, lunch, access to the full ACS meeting (Sunday through Thursday), and entry to the exposition (Sunday to Tuesday). Attendees can track professional development (based on clock hours) for sessions attended at the ACS national meeting. Upon completion and submission of ACS forms, participants will be mailed a certificate documenting their participation in the conference.

### **Sunday, March 13**

### **High School Teachers Program**

8:30 AM to 4:30 PM.

### **Monday, March 14**

### **Potpourri of Polymer Projects: Take a Byte Out of the NGSS, (cosponsored by POLY)**

4 to 8:30 PM

For more information, contact the Office of High School Chemistry at [education@acs.org](mailto:education@acs.org) or call (800) 227-5558 ext. 2105.



## EVENTS & ACTIVITIES

A variety of organizers will host special events during the meeting. Event participation is open to all interested registrants.

Some events require a ticket or registration to participate. The following events are coded to indicate what is required to participate: **(R)** registration, and payment when applicable, required; **SE-##** ticket required. **All nonticketed events require a visible registration badge for entry.**

Tickets are sold on a first-come, first-served basis. Ticket sales will close at 6 PM the evening prior to the event. Some event organizers may offer a limited number of tickets for sale at the door of the events. Cancellations or refund requests are not accepted after March 6.

*Locations and times are subject to change. To learn more about these events and to buy tickets or register, visit [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016).*

### Friday, March 11

#### **CHAS Workshop: Laboratory Waste Management**

7:30 AM to 4:00 PM, San Diego Convention Center, Room 31B

#### **CHAS Workshop: Laboratory Safety**

7:30 AM to 5 PM, San Diego Convention Center, Room 31A

### Saturday, March 12

#### **CHAS Workshop: How To Be a More Effective Chemical Hygiene Officer**

7:30 AM to 5:00 PM, San Diego Convention Center, Room 31C

#### **CHAS Workshop: Reactive Chemical Management for Laboratories & Pilot Plants**

7:30 AM to 5:00 PM, San Diego Convention Center, Room 31B

#### **CHAS Workshop: Meeting Chemical Safety Expectations in Instructional Laboratories**

7:30 AM to 5:00 PM, San Diego Convention Center, Room 31A

#### **CHAS Workshop: Cannabis Extraction & Analysis**

7:30 AM to 5:00 PM, San Diego Convention Center, Room 32A

#### **COACH Workshop: COACH Leadership & Advanced Negotiations**

8:30 AM to 5:00 PM, Hilton Gaslamp Quarter, Marina A

#### **Presidential Outreach Event: Exploring Our World Through Chemistry**

1:00 to 4:00 PM, San Diego Central Library, 330 Park Blvd., San Diego  
In collaboration with the San Diego Festival of Science & Engineering, this event will feature hands-on experiments to engage kids and the community in chemistry.

#### **COACH Reception**

5:00 to 7:00 PM, Hilton Gaslamp Quarter, Marina B

### Sunday, March 13

#### **Undergraduate Hospitality Center**

8:00 AM to 5:00 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

#### **Undergraduate Digital Café**

8:00 AM to 5:00 PM, Marriott Marquis San Diego Marina, Carlsbad

#### **Undergraduate Workshop: Making the Most of Your First National Meeting**

9:00 to 9:45 AM, Marriott Marquis San Diego Marina, San Diego Ballroom B

#### **Undergraduate Workshop: Graduate School Reality Check, Part I: Getting In**

10:00 to 11:15 AM, Marriott Marquis San Diego Marina, San Diego Ballroom A

#### **ACS Career Fair Workshops: Career Pathway Workshop**

10:00 AM to 5:00 PM, San Diego Convention Center, Room 24A

#### **Undergraduate Workshop: Chem Demo Exchange**

11:00 AM to 12:30 PM, San Diego Convention Center, Sails Pavillon

#### **Leading Without Authority**

11:00 AM to 5:00 PM, Embassy Suites San Diego Downtown Bay, Monterey I

#### **Undergraduate Workshop: Graduate School Reality Check, Part II: You're In— Now What?**

11:15 AM to 12:30 PM, Marriott Marquis San Diego Marina, San Diego Ballroom A

#### **SCHB & PROF Luncheon**

11:30 AM to 1:30 PM, Marriott Marquis San Diego Marina, Oceanside Room

#### **ACS Board Open Session & Luncheon**

(Open to staff and attendees)  
11:45 AM to 1:00 PM, San Diego Convention Center, Room 20D

#### **CHED High School/College Interface Luncheon/SE-01/\$45**

(Included at no charge with high school teacher registration)

Noon to 1:00 PM, Manchester Grand Hyatt San Diego, Harbor Ballroom A

#### **BIOT Lunch Seminars**

12:30 to 2:00 PM, Westin San Diego, Topaz Room

#### **CTA National Technician Award Luncheon/SE-02/\$45**

1:00 to 3:00 PM, Hilton San Diego Bayfront, Indigo 204A

#### **Undergraduate Workshop: Networking Social with Graduate School Recruiters**

1:00 to 5:00 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

#### **ACS Career Fair Workshops: Career Pathways I**

1:30 to 5:30 PM, San Diego Convention Center, Room 23A

#### **ACS Career Fair Workshops: Career Pathways II**

1:30 to 5:30 PM, San Diego Convention Center, Room 23B

#### **ACS Career Fair Workshops: Career Pathways III**

1:30 to 5:30 PM, San Diego Convention Center, Room 23C

#### **Undergraduate Workshop: Effective Chemistry Demos for Community Outreach**

2:45 to 4:00 PM, San Diego Convention Center, Sails Pavillon

#### **Graduate & Postdoctoral Scholars Workshop: Faculty & Postdoc Afternoon Networking Coffee Break**

3:00 to 5:00 PM, San Diego Convention Center, Sails Pavillon

#### **Ten Million Thanks (invitation only)**

A tribute to all who made possible the success of the ACS Scholars Program  
3:30 to 5:30 PM, Hilton San Diego Bayfront, Indigo Ballroom D

#### **International Networking Event**

4:00 to 5:30 PM, Hilton San Diego Bayfront, Aqua 300A/B

#### **Undergraduate Workshop: Networking 101 Workshop**

4:00 to 5:30 PM, Marriott Marquis San Diego Marina, San Diego Ballroom A

#### **Nominees Town Hall Meeting**

4:30 to 5:30 PM, Hilton San Diego Bayfront, Indigo Ballroom A

#### **ACS Diversity Reception**

5:00 to 7:00 PM, Hilton San Diego Bayfront, Aqua Salon D

## SOCIAL & EDUCATIONAL EVENTS

### University of Wisconsin, Madison, Alumni & Friends

5:00 to 7:00 PM, Hilton Gaslamp Quarter, Pacific Room

### Chemistry at Illinois Alumni & Friends Reception

5:00 to 8:00 PM, Westin San Diego, Topaz Room

### CHED Social Reception

5:30 to 7:00 PM, Manchester Grand Hyatt San Diego, Coronado Foyer

### International Welcome Reception/ SE-03/no charge

5:30 to 7:30 PM, Hilton San Diego Bayfront, Sapphire Ballroom A/B & E/F

### Joint Research Corporation/Petroleum Research Fund Reception

5:30 to 7:30 PM, Hilton San Diego Bayfront, Indigo Ballroom C/G

### COLL Social Hour/Poster Session/ Open Business Meeting

5:30 to 8:00 PM, San Diego Convention Center, Hall E

### District II Councilor Caucus

6:00 to 7:00 PM, Hilton San Diego Bayfront, Indigo 202B

### District IV Councilor Caucus

6:00 to 7:00 PM, Hilton San Diego Bayfront, Indigo 204A

### District V Councilor Caucus

6:00 to 7:00 PM, Hilton San Diego Bayfront, Indigo 204B

### District VI Councilor Caucus

6:00 to 7:00 PM, Hilton San Diego Bayfront, Indigo 206

### Mid-Atlantic Councilor Caucus

6:00 to 7:00 PM, Hilton San Diego Bayfront, Indigo 202A

### CELL & FLUO Poster Sessions

6:00 to 8:00 PM, San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)

### INOR Poster Sessions

6:00 to 8:00 PM, San Diego Convention Center, Hall D

### Expo Attendee Welcome Reception

6 to 8:30 PM, San Diego Convention Center, Halls B-C

### CINF Welcoming Reception & Poster Session

6:30 to 8:30 PM, San Diego Convention Center, Room 3

### ACS Student Chapter Awards Ceremony

7:00 to 8:30 PM, San Diego Convention Center, Ballroom 20 A/C

### ANYL Poster Session

7:00 to 9:00 PM, San Diego Convention Center, Sails Pavilion

### CHED Poster Session

7:00 to 9:00 PM, San Diego Convention Center, Hall D

### MEDI & BIOL Poster Session

7:00 to 9:00 PM, San Diego Convention Center, Hall F

### ORGN Poster Session

8:00 to 10:00 PM, San Diego Convention Center, Hall D

### Presidential Poster Session

8:00 to 10:00 PM, San Diego Convention Center, Hall D

### Undergraduate Research Social

8:30 to 11:00 PM, San Diego Convention Center, Ballroom 20D

## Monday, March 14

### YCC 5K Fun Run/SE-04/\$25 (regular)/SE-04A/\$15 (student)

6:45 to 8:30 AM, San Diego Convention Center, Lobby D

### WCC Women in the Chemical Enterprise Breakfast/SE-05/\$40 (regular)/SE-05A/\$20 (student)

7:30 to 9:00 AM, Hilton San Diego Bayfront, Indigo Ballroom C/G  
(A limited number of student tickets are available. Students may purchase regular tickets if student tickets are sold out.)

### Engaging Colleagues in Dialogue

8:00 AM to noon, Embassy Suites San Diego Downtown Bay, Monterey I

### Undergraduate Hospitality Center

8:00 AM to 5:00 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

### Undergraduate Digital Café

8:00 AM to 5:00 PM, Marriott Marquis San Diego Marina, Carlsbad Room

### ACS Career Fair Workshop: Career Pathways I

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23A

### ACS Career Fair Workshop: Career Pathways II

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23B

### ACS Career Fair Workshop: Career Pathways III

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23C

### ACS Exposition

9:00 AM to 5 PM, San Diego Convention Center, Halls B/C

### Undergraduate Workshop: Chemists Celebrate Earth Day (cosponsored by Committee on Community Activities)

9:45 to 11:00 AM, San Diego Convention Center, Room 30C/D

### Chem Ambassadors Game & Cafe

10:30 to 11:30 AM, Marriott Marquis San Diego Marina, Carlsbad Room XX

### Diversity Women Chemist of Color Networking Event/SE-06/no charge

10:30 AM to Noon, Hilton San Diego Bayfront, Aqua Salon A/B

### Committee on Minority Affairs Luncheon/SE-07/\$50 (regular)/SE-07A/\$25 (student)

11:30 AM to 1:30 PM, Hilton San Diego Bayfront, Sapphire Ballroom A/B

### SCHB & PROF Luncheon

11:30 AM to 1:30 PM, Marriott Marquis San Diego Marina, Vista Room

### CHAL Drug & Power Luncheon/SE-08/\$40

Noon to 1:30 PM, San Diego Convention Center, Room 20D

### Undergraduate Poster Session

12:00 to 2:00 PM, San Diego Convention Center, Hall D/E

### Purdue University Chemistry Luncheon/SE-09/\$10

12:00 to 2:00 PM, Manchester Grand Hyatt San Diego, Coronado E

### BIOT Lunch Seminars

12:30 to 2:00 PM, Westin San Diego, Topaz Room

### Fostering Innovation

1:00 to 5:00 PM, Embassy Suites San Diego Downtown Bay, Monterey I

### ENFL Poster Session

2:00 to 4:00 PM, San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)

### Undergraduate Workshop: Speed Networking with Chemistry Professionals

3:45 to 5:15 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

### The Kavli Foundation Emerging Leader in Chemistry Lecture

4:00 to 5:10 PM, San Diego Convention Center, Ballroom 20 A/C

### Just Cocktails, WCC Open Meeting

4:00 to 5:30 PM, Hilton San Diego Bayfront, Aqua Salon D

## SOCIAL & EDUCATIONAL EVENTS

### **The Fred Kavli Innovations in Chemistry Lecture**

5:15 to 6:30 PM, San Diego Convention Center, Ballroom 20 A/C

### **CHAL Reception**

6:00 to 8:00 PM, San Diego Convention Center, Room 22

### **Chinese American Chemical Society Dinner Banquet/SE-10/\$35**

6:00 to 9:00 PM, Panda Inn Mandarin Cuisine, 506 Horton Plaza

### **University of Pennsylvania Alumni Reception**

6:30 to 8:30 PM, Cafe Sevilla, 335 5th Ave.

### **CARB Award Dinner/SE-11/\$60**

6:30 to 9:30 PM, Rockin' Baja Lobster—Gaslamp, 310 5th Ave.

### **ACS Graduate & Postdoctoral Scholars Reception**

7:00 to 8:30 PM, San Diego Convention Center, Room 20D

### **Sci-Mix Interdivisional Poster Session & Mixer**

(Drink ticket included with registration)

8:00 to 10:00 PM, San Diego Convention Center, Hall D/E

### **Tuesday, March 15**

### **Senior Chemists Committee Breakfast/SE-12/\$20**

7:30 to 9:30 AM, Hilton San Diego Bayfront, Indigo Ballroom D/H

### **University of Minnesota Alumni & Friends Breakfast/SE-13/\$5.00**

7:30 to 9:30 AM, San Diego Convention Center, Room 20D

### **Coaching & Feedback**

8:00 AM to noon, Embassy Suites San Diego Downtown Bay, Monterey I

### **ACS Career Fair Workshop: Career Pathways I**

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23A

### **ACS Career Fair Workshop: Career Pathways II**

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23B

### **ACS Career Fair Workshop: Career Pathways III**

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23C

### **ACS Exposition**

9:00 AM to 5:00 PM, San Diego Convention Center, Halls B–C

### **Eli Lilly Travel Award Poster Session**

11:00 AM to noon, Hilton San Diego Bayfront, Indigo Ballroom D/H

### **Alpha Chi Sigma Fraternity Luncheon**

11:30 AM to 1:30 PM, San Diego Pier Café, 889 West Harbor Dr.

### **SCHB & PROF Luncheon**

11:30 AM to 1:30 PM, Marriott Marquis San Diego Marina, Vista Room

### **CINF Luncheon/SE-14/\$20 (regular member)/SE-14A/\$25 (nonmember)/SE-14B/\$15 (student)**

Noon to 1:30 PM, San Diego Convention Center, Room 20D

### **COLL Luncheon/SE-18/\$45**

Noon to 1:30 PM, San Diego Convention Center, Room 20B/C

### **WCC Luncheon/SE-15/\$50 (regular)/SE-15A/\$25 (student)**

Noon to 1:30 PM, Hilton San Diego Bayfront, Indigo Ballroom D/H

### **Committee on Environmental Improvement (CEI) Film Series**

Noon to 2:00 PM, San Diego Convention Center, Room 8

### **BIOT Lunch Seminars**

12:30 to 2:00 PM, Westin San Diego, Topaz Room

### **Strategic Planning**

1:00 to 5:00 PM, Embassy Suites San Diego Downtown Bay, Monterey I

### **AGFD C<sup>4</sup> Communicating Chemistry: Caribbean Cuisine/SE-21/\$10**

2:30 to 4:30 PM, San Diego Wine & Culinary Event Center, 200 Harbor Dr.

### **AGFD Poster Session**

3:00 to 5:00 PM, San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)

### **Local Section Officers, Outreach Coordinator & Speakers Reception**

3:30 to 5:30 PM, Hilton San Diego Bayfront, Indigo 204A/B

### **Division Councilors & Division Officers Caucus & Reception**

4:00 to 6:30 PM, San Diego Convention Center, Room 24A

### **I&EC Poster Session**

5:00 to 7:00 PM, San Diego Convention Center, Hall D

### **UCLA Research Showcase**

5:00 to 7:00 PM, San Diego Convention Center, Room 20A

### **District I Councilor Caucus**

5:30 to 7:00 PM, Hilton San Diego Bayfront, Indigo 202A

### **Geochemistry Division Reception**

5:30 to 7:30 PM, Omni San Diego Hotel, Grand Ballroom E

### **ENFL Energy & Fuel Dinner/SE-16/\$60**

6:00 to 9:00 PM, The Prado at Balboa Park, 1549 El Prado

### **PMSE/POLY Joint Poster Session**

6:00 to 8:00 PM, San Diego Convention Center, Hall F

### **INOR Poster Session**

6:00 to 8:00 PM, San Diego Convention Center, Hall D

### **COMP Poster & Awards Session**

6:00 to 8:00 PM, San Diego Convention Center, Hall E

### **BIOT Poster Session**

6:00 to 9:00 PM, San Diego Convention Center, Hall E

### **ENVR Division Reception/SE-19/\$20**

6:30 to 8:00 PM, Meze Greek Fusion Restaurant, 345 5th Ave.

### **ACS National Awards Reception, Banquet Ceremony & General Meeting of the Society/SE-17/\$130**

6:30 to 10:00 PM, Manchester Grand Hyatt San Diego, Harbor Ballroom D-I

### **CELL Awards Banquet/SE-20/\$65**

6:30 to 10:00 PM, Fogo de Chao, 668 6th Ave.

### **BIOL Poster Sessions**

7:00 to 9:00 PM, San Diego Convention Center, Hall E

### **CARB Poster Session**

7:00 to 9:00 PM, San Diego Convention Center, Hall D

### **CATL & ORGN Poster Session**

8:00 to 10:00 PM, San Diego Convention Center, Hall D

### **Wednesday, March 16**

### **ACS Career Fair Workshop: Career Pathways I**

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23A

### **ACS Career Fair Workshop: Career Pathways II**

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23B

### **ACS Career Fair Workshop: Career Pathways III**

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23C

### **POLY/PMSE Awards Reception**

5:30 to 8:30 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

# 251st American Chemical Society National Meeting & Exposition



Computers in Chemistry Thematic Program organized by Dr. Kenneth M. Merz, Jr., Director, Institute for Cyber Enabled Research (iCER), Joseph Zichis Chair in Chemistry, Department of Chemistry and the Department of Biochemistry and Molecular Biology, Michigan State University, and the Editor-in-Chief of the *Journal of Chemical Information and Modeling*.

## Computers in Chemistry

Sunday, March 13, 2016, 3:00 – 6:00 PM  
San Diego Convention Center • Ballroom 20 A – C



### Dr. George C. Schatz

Charles E. and Emma H. Morrison Professor of Chemistry,  
Professor of Chemical and Biological Engineering  
Department of Chemistry, Northwestern University,  
Editor-in-Chief, *Journal of Physical Chemistry*

*Using Self-Assembly to make Functional Materials: Computational Perspectives*



### Dr. Sharon Hammes-Schiffer

Swanlund Chair, Professor of Chemistry  
Department of Chemistry, University of Illinois at Urbana-Champaign

*Proton-coupled electron transfer in catalysis and energy conversion*



### Dr. David Baker

Head of the Institute for Protein Design, Professor of Biochemistry  
Department of Biochemistry, University of Washington

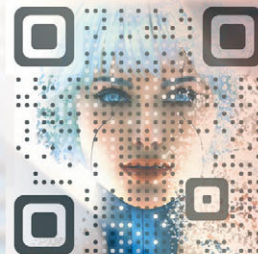
*Post-Evolutionary Biology: Design of novel protein structures, functions and assemblies*



### Dr. William L. Jorgensen

Sterling Professor of Chemistry  
Department of Chemistry, Yale University

*30 Years of Free Energy Perturbation Theory: From Free Energies of Hydration to Drug Discovery*



**ENVR & PHYS Poster Sessions**

6:00 to 8:00 PM, San Diego Convention Center, Hall D

**GEOC Poster Session**

8:00 to 10:00 PM, San Diego Convention Center, Hall D

**Joint MEDI & ORGN Poster Session**

7:00 to 10:00 PM, San Diego Convention Center, Hall F

**WORKSHOPS**

**THE ACS DIVISION OF CHEMICAL HEALTH & SAFETY (CHAS) WORKSHOPS**

are scheduled for the Friday and/or Saturday prior to a national meeting. Workshops begin at 8:30 AM and finish around 4:00 PM, with a 1 hour (no host) lunch break. Coffee is available starting at 8:00 AM.

Register online at [dchas.org](http://dchas.org).

**Laboratory Waste Management.** Friday, March 11, 7:30 AM to 5:00 PM. San Diego Convention Center, 31B. CHAS offers this workshop to assist participants with the various regulatory requirements that apply to laboratories that generate hazardous waste, as well as provide insight into the options for on-site management and off site disposal. Focus will include recycling and reclamation techniques, economical handling of waste, and liability issues.

**Laboratory Safety.** Friday, March 11, 7:30 AM to 5:00 PM. San Diego Convention Center, 31A. The Laboratory Safety Institute and CHAS present an intensive one-day introduction to effective lab safety programs and the fundamentals of lab safety. Through a combination of discussion, video, activities, and instructor presentations, the participants learn ways to identify hazards and convince others that lab safety is important. They learn about the critical components in a lab safety program and techniques for program evaluation.

**How To Be A More Effective Chemical Hygiene Officer (CHO).** Saturday, March 12, 7:30 AM to 5:00 PM. San Diego Convention Center, 31C. CHAS offers this workshop to provide participants with a detailed analysis of the CHO position and to prepare for the CHO certification exam to be held the next day. Participants receive a clear perspective on safety issues in the lab-

oratory, focusing on what a CHO does and how to do it better. The workshop covers all of the content areas of the certification exam, including a sample test in the same format as the real one. Whether you are a new CHO or an experienced one, you will find something to put to real use in this fast-paced presentation.

**Reactive Chemical Management for Laboratories & Pilot Plants.**

Saturday, March 12, 7:30 AM to 5:00 PM. San Diego Convention Center, 31B. Chemical reactivity hazards contribute to a significant number of incidents in laboratories and pilot plants. This workshop will provide participants with the knowledge and skill to screen processes for potential hazards, recognize when reactive hazards are present, and implement appropriate controls to reduce the risk of an incident. Workshop attendees will review case studies of actual incidents and work examples to understand the screening and recognition process. Group discussions of control methods will allow participants to share their experiences and to evaluate methods for controlling reactivity risks.

**Cannabis Extraction & Analysis.** Saturday, March 12, 7:30 AM to 5:00 PM. San Diego Convention Center, 32A. CHAS and CANN (Cannabis Chemistry Subdivision) present a comprehensive review of current methodologies and best practices in the analysis of cannabis products and extraction/processing of cannabis. Participants will learn the latest developments in extraction technologies, how to comply with testing standards, and how to operate safely.

**Meeting New Chemical Safety Expectations in Instructional Laboratories.** Saturday, March 12, 8:30 AM to 4:00 PM. San Diego Convention Center, 31A. The 21st-century chemistry laboratory curriculum includes discovery-based, research-style lab work in addition to traditional "cookbook" procedures. To ensure a safe working environment in this emerging pedagogy, laboratory safety practices must evolve away from a strict focus on safety rules toward risk-assessment and risk-management practices. This transition is outlined in ACS's guidelines for bachelor's degree programs and in the new National Fire Protection Association

(NFPA) 45-2015 safety standards. This workshop will flesh out these ideas in the cultural context of lab safety and then review and provide practice with Job Hazard Analysis and Control Banding tools, as described in ACS's Identifying & Evaluating Hazards in Research Laboratories document. Finally, we will address how these tools can be used to address the new NFPA requirements for a documented hazard/risk assessment and a safety briefing to students in instructional laboratories.

**COAch: Leadership & Advanced Negotiations Skills.** Saturday, March 12, 8:30 AM to 5:00 PM. Hilton San Diego Gaslamp Quarter, Marina A. This academic leadership seminar is designed for university faculty or other academic administrators who are anticipating, considering, or fulfilling academic leadership roles. The advanced negotiations section builds on the basics of negotiations and adds a leadership assessment, as well as advanced skills in negotiating difficult conversations. Participants will also learn how to differentiate types of leadership approaches to change, identify the stages of resistance to change, and learn how to use their network in leading change. The group will be given a model for how to form a high-performance task force to deal with challenging issues, as well as processes for giving feedback. Participants will practice a number of skills to strengthen understanding of the techniques above. As a final exercise, volunteer participants will practice a case study.

**Standard Methods, Materials & Databases for Surface Complexation Measurements.** Wednesday, March 16, 5:30 PM to 7:00 PM, Omni San Diego Hotel, Grand Ballroom D. When combined with chemical equilibrium modeling, the measurement of complexation reactions between material surfaces and target chemical species can result in the calculation of discrete reactive surface site concentrations and intrinsic thermodynamic equilibrium constants. These parameters are critical when modeling and predicting chemical processes associated with industrial separations, water treatment and remediation, and the reactive transport of contaminants in natural geochemical systems. This workshop, sponsored in part by the National Institute of Stan-

dards & Technology, will explore the need for standardized experimental and modeling methods and standard reference materials for surface complexation measurements, as well as their capacity to promote the development and availability of internally consistent datasets.



## ACS CAREER NAVIGATOR

**ACS CAREER NAVIGATOR** is your home for career services, leadership development, in-person and online professional education, and market intelligence resources. We offer comprehensive and easily identified tools that allow you to achieve your career goals by landing a new job, finding a new career path, or comparing your salary and viewing current trends in the field to make better-informed decisions.

Opportunities abound at the ACS national meeting in San Diego to take advantage of the many resources and tools the ACS Career Navigator offers to help you succeed in the global scientific enterprise. Are you ready to get started? Refresh skills and branch into new areas of emerging science and advanced applications with a short course or with an ACS Leadership Development System course that gives you skills that can be immediately applied in school or on the job. If you are an ACS member, stop by the ACS Career Fair in the convention center and speak to a personal career consultant. In short, whatever your career goals, the ACS Career Navigator is here to help you achieve and exceed them. We'll see you in San Diego.

### ACS CAREER FAIR

**JOB SEEKERS**, are you looking to jump-start your job search or enhance your professional development?

**EMPLOYERS**, are you looking to hire scientists and engineers? Then you need to attend the ACS Career Fair, open Sunday, March 13, 9 AM to 5 PM; Monday, March 14, 9 AM to 5 PM; Tuesday, March 15, 9 AM to 5 PM; and Wednesday, March 16, 8:30 AM to 12:30 PM (workshops only) in the San Diego Convention Center. The career fair is the place where the best talent and the best employers in chemistry meet.

**LET ACS HELP YOU REACH YOUR CAREER GOALS.** ACS will help you prepare for your next career move by providing resources that make it possible to map out your personal job search strategy, strengthen your résumé, and build your interview skills, all with the support of career consultants. During the career fair, participants can take full advantage of the following:

- Networking opportunities
- Résumé reviews
- One-on-one career consulting
- Interview practice and skills building
- More than 20 career-related workshops

Job seekers must be ACS members, be registered for the national meeting, and complete career fair registration at [careerfair.acs.org](http://careerfair.acs.org) (pick up a career fair registration badge beginning Sunday, March 13).

**Please note:** We cannot guarantee that you will secure interviews at the ACS Career Fair. Interviewing is strictly contingent on the availability of positions and the credentials and qualifications that employers are seeking.

**ONE-ON-ONE CAREER CONSULTING.** Individual 30-minute appointments with career consultants are available both on-site and online. These consults can help you strengthen your résumé, improve your interviewing skills, and design a job search or comprehensive professional growth strategy. Please bring a copy of your résumé or CV to all appointments. All one-on-one on-site career consulting sessions will take place in the Résumé Review/Mock Interview area. Sign-up begins at 9 AM on Sunday, March 13, on a first-come, first-served basis.

**CAREER AND PROFESSIONAL DEVELOPMENT WORKSHOPS.** More than 20 career-related workshops will help you with everything from your résumé to optimizing job performance to how to ace an interview. Workshop times are subject to change. Please consult the online workshop schedule at [careerfair.acs.org](http://careerfair.acs.org) for location.

#### Sunday, March 13

- Finding Your Path**, 1:30 to 5:30 PM
- Acing the Interview**, 1:30 to 5:30 PM
- Working in Industry**, 1:30 to 5:30 PM
- New Technology to Find Jobs & Manage Your Career**, 10:00 to 11:30 AM
- Soup to Nuts of Entrepreneurship**, Noon to 1:30 PM
- Foreign National Scientist Obtaining a Job in the U.S.**, 1:30 to 3 PM
- Writing Excellent Proposals**, 3:30 to 5:00 PM

#### Monday, March 14

- Working for Yourself**, 8:30 AM to 12:30 PM
- Working in Higher Education**, 8:30 AM to 12:30 PM
- Working in Government**, 8:30 AM to 12:30 PM
- Acing the Interview**, 1:30 to 5:30 PM
- Working in Industry**, 1:30 to 5:30 PM
- Finding Your Path**, 1:30 to 5:30 PM

#### Tuesday, March 15

- Finding Your Path**, 8:30 AM to 12:30 PM
- Acing the Interview**, 8:30 AM to 12:30 PM
- Working in Industry**, 8:30 AM to 12:30 PM
- Working in Government**, 1:30 to 5:30 PM
- Working in Higher Education**, 1:30 to 5:30 PM

#### Wednesday, March 16

- Finding Your Path**, 8:30 AM to 12:30 PM
- Acing the Interview**, 8:30 AM to 12:30 PM
- Working in Industry**, 8:30 AM to 12:30 PM

**EMPLOYERS, ACS HAS THE TALENT YOU ARE LOOKING FOR.**

Leading employers around the world trust and depend on ACS to provide them with the talent they need to innovate and excel. At our last event, approximately 1,000 global job seekers— from recent grads to seasoned professionals— met with on-site recruiters seeking to fill positions in all facets of chemistry, pharmaceuticals, and biotechnology.

The ACS Careers Jobs Database can help manage your employer account, post jobs, search for qualified candidates, and schedule career fair interviews. Moreover, participating in the ACS Career Fair enables you to accomplish the following:

- Connect with top talent via on-site interviews.
- Screen candidates and make appointments in advance.
- Find the personnel your company needs to thrive, from entry- to executive-level positions.
- Meet qualified candidates informally via on-site networking forums.
- Extend your presence for 30 days after the career fair via the ACS jobs database.

**ACS CAREER FAIR AND THE ACS EXPOSITION TEAM HAVE JOINED FORCES.**

Employers can purchase booth space inside the exposition hall, enabling your company to maximize its ability to showcase products and services and connect with job seekers. Employers can sign up for the ACS Career Fair Recruiters Row package by contacting Kimberly Mallory at (202) 452-8918 (U.S./Canada only) or e-mail [k\\_mallory@acs.org](mailto:k_mallory@acs.org).

Employers will receive an e-mail confirmation and must visit the ACS Career Fair Information Booth in the Convention Center to pick up their blue badge. For more information, please visit [careerfair.acs.org](http://careerfair.acs.org) or contact Kimberly Mallory (see above).

**ACS SHORT COURSES**

**REFRESH YOUR SKILLS** or branch into new areas with an ACS Short Course. Held in conjunction with ACS national meeting in San Diego, courses taught by our expert instructors give you the opportunity to stay on top of new technology, growing trends in the industry, and the skills you need to advance your

career. ACS member, advanced registration, and group discount rates are available. A course fee and registration separate from the national meeting are required. For more information on ACS Short Courses in San Diego or to register, visit [proed.acs.org/sandiego](http://proed.acs.org/sandiego). If you have questions, call (202) 872-4508, fax (202) 872-6336, or e-mail [proed@acs.org](mailto:proed@acs.org).

**ANALYTICAL**

**1-D & 2-D NMR Spectroscopy: Structure Determination of Small Molecule Organic Compounds**, March 11–12

**Practical Applications of Mass Spectrometry for Small Molecules**, March 11–12

**BIOLOGICAL/MEDICINAL**

**Applications of Pharmacokinetic & Safety Pharmacology for Chemists in Drug Development**, March 11–12

**Druglike Properties: Optimizing Pharmacokinetics & Safety in Drug Development**, March 11–12

**Essentials of Medicinal Chemistry & Pharmacology**, March 11–12

**Structure Based Drug Design**, March 11–12

**COMPUTERS/STATISTICS/ENGINEERING**

**Experimental Design for Productivity & Quality in Research & Development**, March 11–13

**ORGANIC/PHYSICAL**

**1-D & 2-D NMR Spectroscopy: Structure Determination of Small Molecule Organic Compounds**, March 11–12

**Dispersions in Liquids: Suspensions, Emulsions & Foams**, March 11–12

**Mastering the Art of Writing Reasonable Organic Reaction Mechanisms**, March 11–12

**Organic Synthesis: Methods & Strategies for the 21st Century Chemist**, March 11–12

**POLYMERS**

**Polymeric Coatings**, March 11–12

**Polymer Science & Technology**, March 12–13

**PROFESSIONAL DEVELOPMENT**

**Effective Supervision of Scientists & Technical Staff**, March 11–12

**Effective Technical Writing**, March 11–12

**Project Management for Technical Professionals**, March 11–12

**REGULATORY/ENVIRONMENTAL**

**Write Your Own Patent Applications**, half-day course, March 13

**Intellectual Property Strategies for Technical Professions**, half-day course, March 13

**2016 LEADERSHIP DEVELOPMENT SYSTEM COURSE OFFERINGS**

**WHETHER YOU ARE A** manager, experienced professional, or new to the workforce, we invite you to attend an ACS Leadership Development System course held at the ACS national meeting. The following four-hour facilitated courses require a fee of \$150 each for ACS members and \$300 each for nonmembers. Register for these courses when you register for the meeting. For more information and full course descriptions, visit [www.acs.org/leadershipdevelopment](http://www.acs.org/leadershipdevelopment).

**Leading Without Authority.** Sunday, March 13, 1:00 to 5:00 PM. We've all been in situations where we are leading projects or teams and need to direct everyone's effort but don't have complete control of the project's resources, including the people. Learn practical tools to help you gain cooperation without formal authority and motivate your colleagues or volunteers.

**Engaging Colleagues in Dialogue.** Monday, March 14, 8:00 AM to noon. Communication underlies everything we do and has a direct correlation to the success of a project. It is one of the most important skills we need to be successful in school, on the job, and in volunteer situations. This hands-on, interactive course helps develop your one-to-one communication skills. You will learn how to improve both sides of the communication exchange: first, working to understand how to better communicate your messages and second, working on listening and acknowledging others' messages. You will have an opportunity to assess your own communication skills through conversations with colleagues.

**Fostering Innovation.** Monday, March 14, 1:00 to 5:00 PM. Keeping pace in an environment of constant change requires continuous innovation. Whether you are in a nonprofit, business, or academic environment, the ability to contribute to the creation of new ideas, new processes, and new approaches is a key to personal and organizational success. But coming up with new ideas is challenging, and few of us have the tools and skills. This course teaches a proven, systematic process to generate ideas. You will gain understanding and tools to help you tap into your own innovation style and learn how to stimulate innovative thinking among team members and colleagues.

**Coaching & Feedback.** Tuesday, March 15, 8:00 AM to noon. Most managers will tell you that coaching is important, and yet they avoid actually coaching anyone. Some who try find it harder than expected. The reason? Most managers lack the skills and confidence to be effective in the coaching role. But good coaching is central to your success as a leader and to the success of your team members, employees, and volunteers on ACS committees. Coaching will help you increase performance, expand your team's capabilities, and improve relationships and morale. This course provides leaders with a proven process, practical tools, and a hands-on opportunity to coach volunteers and employees more effectively.

**Strategic Planning.** Tuesday, March 15, 1:00 to 5:00 PM. Among the responsibilities of a leader, none is more critical than setting goals and direction. Whether you are leading at the level of a local section, division, or national committee, your members look to you to establish the strategic plan that will guide the group's activities. This course will help you improve your understanding of the planning process while giving you the opportunity to start developing a strategic plan.

## EXHIBITOR SPONSORED WORKSHOPS

**EXHIBITING COMPANIES** will host free education sessions for attendees to introduce new products and services, build skills with specific tools and techniques, and highlight applica-

tions for existing instrumentation. Visit [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016) to register for workshops.

### Sunday, March 13

**Flow Chemistry Seminar.** Sponsor: ThalesNano Nanotechnology, 3:30 to 6:00 PM, SDCC, Room 12. Join our seminar for a glimpse into the latest advances in continuous-flow reactor technology, and see how it can benefit your chemistry. Information is also available at the ThalesNano booth, #1121.

### Monday, March 14

**Innovative Technologies To Improve Your Students' Learning Experience.** Sponsor: McGraw-Hill Education, 9:30 AM to noon, SDCC, Room 15B.

9:30 to 10:30 AM— **Adaptive Learning To Help Prepare & Engage Your Students for Success.** Adaptive technology is at the forefront of the evolution of digital teaching, allowing instructors to teach and students to learn in ways never before possible. But what does this really mean? And how can you make it work for you and your students? Get answers to these questions from instructors who have years of experience using adaptive technology, including SmartBook and LearnSmart Prep.

11:00 AM to noon— **Revolutionizing the Lab Experience: Introducing LearnSmart Labs for General Chemistry.** LearnSmart Labs provides an adaptive, interactive, personalized lab experience that encourages students to theorize and experiment like scientists do. In the realistic LearnSmart Labs environment, students can practice the scientific method, safely develop and test hypotheses, and think critically about their findings before ever setting foot in a physical lab.

**Waters Technical Workshops.** Sponsor: Waters, 9:30 AM to noon, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2. Join Waters for two educational workshops designed to help improve laboratory effectiveness in your organization.

9:30 to 10:30 AM— **Transforming Sample Preparation.** Waters has developed a new, water-wettable, reversed-phase sorbent and an easy-to-use, streamlined approach that produces high recoveries, improved sample flow capabilities, and reduced matrix effects.

Don't miss this discussion on a new, novel sorbent for small-molecule sample preparation that is easier to use and produces cleaner samples in less time with fewer steps.

10:30 to 11:30 AM— **Empowering Solutions.** We will explore the new features of Empower 3 FR3 in this session. Topics covered will include mass spectrometric peak tracking, new peak labeling options, new component summary reporting options, location fields, new custom field capabilities, Waters's data manager, and qualification and performance enhancements.

**CAS Solutions.** Sponsor: CAS, 9:30 AM to 3 PM, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 1. Visit CAS in the Exhibitor Workshop to learn more about our products and solutions.

**ACS on Campus.** Sponsor: ACS Store, 12:30 to 3 PM, SDCC, Room 15B. Learn from ACS editors and experts in the field about how to maximize your research, get published, and build the skills you need to gain that competitive edge for your career. The event is free, including complimentary food, drinks, and giveaways. The event is open to undergraduates, graduate students, researchers, faculty, and librarians.

**Solutions for Innovation: From Composition to Structure.** Sponsor: JEOL USA, 12:30 to 3:00 PM, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2. In your element: SEM/EDS. Find your formula: ambient ionization mass spectrometry. Verify your structure: NMR. Learn how the latest innovations from JEOL integrate to enhance your science.

**Seamless Integration of 2-D & 3-D SAR To Guide MultiParameter Optimization.** Sponsor: Optibrium, 3:30 to 6:00 PM, SDCC, Room 15B. In this hands-on workshop, we will explore how the combination of two-dimensional structure-activity relationships (SARs) with 3-D structure-based design can be used to guide the optimization of high-quality compounds. Practical examples will illustrate how analyses such as activity-cliff detection and matched molecular pair analysis in StarDrop's Card View system can be linked with a 3-D view of a compound binding to a therapeutic target. We will also use the SeeSAR software platform to demonstrate how 2-D quantitative structure-activity relationship (QSAR) models of



key absorption, distribution, metabolism, and excretion (ADME) properties can monitor potential risks, and we will consider strategies to improve binding affinity using SeeSAR's visual HYDE scoring approach.

### Tuesday, March 15

#### Innovative Technologies To Improve Your Students' Learning Experience.

*Sponsor:* McGraw-Hill Education, SDCC, Room 15B.

9:30 to 10:30 AM — **The Rewards of Technology in Organic Chemistry.** With digital tools designed to streamline tasks and improve student outcomes, educators are free to focus on what matters most: teaching. Help your students come to class more prepared and engaged, increase course retention, study smarter, and get better grades.

#### 11:00 AM to noon — Moving Beyond Traditional Homework with ALEKS.

Jack Eichler from the University of California, Riverside, will present his research findings from his *Journal of Chemical Education* article "Online Homework Put to the Test" (2013, DOI: 10.1021/ed3006264). In his study, Eichler compared two separate online learning systems, ALEKS (responsive-adaptive) and MasteringChemistry (responsive), and measured the impact of each online learning system on student final exam scores for a general chemistry course. Eichler will share his results and as well as his experiences using online homework.

#### Introduction to Protein & Peptide HPLC (Part I) and State-of-the-Art Protein & Peptide Reversed-Phase Separations by UHPLC (Part II).

*Sponsor:* MilliporeSigma (Sigma-Aldrich), 9:30 AM to noon, SDCC, Room 12. Join MilliporeSigma for a two-part workshop focusing on bioanalytical HPLC separations. Learn about the latest technologies, enjoy complimentary refreshments, and be entered to win a free HPLC column for your evaluation.

**CAS Solutions.** *Sponsor:* CAS, 9:30 AM to 3 PM, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 1. See page 46.

**Spinsolve Benchtop NMR for Industry & Academia.** *Sponsor:* Magritek, 10:00 AM to noon, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2. Magritek presents the latest develop-

ments with the Spinsolve benchtop NMR spectrometer. Join us to learn about the extended and improved capabilities of this high-performance NMR instrument, including applications in a range of practical problems of interest for industry and academia.

#### WebAssign 101: Getting Started with WebAssign.

*Sponsor:* WebAssign, 3:30 to 6:00 PM, SDCC, Room 12. This workshop is ideal for new WebAssign users or active users who want to learn more about how to use WebAssign's features to save time, better engage your students, and assess student performance. Join WebAssign's Brad Spiker for a lively and informative introduction to WebAssign. You'll learn how to create a course, build an assignment, and schedule assignments, and you'll get some of Brad's favorite tips for enriching your chemistry classroom experience. You won't want to miss this workshop for a painless way to jump-start your success with WebAssign.

#### Reverse Engineering of Materials & Polymers Using Infrared & Raman Spectroscopy.

*Sponsor:* Bruker, 12:30 to 3:00 PM, SDCC, Room 15B. Product development in the industrial world can be a long and expensive process. In a competitive market, the window of opportunity for significant revenue can close before a new product even exits the development cycle. The obvious solution to keeping up in a competitive market is to acquire the product in question, disassemble it, and analyze it. This reverse engineering process can greatly expedite the immediate introduction of competitive products into the marketplace. The chemical properties can be readily determined by utilizing analytical tools such as gas-phase chromatography and atomic absorption spectroscopy. Molecular spectroscopy (infrared and Raman) is among the most powerful tools in the reverse-engineering process. Each molecule has a unique infrared and Raman signature that provides great specificity in the identification process.

#### New in the Field of Chromatography from Thermo Fisher Scientific

*Sponsor:* Thermo Fisher Scientific, 12:30 to 3:00 PM, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2. **Part I: A New & Exciting Line of High-Pressure Ion Chromatography (HPIC) Instruments.** Ion chromatography is a well established

and accepted analytical technique used for a wide diversity of sample matrices such as foods and beverages, industrial chemicals, and ultra-high-purity water. Learn faster and more cost-effective methods that use a new line of high-pressure-capable IC systems. Examples will include the determination of common ionic pollutants found in environmental samples — organic acids, anions, cations, and carbohydrates in food and beverage matrices — as well as ionic compound determinations in pharmaceutical and biotechnology samples. **Part II: Advances in UHPLC Instrumentation.** Learn how the Vanquish UHPLC system's novel detectors, method transfer tools, and dedicated columns help you solve your toughest scientific challenges.

#### Characterizing Structure & Chemistry of Functional Nanomaterials by Advanced Electron Microscopy.

*Sponsor:* FEI, 12:30 to 3:00 PM, SDCC, Room 12. The development of technologies for efficient resource usage, energy conversion, transportation, environmental protection, and other applications relies heavily on the development of new and improved nanostructures and nanomaterials. Characterization of these materials down to the subnanometer scale — while focusing on structural evolution with a link to the nanomaterial's performance — plays a crucial role in obtaining detailed knowledge about the relationship among structure, unique properties, and function in these systems. FEI's solutions can help you to visualize and analyze structure and morphology as well as the chemical composition of those materials under a variety of conditions. In this workshop, we will profile use cases in nanostructure characterization — including 2-D materials, catalysts, and polymers — and take you through different electron microscopy characterization methods that will enable you to get more insight.

#### Exploiting Matched Molecular Pairs in Drug Discovery.

*Sponsor:* Simulations Plus, 3:30 to 6:00 PM, SDCC, Room 15B. This hands-on workshop will guide attendees through the design of potential BACE1 inhibitors using state-of-the-art ADMET Predictor 8.0 software. BACE1 is a classic target for Alzheimer's disease, a progressive neurodegenerative disorder. The binding site of BACE1 contains two acidic

amino acids (Asp32 and Asp228) where inhibitors that contain a basic moiety can form salt bridge/hydrogen binding interactions. Modification of the ligand's p*K*<sub>a</sub> is important not only for binding to the enzyme but also because it affects the ligand's ability to penetrate the blood-brain barrier. The initial step in the design phase is to analyze the available data for structure-activity relationships (SARs). The attendees will learn how to cluster compounds according to their maximum common substructure, create R tables, and use matched molecular pair analysis to extract SARs. Presenters will demonstrate a QSAR model that predicts BACE1 enzymatic inhibition. Virtual libraries containing amidine-like functionality will be generated and then be filtered based on their predicted BACE1 inhibition, solubility, permeability, metabolic stability, and other ADMET properties using an ADMET liability scoring function. The workshop will conclude with physiologically based pharmacokinetic (PBPK) simulations for the filtered analogs.

**Wednesday, March 16**

**Inhibitor Design Using MOE Structure-Based Drug Design Applications.** *Sponsor:* Chemical Computing Group, 3:30 to 6:00 PM, SDCC, Room 15B. This hands-on workshop will cover in silico structure-based drug design (SBDD) methods for the rational design of EGFR kinase inhibitors. Starting with raw PDB protein-ligand 3-D structures,

all the steps required to initiate and advance an SBDD modeling study will be covered: preparing PDB structures for modeling, binding pocket visualization, and 2-D and 3-D protein-ligand contact analyses. We will cover advanced topics such as pharmacophore query generation, protein-ligand docking, protein alignments for binding-site comparative analysis and SAR evaluation, and combinatorial synthesis. In silico ligand modification and derivatization will also be covered in the context of ligand optimization.

**Automated HPLC & LCMS Workflows Implemented in Complex Analytical Challenges.** *Sponsor:* Agilent Technologies, 9:30 AM to noon, SDCC, Room 12.

**Simplifying 2D-LC & 2D-LC/MS Automated Workflows.** Two-dimensional Liquid Chromatography (2D-LC) allows chromatographers to extract more information from their samples than one dimensional chromatography. In addition, a two dimensional analysis will allow the user to change a mobile phase that may not be suitable for a mass spectrometer into a more mass spec amenable composition. We will discuss a unique software and hardware approach to 2D-LC and 2D-LC-MS as well as providing examples of how this technique can provide further elucidation of complex samples.

**Accelerate ADC characterization with the new DAR Calculator.** Discover comprehensive protein characterization

using the Drug-to-Antibody Ratio (DAR) calculator, a new tool in the MassHunter Bioconfirm software. It complements your LC/MS biopharma toolbox which includes best-in-class automated sample prep with AssayMAP Bravo and high resolution TOF and Q-TOF LC/MS.

**Elemental Impurity & Extractables and Leachables.** *Sponsor:* Agilent Technologies, 12:30 PM to 3:00 PM, SDCC, Room 12. Elemental Impurities Analysis of Pharmaceutical and Nutraceutical Products: Updates on 232/233 and 2232 Control of impurities, including inorganic contaminants, has always been a concern in the development and production of pharmaceutical and nutraceutical products, and dietary supplements. Join us for a discussion on the latest updates and requirements, implementing techniques for measuring tough samples, and tips to achieve the lowest sensitivity. A review of the next steps in meeting the upcoming requirements will be provided. The Innovation of Workflows for Extractables and Leachables One of the most written about topics in the industry today. Gain a fresh perspective on the workflows and analytical solutions required to be in compliance. A Discussion on some of the latest regulations and the automated workflows necessary to perform these critical analysis utilizing techniques such as HPLC/MS , GC/MS and Atomic Spectroscopy.

## SPEAKER INSTRUCTIONS

**ALL SPEAKERS** and poster presenters must register and pay the appropriate registration fee to attend the meeting. Invited speakers should contact their symposium organizer or division program chair to clarify terms of their invitation.

All presenters should prepare for their presentation by verifying the following details: the status of your abstract at [maps.acs.org](http://maps.acs.org) (using your ACS ID to log in to the system); mode of presentation (oral or poster); and the time, length, and location of your presentation. Speakers should arrive in their presentation rooms at least 30 minutes before their scheduled speaking time. Poster presenters should set up their poster at least one hour before the start of their poster session. If you need to withdraw your presentation, please send a withdrawal notice to [maps@acs.org](mailto:maps@acs.org) and contact your symposium organizer immediately.

### TECHNICAL SESSION EQUIPMENT.

Each technical session meeting room will be equipped with the following: LCD projector, screen, podium, podium microphone or lapel microphone, and laser pointer. Speakers need to provide their own laptops or arrange for specialty equipment directly with their symposium organizer and/or division program chair. To request other specialty equipment (at the standard fee), contact an ACS Operations Office during the meeting.

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### SCI-MIX POSTER SESSION ONLY.

Sci-Mix presenters may begin poster setup at 7:15 PM (45 minutes before the session begins). Each presenter may be accompanied by one assistant only, and both people are required to check in before entering the hall. After exiting, presenters will not be permitted to reenter the hall until the session begins at 8:00 PM.

## ABSTRACTS & PREPRINTS

### ONLINE TECHNICAL PROGRAM.

The technical program for the 251st national meeting is now available at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016). You can search by divisions or committees, symposia, speakers, or keywords from abstracts as well as presidential events and the multidisciplinary theme of "Computers in Chemistry."

### ABSTRACTS (USB FLASH DRIVE).

Abstracts of all scientific sessions at the meeting can be purchased in USB flash drive (thumb drive) format through ACS Attendee Registration either online by Jan. 24 or on-site in San Diego from March 13 to 17. The ACS member fee is \$65 each; the nonmember fee is \$90 each. Attendees can pick up their abstracts on-site at ACS Attendee Registration at the San Diego Convention Center. You can have a USB flash drive shipped to you if you place your order by January 24, pay an \$8.00 postage fee per item, and provide a valid street address within the U.S. or Canada. If you are not attending the meeting, you can purchase abstracts only from the ACS Office of Society Services, 1155—16th St., N.W., Washington, DC 20036; (800) 227-5558. Abstract USB flash drives and their shipping costs are nonrefundable.

### PREPRINTS/GRAPHICAL ABSTRACTS.

Preprints and graphical abstracts from the following divisions may be ordered directly from each division. You can purchase them via the information below or inquire about these products at the hospitality table for each division near their meeting rooms.

#### Energy & Fuels.

Visit [proceedings.com/2256.html](http://proceedings.com/2256.html).

#### Polymer Chemistry.

Kathy Mitchem, e-mail: [kathy@vt.edu](mailto:kathy@vt.edu)

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Monday, March 14, 8 - 10PM

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# 251st American Chemical Society National Meeting & Exposition

March 13–17, 2016 • San Diego, CA

Marriott Marquis San Diego Marina  
(Unless Otherwise Noted)

#acsSanDiego • #ACSSanDiegoUG



All events are sponsored or cosponsored by the Society Committee on Education Undergraduate Programs Advisory Board

CHAIR: Michael R. Adams, *Xavier University of Louisiana, New Orleans.*

PROGRAM CHAIR: Steven Emory, *Western Washington University, Bellingham.*

## UNDERGRADUATE PROGRAM

### Sunday, March 13

#### Hospitality Center

8:00 AM – 5:00 PM • San Diego Ballroom B

#### Undergraduate Research Oral Session

8:30 AM – 5:00 PM • Manchester Grand Hyatt San Diego, Promenade A

#### The Two-Year College Guidelines: What's New?

8:30 – 12:00 NOON • Manchester Grant Hyatt Promenade B

#### Making the Most of Your First National Meeting

9:00 – 9:45 AM • San Diego Ballroom B

#### Graduate School Reality Check, Part I: Getting In

10:00 – 11:15 AM • San Diego Ballroom A  
*Cosponsored by the ACS Younger Chemists Committee*

#### Chem Demo Exchange

11:00 AM – 12:30 PM • San Diego Convention Center, Sails Pavilion

#### Graduate School Reality Check, Part II: You're In – Now What?

11:15 AM – 12:30 PM • San Diego Ballroom A  
*Cosponsored by the ACS Younger Chemists Committee*

#### Symposium: Trends in Computational Chemistry

1:00 – 2:30 PM  
San Diego Ballroom C  
*Cosponsored by the ACS Computers in Chemistry Division*

#### Networking Social with Graduate School Recruiters

1:00 – 5:00 PM • San Diego Ballroom B

#### Workshop: Effective Chemistry Demos for Community Outreach

2:45 – 4:00 PM • San Diego Convention Center, Sails Pavilion

#### Workshop: Improving Scientific Communications

3:00 – 4:15 PM • San Diego Ballroom A  
*Cosponsored by the ACS Younger Chemists Committee*

#### Workshop: Networking 101

4:15 – 5:45 PM • San Diego Ballroom A  
*Cosponsored by the ACS Division of Professional Relations and Younger Chemists Committee*

#### Student Chapter Awards Ceremony

7:00 – 8:30 PM • San Diego Convention Center, Ballroom 20A – C

#### Undergraduate Social

8:30 – 11:00 PM • San Diego Convention Center, Ballroom 20D

### Monday, March 14

#### Hospitality Center

8:00 AM – 5:00 PM • San Diego Ballroom B

#### Realities of the Chemical Industry: Career Paths and Opportunities

8:30 AM – 5:00 PM • Coronado Room  
*Cosponsored by the ACS Industrial & Engineering Chemistry Division*

#### Undergraduate Research Oral Session

8:30 AM – 5:00 PM • Manchester Grand Hyatt San Diego, Promenade A

#### Symposium: Advances in Chemical Imaging: Ultra-Resolution to Single Molecules

9:00 – 10:30 AM • San Diego Convention Center, Room 33B  
*Cosponsored by the ACS Division of Analytical Chemistry and the Physical Chemistry Division of the ACS*

#### Symposium: Frontiers in Inorganic Chemistry

9:30 – 11:30 AM • San Diego Convention Center, Room 33C  
*Cosponsored by the Division of Inorganic Chemistry of the ACS*

#### Chemists Celebrate Earth Day Outreach Ideas

9:45 – 11:00 AM • San Diego Convention Center, Room 30C/D  
*Cosponsored by the ACS Committee on Community Activities*

#### Chemistry Ambassadors Game & Café

10:30 – 11:30 AM • Carlsbad Room

#### Undergraduate Research Poster Session

12:00 NOON – 2:00 PM • San Diego Convention Center, Hall D  
*Cosponsored by the ACS Divisions of Agricultural and Food Chemistry, Analytical, Environmental, Inorganic, Medicinal, Physical, and Polymer Chemistry, Biological Chemistry, and Geochemistry*

#### Eminent Scientist Lecture

Featuring Richard N. Zare, Stanford University, "My Life with Lasers"  
*Cosponsored by the ACS Division of Analytical Chemistry and the Physical Chemistry Division of ACS*  
2:30 – 3:30 PM • San Diego Ballroom A

#### Student Speed Networking with Chemistry Professionals

3:45 – 5:15 PM • San Diego Ballroom B

#### Kavli Lecture

5:30 – 6:30 PM • San Diego Convention Center, Ballroom 20A – C

#### Sci-Mix/Successful Student Chapter Posters

8:00 – 10:00 PM • San Diego Convention Center, Hall D/E

### Tuesday, March 15

#### Realities of the Chemical Industry: Career Paths and Opportunities

8:30 AM – 5:00 PM • Coronado Room

#### Workshop: ChemIDP: A New Career Planning Tool

10:00 AM – 12 NOON • Ballroom 20A

#### Chemistry and the Environment Film Series

12:00 NOON – 2:00 PM • San Diego Convention Center, Room 8

# TECHNICAL PROGRAM SUMMARY

## Presidential Events

PRES

D. Nelson, Program Chair

San Diego Convention Center	S	M	Tu	W	Th
Discussions with the President's Task Force on Employment**	P				
My Comments to the President's Task Force on Employment**	E				
My Experiences in & Advice for Organic Chemistry Courses**	E				
My Experience with & Advice for Improving Diversity in Chemistry**	E				
Is There a Crisis in Organic Chemistry Education?*		A			
How To Foster Diversity in the Chemical Sciences: Lessons Learned & Taught from the Stories of Recipients of the Stanley C. Israel Award**		A			
Diversity-Quantification-Success?*		P			
Sci-Mix		E			
Dreyfus Award Symposium			D		
New Reality of the Chemical Enterprise: Traditional & Nontraditional Career Paths* (I&EC)		D	D		
Excellence in Graduate Polymer Research* (POLY)		D	DE		
LGBT Chemists' Symposium on Chemical Biology* (PROF)		P			

## Multidisciplinary Program Planning Group (continued)

MPPG

K. Merz, Program Chair

San Diego Convention Center	S	M	Tu	W	Th
The Fred Kavli Innovations in Chemistry Lecture <b>cc</b>		P			
Computers in Nanoscience & Nanotechnology <b>cc</b>		P			
Computer-Aided Drug Design** <b>cc</b>			D	D	A
The Centrality of Computing across Chemistry <b>cc</b>			P		
The History of Chemistry & Computing** <b>cc</b>				A	
Big Data Science** <b>cc</b>					D
Fall 2015 InterCollegiate Cheminformatics Course* (CHED)	D				
Analytical & Computational Isotope Geochemistry* (GEOC)	D				
Environmental Interfaces* (GEOC)	P	D	D	DE	
Molecular Modeling at the Undergraduate Level* (CHED)	P				
Current Topics in Chemical Business Development & Management* (BMGT)	P				
GSSPC: Resolving the Big Picture: Bringing Molecules into Focus* (CHED)		D			
Adsorption of Metals by Geomedia* (GEOC)	P	D	DE	A	
Nonlinear Spectroscopy & Modeling* (ANYL)	P				
Communicating Chemistry through Social Media* (CHED)		P			
Advances in E-Learning* (CHED)			D		
Teaching & Implementing Effective Data Analysis & Computational Approaches across the Undergraduate Chemistry Program* (CHED)			P		
Homework: Past, Present & Future* (CHED)				A	
Know Your Unknowns: Estimating the Reliability of Individual Activity & Property Predictions* (COMP)				A	
Chemical Imaging: Applications, Advances & Challenges* (ANYL)				D	A
Big Data & Small Data* (ANYL)				D	
Computer-Aided Data Analysis in Chemical Education Research (CADACER)* (CHED)				D	

## Multidisciplinary Program Planning Group

MPPG

K. Merz, Program Chair

San Diego Convention Center	S	M	Tu	W	Th
Computational Materials & Nanoscience: Theory Meets Experiment** <b>cc</b>				D	D
Multiscales Chemistry** <b>cc</b>	D	D	D	P	
Computers in Chemistry Plenary Session <b>cc</b>	P				
Preparing for the Real World: Challenges Faced by Young Investigators** <b>cc</b>		D			
The Kavli Foundation Emerging Leader in Chemistry Lecture <b>cc</b>		P			

# PROGRAM SUMMARY

## Multidisciplinary Program Planning Group (continued)

MPPG

*K. Merz, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Online Approaches in Chemical Education* (CHED)				D	
Peptide Modeling* (COMP)				P	
Applied Geochemical Modeling* (GEOC)				E	D

## Division of Agricultural & Food Chemistry

AGFD

*B. Park, Program Chair*

US Grant Hotel	S	M	Tu	W	Th
Undergraduate Symposium	A				
Flavor Chemistry of Alcoholic Beverages	D	A			
Bioactives & Neurodegenerative Diseases	D	D			
Graduate Student Symposium	P				
Cannabis: Exploring the Chemistry, History & Future**		D			
Advances in Food Peptide & Food Protein Research: Nutrition, Functionality & Food Safety		P			
Sci-Mix		E			
Chemical Modification of Natural Bio-based Material: Design & Application for Value-Added Products			A		
Public Health Perspectives of Mycotoxins in Food**			D	D	
Applied Nanotechnology for Food & Agriculture			D		
General Posters			P		
Metabolomics in Agriculture & Food Chemistry: Current Status & Future Scopes			P		
General Papers				D	
Natural & Modified Carbohydrate Polymers: Effects on Obesity-Related Metabolic Diseases				D	
Advances & Applications in Water-Sensing Technologies for Drinking Water, Reuse, Agri-Tech & Research* (ENVR)	D				
Undergraduate Research Posters* (CHED)		P			
Cannabis: Exploring the Chemistry, History & Future* (SCHB)			A		

## Division of Agrochemicals

AGRO

*J. Gan, P. Rice, Program Chairs*

Located with Primary Sponsor	S	M	Tu	W	Th
Wolfrom Award* (CARB)	A				
Public Health Perspectives of Mycotoxins in Food* (AGFD)			D	D	

## Division of Analytical Chemistry

ANYL

*J. Harris, L. Baker, Program Chairs*

Wyndham San Diego Bayfront	S	M	Tu	W	Th
Sampling & Processing of Biological Particles Enabled by Micro- or Nano-Fluidics	A				
Luminescent Proteins, Dyes & Sensors	D				
XRF: Cutting-Edge Elemental Spectrometry	P	A			
Capillary Electrophoresis Applied to Bioanalysis	P				
Analytical Division Poster Session	E				
Electrochemical Measurements at Biological Interfaces		A			
Protein Structure & Folding: From Solution to the Gas Phase**		D			
Analytical Methodologies & Research Partnerships at the Interface of Chemistry & Art/Archaeology		P	D		
Nonlinear Spectroscopy & Modeling**		P			
Sci-Mix		E			
Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Honoring Albert J. R. Heck**			A		
Biosensing of Proteins, Peptides, DNAs & RNAs			D	D	
Approaches for Engaging Students in Analytical Chemistry Courses**			P		
Chemical Imaging: Applications, Advances & Challenges**				D	A
Big Data & Small Data** <span style="color: red;">cc</span>				D	
Advances in Analytical Separations					D
Advances in Structural Mass Spectrometry					P
Multiscales Chemistry* (MPPG)	D	D	D	P	
Global Initiatives in Research Data Management & Discovery* (CINF)	P	D			
Advances in Chemical Imaging: Ultra-Resolution to Single Molecules* (SOCED)		A			



## PROGRAM SUMMARY

### Division of Analytical Chemistry (continued)

A N Y L

*J. Harris, L. Baker, Program Chairs*

Wyndham San Diego Bayfront	S	M	Tu	W	Th
GSSPC: Resolving the Big Picture: Bringing Molecules into Focus* (CHED)		D			
Undergraduate Research Posters* (CHED)		P			
Public Health Perspectives of Mycotoxins in Food* (AGFD)			D	D	

### Division of Biochemical Technology

B I O T

*S. Tobler, P. Tessier, Program Chairs*

Westin San Diego	S	M	Tu	W	Th
David Perlman Memorial Lectureship & Van Lanen Service Award Presentation	A				
Biomolecular & Biophysical Processes	D	D	D	D	D
Upstream Processes	D	D	D	D	D
Biofuel & Biobased Chemical Production	D	D			
Downstream Processes	DE	D	D	D	D
Computationally Enabled Biotechnology at the Molecular, Cellular & Process Scales <sup>cc</sup>	P	D			
Marvin J. Johnson Award in Microbial & Biochemical Technology Presentation		A			
Sci-Mix		E			
BIOT Young Investigator & Peterson Awards Presentations			A		
Emerging Technologies			D	D	D
Biosimilars			D		
Poster Session			E		
BIOT Industrial Biotechnology Award			E		
Quality by Design for Biopharmaceuticals				D	A
Biotechnology & Bioengineering Daniel I. C. Wang Award				E	
Biotechnology & Bioengineering Elmer Gaden Award					A
ACS Award in Separations Science & Technology: Honoring Steven M. Cramer* (I&EC)	A				
Undergraduate Research Posters* (CHED)		P			
LGBT Chemists' Symposium on Chemical Biology* (PROF)		P			

### Division of Biological Chemistry

B I O L

*V. Bandarian, L. Hedstrom, Program Chairs*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Computational Enzymology <sup>cc</sup>	A				
Young Investigators in Biological Chemistry	D	P		A	A
E. Bright Wilson Award in Spectroscopy: Honoring Robert G. Griffin**	P				
Current Topics in Biochemistry	E		E		
Frontiers in Biomolecular Recognition: From Materials to Cells		A			
Sci-Mix		E			
Chemistry in Service of Biology: Tools for Probing Cellular Processes			A		
ACS Chemical Biology Award Symposium			P		
RNA Structure & Function: Perspectives from Inside the Cell & Out				A	
Goodman Award: Honoring Joan Steitz				P	
Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory* (PHYS)	D	D	A	A	
Multiscales Chemistry* (MPPG)	D	D	D	P	
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Undergraduate Research Posters* (CHED)		P			
LGBT Chemists' Symposium on Chemical Biology* (PROF)		P			
Diversity-Quantification-Success?* (PRES)		P			
ACS Award for Encouraging Women into Careers in the Chemical Sciences: Honoring Carol A. Fierke* (WCC)			A		
Computer-Aided Drug Design* (MPPG)			D	D	A
Big Data Science* (MPPG)					D

# PROGRAM SUMMARY

## Division of Business Development & Management

BMGT

*D. Daly, Program Chair*

Westin San Diego Gaslamp Quarter	S	M	Tu	W	Th
Current Topics in Chemical Business Development & Management** <span style="color: red;">cc</span>	P				
Industrial Research at the Interface of Inorganic Chemistry & Polymer Science* (POLY)	P		E		
Discussions with the President's Task Force on Employment* (PRES)	P				
My Comments to the President's Task Force on Employment* (PRES)	E				
Women in Innovation: Science & Technology* (PROF)		A			
Industrial Innovation in Polymer Chemistry: Sustainable Polymerization Feedstocks & Process Technology* (POLY)	P				
Chemical Angel Network* (PROF)			P		

## Division of Carbohydrate Chemistry

CARB

*N. Snyder, Program Chair*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Wolfrom Award**	A				
Isbell Award	P				
Gin New Investigator Award	P				
Glycosylases: Inhibition & Therapeutic Applications**		D			
Sci-Mix		E			
Carbohydrate Research at Predominantly Undergraduate Institutions**			D		
General Posters			E		
From mAb to ADCs: Tailored Antibodies & Dedicated Chemistry Technologies for Site-Specific ADCs**				A	
Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Honoring Professor Sharpless's 75th Birthday**				D	A

\*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

\*\*Primary organizer of a cosponsored symposium.

CC = Computers in Chemistry

A = AM AE = AM/EVE P = PM D = AM/PM

E = EVE DE = AM/PM/EVE PE = PM/EVE

## Division of Carbohydrate Chemistry (continued)

CARB

*N. Snyder, Program Chair*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Functional Lignocellulosics & Nanotechnology* (CELL)	D	D	A	D	
Discussions with the President's Task Force on Employment* (PRES)	P				
My Comments to the President's Task Force on Employment* (PRES)	E				
Biomedical & Drug Delivery Applications of Polysaccharide-Based Materials* (CELL)				D	A

## Division of Catalysis Science & Technology

CATL

*E. Nikolla, K. Ramasamy, Program Chairs*

Manchester Grand Hyatt San Diego	S	M	Tu	W	Th
Catalytic Materials for Methane Conversion** <span style="color: red;">cc</span>	D	A			
Catalysis at the Subnanometer Scale**	D	A			
Computational Chemistry across Catalysis** <span style="color: red;">cc</span>	D	D	D	A	
Amorphous Catalytic Materials <span style="color: red;">cc</span>	D	D			
Fundamental Surface Chemistry of Non-oxide Transition-Metal Ceramic Catalysts: Carbides, Nitrides, Sulfides, Phosphides, Selenides** <span style="color: red;">cc</span>	D				
Ipatieff Prize: Honoring Aditya Bhan		D	D		
Elucidation of Mechanisms & Kinetics on Surfaces**		P	D	D	D
Surface Chemistry & Catalysis of Metal Oxides <span style="color: red;">cc</span>		P	D	D	
Sci-Mix		E			
Condensed Phase Catalysis** <span style="color: red;">cc</span>			A		
Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice**			P	D	D
Poster Session			E		
Catalytic Processes at Interfaces: Fundamentals & Applications <span style="color: red;">cc</span>				D	A
James Flack Norris Award in Physical Organic Chemistry: Honoring Juan C. Scaiano				D	
General Papers					D
Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications* (COMP)	D	D			

PROGRAM SUMMARY

**Division of Catalysis Science & Technology (continued)**

CATL

*E. Nikolla, K. Ramasamy, Program Chairs*

Manchester Grand Hyatt San Diego	S	M	Tu	W	Th
Alpha-Olefin Catalysis: Production & Transformations* (I&EC)	D				
Fuel Cells* (ENFL)	D				
CO <sub>2</sub> Conversion & Utilization* (ENFL)		D	D	D	
WCC 2016 Rising Stars Awards Symposium* (WCC)		D			
Nanomaterials for Energy Conversion & Storage* (ENFL)		P	D	A	
Application of Computational Chemistry for Energy & Fuel Production* (ENFL)			D	D	A
Gabor A. Somorjai Award for Creative Research in Catalysis: Honoring Donna G. Blackmond* (ORGN)				A	
In Situ & Operando Characterization & Modeling of Reaction Kinetics* (ENFL)				D	A
George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Honoring Mieczyslaw M. Boduszynski* (ENFL)				P	

**Division of Cellulose & Renewable Materials (continued)**

CELL

*C. Frazier, Program Chair*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Biomedical & Drug Delivery Applications of Polysaccharide-Based Materials**				D	A
Cellulose Nanocrystal Fundamentals				D	D
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Glycosylases: Inhibition & Therapeutic Applications* (CARB)		D			
Diversity-Quantification-Success?* (PRES)		P			
Carbohydrate Research at Predominantly Undergraduate Institutions* (CARB)			D		
Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Honoring Professor Sharpless's 75th Birthday* (CARB)				D	A

**Division of Cellulose & Renewable Materials**

CELL

*C. Frazier, Program Chair*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Functional Lignocellulosics & Nanotechnology**	D	D	A	D	
Lignin Refining, Functionalization & Utilization	D	D	A		
Structure of Native Celluloses & Variety of Nanocelluloses that Can Be Formed from Them: Anselme Payen Award Symposium in Honor of Akira Isogai	D	D	D		
New Horizons in Sustainable Materials**	D	D			
Biomass & Polymer Extrusion, Composite & Reaction Technologies: New Insights, Future Potential & Principles to Practice**	D				
General Posters	E				
Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems		D	A	D	D
Sci-Mix		E			
Cellulose Nanocomposites: Processing, Development & Their Structure-Property Relations			A	D	D

**Division of Chemical Education**

CHED

*I. Levy, I. Black, D. Wicht, Program Chairs*

Manchester Grand Hyatt San Diego	S	M	Tu	W	Th
Cottrell Scholars Collaborative: Innovating the Integration of Research & Teaching	A				
The Two-Year Guidelines: What's New**	A				
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment**	D	A			
Undergraduate Research Papers**	D	D			
Chemistry Education Research: Graduate Student Research Forum	D				
Fall 2015 InterCollegiate Cheminformatics Course** <small>cc</small>	D				
High School Program**	D				
NMR Spectroscopy in the Undergraduate Curriculum	D				
Molecular Modeling at the Undergraduate Level** <small>cc</small>	P				

## PROGRAM SUMMARY

### Division of Chemical Education (continued)

CHED

*I. Levy, I. Black, D. Wicht, Program Chairs*

Manchester Grand Hyatt San Diego	S	M	Tu	W	Th
Perspectives on Climate Change Literacy & Education: Local to International**	P				
General Posters	E				
Strategies Promoting Success of Two-Year College Students		A	A		
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Honoring Avi Hofstein		A			
Chemistry Education Research		D	D	D	A
Chemists Helping Teachers Incorporate Next Generation Science Standards (NGSS) into Their K-12 Classrooms		D			
GSSPC: Resolving the Big Picture: Bringing Molecules into Focus** <i>cc</i>		D			
Communicating Chemistry through Social Media** <i>cc</i>		P			
Integration of STEM & the Liberal Arts		P			
Research on Learning in the Lab		P			
Undergraduate Research Posters** <i>cc</i>		P			
Potpourri of Polymer Projects: Take a Byte out of the NGSS**		E			
Successful Student Chapters**		E			
Sci-Mix		E			
ACS-CEI Award for Incorporating Sustainability into Chemistry Education**			A		
General Papers			D		A
Advances in E-Learning** <i>cc</i>			D		
George C. Pimentel Award in Chemical Education: Honoring Richard S. Moog			D		
Green Chemistry: Theory & Practice**			D		
International & Multicultural Perspective**			P		
Teaching & Implementing Effective Data Analysis & Computational Approaches across the Undergraduate Chemistry Program** <i>cc</i>			P		
Homework: Past, Present & Future** <i>cc</i>				A	
Computer-Aided Data Analysis in Chemical Education Research (CADACER)** <i>cc</i>				D	
Curricular Innovations in Undergraduate Chemical Education Impacted by NSF				D	
Implementing Discovery-Based Research Experiences in Undergraduate Chemistry Courses				D	

### Division of Chemical Education (continued)

CHED

*I. Levy, I. Black, D. Wicht, Program Chairs*

Manchester Grand Hyatt San Diego	S	M	Tu	W	Th
Online Approaches in Chemical Education** <i>cc</i>				D	
Process Oriented Guided Inquiry Learning (POGIL)				D	
Citizens First!**				P	
Instructors & Researchers Advancing Graduate Student Education					A
Supporting & Expanding Undergraduate Research in Chemistry					A
Ethics 101* (PROF)	A				
Undergraduate Teaching at the Frontiers of Inorganic Chemistry* (INOR)	AE	P			
Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Safety Begins in the Classroom: Demonstrations, Awareness & Prelab Planning* (CHAS)	P				
Preceptors of Chemistry* (HIST)	P				
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Preparing for the Real World: Challenges Faced by Young Investigators* (MPPG)		D			
Diversity-Quantification-Success?* (PRES)		P			
Successful REU Programs* (PROF)			A		
Developing, Implementing & Teaching Hazard Assessment Tools* (CHAS)			D		
Approaches for Engaging Students in Analytical Chemistry Courses* (ANYL)			P		
James Bryant Conant Award in High School Chemistry Teaching: Honoring Julia Winter* (ORGN)			P		

# PROGRAM SUMMARY

## Division of Chemical Health & Safety

CHAS

*D. Decker, F. Wood-Black, J. Pickel, Program Chairs*

Hilton Gaslamp San Diego	S	M	Tu	W	Th
Ask Dr. Safety: Incident Reporting**	P				
Safety Begins in the Classroom: Demonstrations, Awareness & Prelab Planning**	P				
How Texas Tech & UCLA Have Affected Laboratory Safety Nationwide**		P			
Sci-Mix		E			
Developing, Implementing & Teaching Hazard Assessment Tools**			D		
Chemical, Sample & Asset Management Tools**				D	
Cannabis: Exploring the Chemistry, History & Future* (SCHB)			A		

## Division of Chemical Information

CINF

*E. Davis, E. Alvaro, Program Chairs*

San Diego Convention Center	S	M	Tu	W	Th
Tomayto versus Tomahto: Overcoming Incompatibilities in Scientific Data <b>cc</b>	A				
From Data to Prediction: Applying Structural Knowledge in Drug Discovery & Development <b>cc</b>	D				
Global Initiatives in Research Data Management & Discovery** <b>cc</b>	P	D			
Data Mining: Searching Noncovalent Interactions in Chemical Databases** <b>cc</b>	P				
CINF Scholarships for Scientific Excellence: Student Poster Competition <b>cc</b>	E				
Beyond Digitized Paper: The Next Generation of ELNs <b>cc</b>		A			
Informatics & Quantum Mechanics: Combining Big Data & DFT in Pharma & Materials <b>cc</b>			D		
Chemical Information for Small Businesses & Start-ups** <b>cc</b>		P			
Sci-Mix		E			
Chemistry, Data & the Semantic Web: An Important Triple to Advance Science <b>cc</b>			D	D	D
Driving Change: Impact of Funders on the Research Data & Publications Landscape** <b>cc</b>			D		

## Division of Chemical Information (continued)

CINF

*E. Davis, E. Alvaro, Program Chairs*

San Diego Convention Center	S	M	Tu	W	Th
Linking Big Data with Chemistry: Databases Connecting Genomics, Biological Pathways & Targets to Chemistry <b>cc</b>			D		
Reimagining Libraries as Innovation Centers: Enabling, Facilitating & Collaborating throughout the Research Life Cycle <b>cc</b>				D	
General Papers					A
From Synthesis to Design: Modeling Tools for Medicinal Chemists* (COMP)	A				
Ethics 101* (PROF)	A				
Fall 2015 InterCollegiate Cheminformatics Course* (CHED)	D				
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Preparing for the Real World: Challenges Faced by Young Investigators* (MPPG)			D		
Computers in Chemistry: Bridging the Gap between Clients & Software* (SCHB)		P			
Diversity-Quantification-Success?* (PRES)		P			
Computer-Aided Drug Design* (MPPG)				D	D
Chemical Imaging: Applications, Advances & Challenges* (ANYL)					A
Big Data & Small Data* (ANYL)					D
Chemical, Sample & Asset Management Tools* (CHAS)					D
Big Data Science* (MPPG)					D

\*Cospresented symposium with primary organizer shown in parentheses; located with primary organizer.

\*\*Primary organizer of a cospresented symposium.

CC = Computers in Chemistry

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E = EVE DE = AM/PM/EVE PE = PM/EVE

# PROGRAM SUMMARY

## Division of Chemistry & the Law

CHAL

*K. Bianco, J. Kennedy, J. Hasford, Program Chairs*

San Diego Convention Center	S	M	Tu	W	Th
Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions	P				
Patenting Gene Sequences: What Is Patentable in Australia, Europe, Mexico & the U.S.	P				
Symposium on the Generic Drug User Fee Program (GDUFA) of 2012 & ANDA Review Process		A			
The Role of Scientific Patent Information in the Innovation Process		P			
Sci-Mix		E			
Recent Developments in Chemical & Pharmaceutical Patent Law			D		
Building & Protecting Intellectual Property				A	
Chemistry of Peace				P	
The Many Faces of CHAL: Where Chemistry Meets the Law					A

## Division of Colloid & Surface Chemistry (continued)

COLL

*R. Nagarajan, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Surface Characterization & Manipulation for Electronic Applications			A	D	A
Computational Modeling & Simulations in Colloid & Surface Chemistry <sup>cc</sup>			A	D	
Physical Chemistry of Complex Environmental Interfaces* (PHYS)	D	D	A	P	D
Applications of Polymer Surfaces & Interfaces* (POLY)	D	P	DE	D	A
Environmental Interfaces* (GEOC)	P	D	D	DE	
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
Elucidation of Mechanisms & Kinetics on Surfaces* (CATL)		P	D	D	D
Diversity-Quantification-Success?* (PRES)		P			

## Division of Colloid & Surface Chemistry

COLL

*R. Nagarajan, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Colloids for Medical Imaging	D	D	A	A	
Biomembrane Synthesis, Structure, Mechanics & Dynamics	D	D	A	D	A
Nanomedicines: Targeting & Clearance	D	D	A	D	
Nanometal: Synthesis, Structure, Property & Application	D	D	A	D	
ACS Award in Colloid & Surface Chemistry: Honoring Nicholas L. Abbott	D	D	D		
Basic Research in Colloids, Surfactants & Nanomaterials	D	D		D	A
Frontier of the Interface of Materials & Biology: Protein-Based Nanomaterials	D	D			
Proteins & Polymers Under Confinement	P				
Fundamental Research in Colloids, Surfaces & Nanomaterials	E				
Computational & Experimental Advances Toward Design of Energy-Efficient Catalysts		D	A		
Sci-Mix		E			

## Division of Computers in Chemistry

COMP

*H. L. Woodcock, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
From Synthesis to Design: Modeling Tools for Medicinal Chemists** <sup>cc</sup>	A				
Drug Discovery <sup>cc</sup>	D	D	D		D
From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules**	D	D		D	
Computational Materials Chemistry	D	D			
Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications**	D	D			
COMP Undergraduate Research & National Meeting Roundtable	P				
Molecular Mechanics		D	D	D	D
Sci-Mix		E			
Materials Science			D	A	
Quantum Mechanics**			D	D	D
ACS Award for Computers in Chemical & Pharmaceutical Research: Honoring Warren J. Hehre			D		

PROGRAM SUMMARY

**Division of Computers in Chemistry (continued)**

**COMP**

*H. L. Woodcock, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Chemical Computing Group Excellence Award for Graduate Students			E		
NVIDIA GPU Award			E		
OpenEye Outstanding Junior Faculty Award in Computational Chemistry			E		
Poster Session			E		
Know Your Unknowns: Estimating the Reliability of Individual Activity & Property Predictions**				A	
Advances in Computer-Aided Biologics Design <sup>cc</sup>				D	
Time-Dependent Dynamics & Electronic Excited States				P	D
Peptide Modeling**				P	
Computational Materials & Nanoscience: Theory Meets Experiment* (MPPG)	A			P	P
Computational Chemistry across Catalysis* (CATL)	D	D	D	A	
Multiscales Chemistry* (MPPG)	D	D	D	P	
Global Initiatives in Research Data Management & Discovery* (CINF)	P	D			
Data Mining: Searching Noncovalent Interactions in Chemical Databases* (CINF)	P				
Trends in Computational Chemistry: Biophysical to Materials Chemistry* (SOCED)	P				
Preparing for the Real World: Challenges Faced by Young Investigators* (MPPG)		D			
WCC 2016 Rising Stars Awards Symposium* (WCC)		D			
Undergraduate Research Posters* (CHED)		P			
Computational Design of Advanced Materials* (COMSCI)			A		
Computer-Aided Drug Design* (MPPG)			D	D	A
Opportunities & Progress in Computational Prediction of Contaminant Toxicity, Fate & Transport Properties* (ENVR)			P		
The History of Chemistry & Computing* (MPPG)				A	
Computational Materials & Nanoscience: Theory Meets Experiment* (MPPG)				D	D
Big Data Science* (MPPG)					D

**Division of Energy & Fuels**

**ENFL**

*X. Wang, D. Heldebrant, Program Chairs*

Wyndham San Diego Bayfront	S	M	Tu	W	Th
Advances in Methane Technology	D	A			
Solar Cells	D	D			
Advances in Chemistry of Energy & Fuels	D	D			
Fuel Cells**	D				
Heavy Oil Upgrading, Production & Characterization	P				
Research Opportunities for Future Energy Technologies	P				
CO <sub>2</sub> Conversion & Utilization**		D	D	D	
Novel Materials for Energy & Fuels		D	D	D	
ENFL Distinguished Researcher Award: Honoring Stu Soled		D	D		
Nanomaterials for Energy Conversion & Storage**		P	D	A	
Sci-Mix		E			
Application of Computational Chemistry for Energy & Fuel Production**			D	D	A
Batteries & Supercapacitors			D	D	A
In Situ & Operando Characterization & Modeling of Reaction Kinetics**				D	A
George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Honoring Mieczyslaw M. Boduszynski**				P	
Catalytic Materials for Methane Conversion* (CATL)	D	A			
Computational Chemistry across Catalysis* (CATL)	D	D	D	A	
Fundamental Surface Chemistry of Non-oxide Transition-Metal Ceramic Catalysts: Carbides, Nitrides, Sulfides, Phosphides, Selenides* (CATL)	D				
Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing* (ENVR)		D	D	D	D
WCC 2016 Rising Stars Awards Symposium* (WCC)		D			
Condensed Phase Catalysis* (CATL)			A		
Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice* (CATL)			P	D	D
Computational Materials & Nanoscience: Theory Meets Experiment* (MPPG)				D	D

## PROGRAM SUMMARY

### Division of Environmental Chemistry

ENVR

*S. Al-Abed, Program Chair*

Omni San Diego Hotel	S	M	Tu	W	Th
Characterization & Toxicity of Airborne Particulate Matters (PMs) in East Asia	D			E	
Sources, Fate & Transport of Perfluorinated Alkyl Substances in the Environment: Theory, Practice & Innovation	D			E	
Detection of Engineered Nanomaterials in Environmentally Relevant Media	D				
Flue Gas Cleaning & Climate Control	D				
New Challenges on Metals & Metalloids: Chemistry, Treatment & the Impacts on Water Quality	D				
Advances & Applications in Water-Sensing Technologies for Drinking Water, Reuse, Agri-Tech & Research**	D				
Water Treatment Technologies To Support Food-Energy-Water Nexus Water Conservation Needs**		P			
Carbonate & Sulfate Minerals: Nucleation, Growth & Control of Scale Formation** <span style="color: red;">cc</span>	D	A			
Per- & Polyfluoroalkyl Substances Associated with Aqueous Film-Forming Foams (AFFF): Chemistry, Remediation & Regulatory Issues	D	A			
Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing** <span style="color: red;">cc</span>	D	D	D	D	D
Treatment of Contaminants of Emerging Concern & Their Transformation Products**	D	D	E		
Innovative Materials & Technologies for Water Purification	D	D			
Chemistry of Materials Management: Mitigation & Reuse for Sustainable Environment**	P				
Sci-Mix	E				
Chemistry & Application of Advanced Oxidation Processes for Water Purification, Treatment & Reuse			D	DE	A
Science & Perception of Climate Change**			P	E	
Opportunities & Progress in Computational Prediction of Contaminant Toxicity, Fate & Transport Properties** <span style="color: red;">cc</span>			P		
ES&T @ 50: Award-Winning Researchers Past, Present & Future				A	
Aquatic Photochemistry**				DE	D
Green Chemistry & the Environment**				DE	

### Division of Environmental Chemistry (continued)

ENVR

*S. Al-Abed, Program Chair*

Omni San Diego Hotel	S	M	Tu	W	Th
Advances in In Situ Pollutant Destruction by Nanoscale Zero-Valent Iron & Other Engineered Nanoparticles				P	D
Membrane Technology for Water-Energy Sustainability**				P	D
General Posters				E	
Analytical & Computational Isotope Geochemistry* (GEOC)	D				
Environmental Interfaces* (GEOC)	P	D	D	DE	
Francis P. Garvan-John M. Olin Medal: Honoring Annie Kersting* (NUCL)		D			
Earle B. Barnes Award for Leadership in Chemical Research Management: Honoring Henry E. Bryndza* (INOR)		P	A		
Elucidation of Mechanisms & Kinetics on Surfaces* (CATL)		P	D	D	D
Adsorption of Metals by Geomedia* (GEOC)		P	D	DE	A
Undergraduate Research Posters* (CHED)		P			
Greener Pathways to Organics & Nanomaterials: Sustainable Applications of Magnetic Nanocatalysts* (I&EC)				D	A

### Division of Fluorine Chemistry

FLUO

*V. Petrov, Program Chair*

Westin San Diego Gaslamp Quarter	S	M	Tu	W	Th
ACS Award for Creative Work in Fluorine Chemistry: Honoring Steven H. Strauss	DE	DE			

### Division of Geochemistry

GEOC

*Y. Jun, Program Chair*

Omni San Diego Hotel	S	M	Tu	W	Th
Geochemical Reactivity of Nanoparticles, Aggregates, Coatings & Organo-Nanoparticulate Flocculates	A			E	
Closing the Human Phosphorus Cycle: Biogeochemistry, Sustainable Phosphorus Recovery, Speciation, Detection & Reuse	A			E	
Analytical & Computational Isotope Geochemistry**	D				
Frontiers in Microscopic Techniques & Applications to Geochemical Reactions	P	A			



# PROGRAM SUMMARY

## Division of Geochemistry (continued)

### GEOC

*Y. Jun, Program Chair*

Omni San Diego Hotel	S	M	Tu	W	Th
Environmental Interfaces**	P	D	D	DE	
Adsorption of Metals by Geomedia**		P	D	DE	A
Sci-Mix		E			
General Geochemistry			A	E	
Environmental Consequences of Resource Development				AE	
Applied Geochemical Modeling** <i>cc</i>				E	D
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Carbonate & Sulfate Minerals: Nucleation, Growth & Control of Scale Formation* (ENVR)		D	A		
Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing* (ENVR)		D	D	D	D
Undergraduate Research Posters* (CHED)		P			
Diversity-Quantification-Success?* (PRES)		P			
Aquatic Photochemistry* (ENVR)				DE	D

## Division of the History of Chemistry

### HIST

*S. Rasmussen, Program Chair*

Hilton San Diego Bayfront	S	M	Tu	W	Th
HIST Tutorial & General Papers	A		A		
Preceptors of Chemistry**	P				
The Posthumous Nobel Prize in Chemistry: Correcting the Errors & Oversights of the Nobel Prize Committee			D		
Sci-Mix		E			
Memorial Symposium Honoring Karen J. Brewer* (INOR)			D	D	
The History of Chemistry & Computing* (MPPG)				A	

## Division of Industrial & Engineering Chemistry

### I & EC

*P. Smith, E. Rosenburg, Program Chair*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
ACS Award in Separations Science & Technology: Honoring Steven M. Cramer**	A				
Alpha-Olefin Catalysis: Production & Transformations**	D				
Industrial & Engineering Fellow: Honoring Bala Subramaniam	P				
New Reality of the Chemical Enterprise: Traditional & Nontraditional Career Paths**		D	D		
Industrial & Engineering Fellow: Honoring Mark B. Shiflett		D			
Sci-Mix		E			
ACS Award in Industrial Chemistry: Honoring Ted C. Germroth**			A		
Separations for the Nuclear Fuel Cycle in the 21st Century Revisited**			P	D	
General Posters			E		
Greener Pathways to Organics & Nanomaterials: Sustainable Applications of Magnetic Nanocatalysts**				D	A
General Papers					D
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Undergraduate Research Posters* (CHED)		P			
Diversity-Quantification-Success?* (PRES)		P			
Green Chemistry: Theory & Practice* (CHED)			D		

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PROGRAM SUMMARY

Division of Inorganic Chemistry

INOR

*N. Radu, S. Koch, Program Chairs*

San Diego Convention Center	S	M	Tu	W	Th
Lanthanide & Actinide Chemistry	A		E	A	A
Coordination Chemistry	AE		E		D
Chemistry of Materials	AE	P		D	D
Undergraduate Teaching at the Frontiers of Inorganic Chemistry**	AE	P			
Bioinorganic Chemistry	AE		PE	D	A
Organometallic Chemistry	DE		DE	D	D
Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Honoring Eric J. Schelter	D	P	A		
ACS Award in Inorganic Chemistry: Honoring Mercouri G. Kanatzidis	D	P	A		
ACS Award in Organometallic Chemistry: Honoring Karen I. Goldberg**	D	P			
ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Honoring Vincent L. Pecoraro	DE	P			
Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Honoring Edward I. Solomon	P	P	A		
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Honoring François P. Gabbaï	P	P	D		
ACS Award in Pure Chemistry: Honoring Jonathan S. Owen	P	P			
Inorganic Catalysts	P		E	A	
Nanoscience	P		E		P
ExxonMobil Solid State Chemistry Faculty Fellow Award: Honoring Mircea Dincă	P				
Undergraduate Research at the Frontiers of Inorganic Chemistry	PE		D		
Main-Group Chemistry	E			A	P
ACS Awards in Inorganic Chemistry: Plenary Session		A			
Earle B. Barnes Award for Leadership in Chemical Research Management: Honoring Henry E. Bryndza**		P	A		
Organometallic Compounds & Catalysts: Influence on Polymer Science & Synthesis		P	A		
Frontiers in Heavy-Element Inorganic Chemistry**		P	D		
Sci-Mix		E			
Memorial Symposium Honoring Karen J. Brewer**			D	D	

Division of Inorganic Chemistry (continued)

INOR

*N. Radu, S. Koch, Program Chairs*

San Diego Convention Center	S	M	Tu	W	Th
Transition-Metal Chemistry in DNA & RNA Regulation			DE	A	
Supramolecular Chemistry: A Crown & Anchor Approach**			DE		
Metal-Oxygen Oxidants in Synthesis & Biology: Beyond Metal-Oxo Species			PE	A	
Environmental & Energy-Related Inorganic Chemistry			PE		A
Solid-State Inorganic Chemistry			PE		A
Interplay of Structure & Transport Properties in Materials for Energy			E	D	
Electrochemistry			E	P	
Inorganic Spectroscopy			E	P	
Computational Materials & Nanoscience: Theory Meets Experiment* (MPPG)	A			P	P
Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in Honor of Matthew J. Polinski & Thomas E. Albrecht-Schmitt* (NUCL)	A				
Alpha-Olefin Catalysis: Production & Transformations* (I&EC)	D				
Industrial Research at the Interface of Inorganic Chemistry & Polymer Science* (POLY)	P		E		
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Frontiers in Inorganic Chemistry* (SOCED)	A				
Undergraduate Research Posters* (CHED)		P			
Diversity-Quantification-Success?* (PRES)		P			
Heavy-Element Inorganic Chemistry: A Tribute to Al Sattelberger* (NUCL)				D	A
Supramolecular Chemistry* (ORGN)				D	

## PROGRAM SUMMARY

### Division of Medicinal Chemistry

M E D I

*W. Young, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Bromodomain Inhibition: BETs & Beyond	A				
General Oral	D		P	P	
Medicinal Chemists' Toolbox: Recent Strategies & Tactics for Resolving Off-Target Liabilities	P				
General Poster	E			E	
Medicinal Chemistry Challenges in the Development of Countermeasures to Highly Lethal Chemicals & Biologicals		A			
Neuroactive Steroids: New Drugs with Old Scaffolds		A			
Young Investigator Symposium		A			
Design of Radioligands & Molecular Probes		P			
Discovery, Pharmacology & Medicinal Chemistry of Rapidly Acting Antidepressants		P			
Medicinal Chemistry Driven by Phenotypic Assays		P			
Sci-Mix		E			
MEDI Award Symposium			A		
Progress & New Approaches in the Ongoing Battle against Multidrug-Resistant Bacteria			A		
Advances in the Development of Type II Kinase Inhibitors			P		
Blood-Brain Barrier in Drug Discovery			P		
Accelerating Medicinal Chemistry by Trusting Genetics				A	
First-Time Disclosures				D	
From Synthesis to Design: Modeling Tools for Medicinal Chemists* (COMP)	A				
Global Initiatives in Research Data Management & Discovery* (CINF)	P	D			
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Undergraduate Research Posters* (CHED)		P			

### Division of Medicinal Chemistry (continued)

M E D I

*W. Young, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
LGBT Chemists' Symposium on Chemical Biology* (PROF)		P			
Diversity-Quantification-Success?* (PRES)		P			
Computer-Aided Drug Design* (MPPG)			D	D	A
Driving Change: Impact of Funders on the Research Data & Publications Landscape* (CINF)			D		
From mAb to ADCs: Tailored Antibodies & Dedicated Chemistry Technologies for Site-Specific ADCs* (CARB)				A	
Big Data Science* (MPPG)					D

### Division of Nuclear Chemistry & Technology

N U C L

*A. Hixon, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Nobel Laureate Signature Award for Graduate Education in Chemistry: Honoring Matthew J. Polinski & Thomas E. Albrecht-Schmitt**	A				
Tackling the Challenging Electronic Structure of Actinides: Honoring Richard Martin <i>cc</i>	P	D	A		
Francis P. Garvan-John M. Olin Medal: Honoring Annie Kersting**		D			
Young Investigators in Nuclear & Radiochemistry**			D	A	
Heavy-Element Inorganic Chemistry: A Tribute to Al Sattelberger**				D	A
General Topics in Nuclear & Radiochemistry					P
Adsorption of Metals by Geomedia* (GEOC)		P	D	DE	A
Frontiers in Heavy-Element Inorganic Chemistry* (INOR)		P	D		
Separations for the Nuclear Fuel Cycle in the 21st Century Revisited* (I&EC)			P	D	

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PROGRAM SUMMARY

Division of Organic Chemistry

ORGN

R. Broene, M. McIntosh, Program Chairs

San Diego Convention Center	S	M	Tu	W	Th
Peptides, Proteins & Amino Acids	A		E		
Nanomaterials	AE				
Biologically Related Molecules & Processes	D	A	E		
New Reactions & Methodology	D	D	D	AE	
Metal-Mediated Reactions & Syntheses	D		E		
Asymmetric Reactions & Syntheses	DE	A			
ACS Award for Creative Work in Synthetic Organic Chemistry: Honoring Scott J. Miller	P				
Lewis Base-Catalyzed Asymmetric Transformations	P				
Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species	E	D	A		
Total Synthesis of Complex Molecules	E		P	D	
Flow Chemistry & Continuous Processes	E			P	
Materials, Devices & Switches	E			P	
Chemistry & Computers	E				
Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Honoring Phil S. Baran		A			
ACS Award for Affordable Green Chemistry: Honoring Martin D. Johnson, Joseph R. Martinelli & Shannon S. Stahl		A			
Molecular Recognition & Self-Assembly		P	DE		
Ernest Guenther Award in the Chemistry of Natural Products: Honoring Eric Block		P			
Frontiers in Molecular Recognition		P			
Green Chemistry: Enhancing Organic Synthesis in Pharma		P			
Sci-Mix		E			
ACS Award for Research at an Undergraduate Institution: Honoring Thomas E. Goodwin			A		
Josef Michl ACS Award in Photochemistry: Honoring Frederick D. Lewis			A		
Chemical Methods To Investigate Protein Posttranslational Modifications			D		
Herbert C. Brown Award for Creative Research in Synthetic Methods: Honoring Alois Fürstner			P		

Division of Organic Chemistry  
(continued)

ORGN

R. Broene, M. McIntosh, Program Chairs

San Diego Convention Center	S	M	Tu	W	Th
James Bryant Conant Award in High School Chemistry Teaching: Honoring Julia Winter** <sup>cc</sup>			P		
Chemistry of Fullerenes, Carbon Nanotubes & Graphene				A	
Gabor A. Somorjai Award for Creative Research in Catalysis: Honoring Donna G. Blackmond**				A	
Supramolecular Chemistry**				D	
Heterocycles & Aromatics				DE	
Ralph F. Hirschmann Award in Peptide Chemistry: Honoring Ronald T. Raines				P	
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Start-up Businesses in Drug Discovery* (SCHB)		A			
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Earle B. Barnes Award for Leadership in Chemical Research Management: Honoring Henry E. Bryndza* (INOR)		P	A		
Computers in Chemistry: Bridging the Gap between Clients & Software* (SCHB)		P			
LGBT Chemists' Symposium on Chemical Biology* (PROF)		P			
Diversity-Quantification-Success?* (PRES)		P			
Cannabis: Exploring the Chemistry, History & Future* (SCHB)			A		
Driving Change: Impact of Funders on the Research Data & Publications Landscape* (CINF)			D		
Supramolecular Chemistry: A Crown & Anchor Approach* (INOR)			DE		
Computational Materials & Nanoscience: Theory Meets Experiment* (MPPG)				D	D

# PROGRAM SUMMARY

## Division of Physical Chemistry

# PHYS

*G. Engel, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Decoding the Spectroscopic Signatures of Large-Amplitude Motions: Challenges & Opportunities for Theory & Experiment <b>cc</b>	D	A		D	D
Toward Predictive Calculations in Strongly Correlated Molecules & Materials <b>cc</b>	D	D	A	A	D
Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory**	D	D	A	A	
Computer Simulations of Thermodynamics & Long time Kinetics of Molecular Events <b>cc</b>	D	D	A	D	D
Frontiers in Solar Light-Harvesting Processes	D	D	A	D	D
Physical Chemistry of Complex Environmental Interfaces**	D	D	A	P	D
Electrochemistry at Solid-Liquid Interfaces	D	D	A		
Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials		D	A	D	A
Physical Principles in Functional Nanoscience: Honoring Mostafa A. El-Sayed		P	A	D	D
Sci-Mix		E			
PHYS Division National Awards Symposium			P		
Electronic Structure & Dynamics of Metastable States <b>cc</b>				D	D
Poster Session				E	
Multiscales Chemistry* (MPPG)	D	D	D	P	
From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules* (COMP)	D	D		D	
Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications* (COMP)	D	D			
Global Initiatives in Research Data Management & Discovery* (CINF)	P	D			
Discussions with the President's Task Force on Employment* (PRES)	P				
E. Bright Wilson Award in Spectroscopy: Honoring Robert G. Griffin* (BIOL)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				

## Division of Physical Chemistry (continued)

# PHYS

*G. Engel, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Advances in Chemical Imaging: Ultra-Resolution to Single Molecules* (SOCED)		A			
Protein Structure & Folding: From Solution to the Gas Phase* (ANYL)		D			
Preparing for the Real World: Challenges Faced by Young Investigators* (MPPG)		D			
Elucidation of Mechanisms & Kinetics on Surfaces* (CATL)		P	D	D	D
Nonlinear Spectroscopy & Modeling* (ANYL)		P			
Diversity-Quantification-Success* (PRES)		P			
Computational Design of Advanced Materials* (COMSCI)			A		
Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Honoring Albert J. R. Heck* (ANYL)			A		
Computer-Aided Drug Design* (MPPG)			D	D	A
Quantum Mechanics* (COMP)			D	D	D
The History of Chemistry & Computing* (MPPG)				A	
Big Data Science* (MPPG)					D

## Division of Polymer Chemistry

# POLY

*M. Jeffries-El, T. White, C. Lipscomb, Program Chairs*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
General Topics: New Synthesis & Characterization of Polymers	A	A	AE	P	A
Polymer Applications & Characterization in Medical Devices Industry	A	A			
Responsive Nanostructures & Nanocomposites	D	D	AE	A	
Sustainable Polymers, Processes & Applications**	D	D	AE		
Applications of Polymer Surfaces & Interfaces**	D	P	DE	D	A
Polymer Additive Manufacturing: Materials, Processes & Simulation	D				
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Scott D. Allen, Geoffrey W. Coates & Anthony R. Eisenhut**	D				

PROGRAM SUMMARY

**Division of Polymer Chemistry  
(continued)**

POLY

*M. Jeffries-El, T. White, C. Lipscomb, Program Chairs*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Industrial Research at the Interface of Inorganic Chemistry & Polymer Science**	P		E		
Paul J. Flory Polymer Education Award: Honoring Kenneth B. Wagener	P				
Frederic Stanley Kipping Award in Silicon Chemistry: Honoring Michael A. Brook**		A			
Excellence in Graduate Polymer Research**	D	DE			
ACS Award in Polymer Chemistry: Honoring Edmund M. Carnahan	D				
Supramolecular Polymers: From Structure to Advanced Functionality		P	DE	D	A
Industrial Innovation in Polymer Chemistry: Sustainable Polymerization Feedstocks & Process Technology**		P			
Sci-Mix		E			
Undergraduate Research in Polymer Science			DE		
Anionic Polymerization: Still Living After 60 Years**			PE	D	A
Click Reactions for Producing Advanced Materials			PE	D	A
13th International Symposium on Biorelated Polymers			PE	D	A
Controlled Depolymerization				D	
POLY/PMSE Plenary Lecture & Awards Reception**				E	
New Horizons in Sustainable Materials* (CELL)	D	D			
Biomass & Polymer Extrusion, Composite & Reaction Technologies: New Insights, Future Potential & Principles to Practice* (CELL)	D				
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
ACS Award for Creative Invention: Honoring Antonio Facchetti* (PMSE)		D	D		

**Division of Polymer Chemistry  
(continued)**

POLY

*M. Jeffries-El, T. White, C. Lipscomb, Program Chairs*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
ACS Award in Applied Polymer Science: Honoring Thomas P. Russell* (PMSE)		D			
Earle B. Barnes Award for Leadership in Chemical Research Management: Honoring Henry E. Bryndza* (INOR)		P	A		
Undergraduate Research Posters* (CHED)		P			
Diversity-Quantification-Success?* (PRES)		P			
Potpourri of Polymer Projects: Take a Byte out of the NGSS* (CHED)		E			
ACS Award in Industrial Chemistry: Honoring Ted C. Germroth* (I&EC)			A		
Computational Materials & Nanoscience: Theory Meets Experiment* (MPPG)				D	D

**Division of Polymeric Materials:  
Science & Engineering**

PMSE

*A. Tsou, B. Olsen, C. Stafford, X. Jia, C. Soles, Program Chairs*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Directed Polymer Assembly	D	A			
Flow-Induced Crystallization of Polymers	D	A			
Clay/Polymer Composites: Nanoclays & Other Natural Nanoparticles	D	D	A		
Bioresponsive & Biomimetic Synthetic Polymers & Materials	D	D			
Dynamic & Tunable Biomaterials	D	D			
James V. Crivello Memorial Symposium	D				
ACS Award for Creative Invention: Honoring Antonio Facchetti**		D	D		
ACS Award in Applied Polymer Science: Honoring Thomas P. Russell**		D			
Hybrid Polymers & Nanocomposites		P	D	D	A
General Papers/New Concepts in Polymeric Materials		P	P	D	A
Sci-Mix		E			
Cooperative Research Award: Honoring Brian Benicewicz & Gordon Calundann			A		
Polymer-Related Energy Conversion & Storage			D	D	A
Polyethylene**			D	D	
Computation & Cheminformatics in Polymers Research			P	D	A

## PROGRAM SUMMARY

### Division of Polymeric Materials: Science & Engineering (continued)

PMSE

*A. Tsou, B. Olsen, C. Stafford, X. Jia, C. Soles, Program Chairs*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Joint PMSE/POLY Poster Session			E		
Sustainable Polymers, Processes & Applications* (POLY)	D	D	AE		
Applications of Polymer Surfaces & Interfaces* (POLY)	D	P	DE	D	A
Biomass & Polymer Extrusion, Composite & Reaction Technologies: New Insights, Future Potential & Principles to Practice* (CELL)	D				
Discussions with the President's Task Force on Employment* (PRES)	P				
My Comments to the President's Task Force on Employment* (PRES)	E				
Frederic Stanley Kipping Award in Silicon Chemistry: Honoring Michael A. Brook* (POLY)		A			
WCC 2016 Rising Stars Awards Symposium* (WCC)		D			
Undergraduate Research Posters* (CHED)		P			
Potpourri of Polymer Projects: Take a Byte out of the NGSS* (CHED)		E			
Anionic Polymerization: Still Living After 60 Years* (POLY)			PE	D	A
POLY/PMSE Plenary Lecture & Awards Reception* (POLY)				E	

### Division of Professional Relations (continued)

PROF

*R. D. Libby, Program Chair*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
My Experiences in & Advice for Organic Chemistry Courses* (PRES)	E				
How To Foster Diversity in the Chemical Sciences: Lessons Learned & Taught from the Stories of Recipients of the Stanley C. Israel Award* (PRES)		A			
Is There a Crisis in Organic Chemistry Education?* (PRES)		A			
Excellence in Graduate Polymer Research* (POLY)		D	DE		
GSSPC: Resolving the Big Picture: Bringing Molecules into Focus* (CHED)		D			
Diversity-Quantification-Success?* (PRES)		P			

### Division of Professional Relations

PROF

*R. D. Libby, Program Chair*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Ethics 101**	A				
Enough to be Dangerous: A Chemist's Handbook to Cross-Functional Development**	P				
Women in Innovation: Science & Technology**		A			
LGBT Chemists' Symposium on Chemical Biology**		P			
Successful REU Programs**			A		
Chemical Angel Network**			P		
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Scott D. Allen, Geoffrey W. Coates & Anthony R. Eisenhut* (POLY)	D				

### Rubber Division

RUBB

*T. DeLapa, Program Chair*

Located with Primary Sponsor	S	M	Tu	W	Th
Potpourri of Polymer Projects: Take a Byte out of the NGSS* (CHED)		E			
Anionic Polymerization: Still Living After 60 Years* (POLY)			PE	D	A

\*Cospponsored symposium with primary organizer shown in parentheses; located with primary organizer.

\*\*Primary organizer of a cospponsored symposium.

CC = Computers in Chemistry  
 A = AM AE = AM/EVE P = PM D = AM/PM  
 E = EVE DE = AM/PM/EVE PE = PM/EVE

# PROGRAM SUMMARY

## Division of Small Chemical Businesses

### SCHB

*J. Sabol, Program Chair*

Marriott Marquis San Diego Marina	S	M	Tu	W	Th
Entrepreneurs' Poster Session		A			
Start-up Businesses in Drug Discovery**		A			
Computers in Chemistry: Bridging the Gap between Clients & Software** <small>cc</small>		P			
Sci-Mix		E			
Cannabis: Exploring the Chemistry, History & Future**			A		
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Scott D. Allen, Geoffrey W. Coates & Anthony R. Eisenhut* (POLY)	D				
Discussions with the President's Task Force on Employment* (PRES)	P				
My Comments to the President's Task Force on Employment* (PRES)	E				
Cannabis: Exploring the Chemistry, History & Future* (AGFD)			D		
Chemical Information for Small Businesses & Start-ups* (CINF)			P		
Chemical Angel Network* (PROF)				P	

## Committee on Science

### COMSCI

*M. Berman, Program Chair*

San Diego Convention Center	S	M	Tu	W	Th
Computational Design of Advanced Materials** <small>cc</small>		A			
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
Diversity-Quantification-Success?* (PRES)		P			

\*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

\*\*Primary organizer of a cosponsored symposium.

CC = Computers in Chemistry  
 A = AM AE = AM/EVE P = PM D = AM/PM  
 E = EVE DE = AM/PM/EVE PE = PM/EVE

## International Activities Committee

### I A C

*E. Contis, Program Chair*

Hilton San Diego Bayfront	S	M	Tu	W	Th
Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences**	D				
Eli Pearce Memorial Symposium			A		
Discussions with the President's Task Force on Employment* (PRES)	P				
My Comments to the President's Task Force on Employment* (PRES)	E				
International & Multicultural Perspective* (CHED)			P		

## Women Chemists Committee

### W C C

*K. Woznick, A. Debaillie, Program Chairs*

Hilton San Diego Bayfront / San Diego Convention Center	S	M	Tu	W	Th
WCC 2016 Rising Stars Awards Symposium**		D			
ACS Award for Encouraging Women into Careers in the Chemical Sciences: Honoring Carol A. Fierke**			A		
Catalysis at the Subnanometer Scale* (CATL)	D	A			
Computational Chemistry across Catalysis* (CATL)	D	D	D	A	
ACS Award in Organometallic Chemistry: Honoring Karen I. Goldberg* (INOR)	D	P			
Discussions with the President's Task Force on Employment* (PRES)	P				
My Experience with & Advice for Improving Diversity in Chemistry* (PRES)	E				
My Comments to the President's Task Force on Employment* (PRES)	E				
Women in Innovation: Science & Technology* (PROF)		A			
LGBT Chemists' Symposium on Chemical Biology* (PROF)		P			
Diversity-Quantification-Success?* (PRES)		P			
Polyethylene* (PMSE)			D	D	
Gabor A. Somorjai Award for Creative Research in Catalysis: Honoring Donna G. Blackmond* (ORGN)				A	



## PROGRAM SUMMARY

### Younger Chemists Committee

Y C C

*M. Druelinger, T. Matos, Program Chairs*

Hilton San Diego Bayfront	S	M	Tu	W	Th
Starting a Successful Research Program at a Predominantly Undergraduate Institution	P				
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment* (CHED)	D	A			
Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Enough to be Dangerous: A Chemist's Handbook to Cross-Functional Development* (PROF)	P				
Excellence in Graduate Polymer Research* (POLY)		D	DE		
Preparing for the Real World: Challenges Faced by Young Investigators* (MPPG)		D			
Young Investigators in Nuclear & Radiochemistry* (NUCL)			D	A	

## How to Read the Technical Program

**1.**  
**Search for the Division—**  
listed in alphabetical order

**ANYL**

### **Division of Analytical Chemistry**

*J. Harris and L. Baker, Program Chairs*

**Note:**

*Times represent the start of oral presentations and numbers represent poster numbers.*

**3.**  
**Locate the session name**

### **SUNDAY MORNING**

**2.**  
**Locate the day**

**4.**  
**Locate the time or poster #**

#### Section A

Wyndham San Diego Bayfront  
East Coast

#### **Luminescent Proteins, Dyes & Sensors**

*H. Ai, Organizer, Presiding*

**5.**  
**Locate the venue and room for each session**

**8:10 ANYL 1.** Radioisotope-responsive polystyrene-silica core-shell nanoparticles used in scintillation proximity assay for tritium. I. Calderon, C. Janczak,

## FULL TECHNICAL PROGRAM

**TWENTY-NINE OF THE SOCIETY'S** technical divisions and four committees are hosting original technical programming during the meeting. More than 12,000 papers have been accepted for this meeting.

Each organizing group's programming is detailed on the following pages.

Nearly 4,000 chemical professionals and students are expected to attend the ever-popular Sci-Mix Interdivisional Poster Session & Mixer on Monday,

March 14 from 8:00 to 10:00 PM at the San Diego Convention Center, Halls D/E. More than 500 noteworthy poster presentations, networking with colleagues, and light refreshments make up this enjoyable event.

Organizing Group	Acronym	Page
<b>PRESIDENTIAL &amp; CROSS-DIVISION PROGRAMMING</b>		
Presidential Events	PRES	TECH-76
Multidisciplinary Program Planning Group	MPPG	TECH-77

### DIVISION PROGRAMMING

Agricultural & Food Chemistry	AGFD	TECH-81
Agrochemicals	AGRO	TECH-85
Analytical Chemistry	ANYL	TECH-85
Biochemical Technology	BIOT	TECH-91
Biological Chemistry	BIOL	TECH-102
Business Development & Management	BMGT	TECH-106
Carbohydrate Chemistry	CARB	TECH-107
Catalysis Science and Technology	CATL	TECH-109
Cellulose & Renewable Materials	CELL	TECH-118
Chemical Education	CHED	TECH-125
Chemical Health & Safety	CHAS	TECH-154
Chemical Information	CINF	TECH-155
Chemistry & the Law	CHAL	TECH-158
Colloid & Surface Chemistry	COLL	TECH-159
Computers in Chemistry	COMP	TECH-177
Energy & Fuels	ENFL	TECH-183
Environmental Chemistry	ENVR	TECH-191
Fluorine Chemistry	FLUO	TECH-203
Geochemistry	GEOC	TECH-204
History of Chemistry	HIST	TECH-209
Industrial & Engineering Chemistry	I&EC	TECH-209
Inorganic Chemistry	INOR	TECH-213

Organizing Group	Acronym	Page
Medicinal Chemistry	MEDI	TECH-236
Nuclear Chemistry & Technology	NUCL	TECH-243
Organic Chemistry	ORGN	TECH-246
Physical Chemistry	PHYS	TECH-258
Polymer Chemistry	POLY	TECH-270
Polymeric Materials Science & Engineering	PMSE	TECH-282
Professional Relations	PROF	TECH-293
Rubber	RUBB	TECH-294
Small Chemical Businesses	SCHB	TECH-294

### COMMITTEE PROGRAMMING (In order of appearance)

Committee on Chemical Safety	CCS	TECH-295
Committee on Community Activities	CCA	TECH-295
Committee on Divisional Activities	DAC	TECH-295
Committee on Environmental Improvement	CEI	TECH-296
Committee on Ethics	ETHC	TECH-296
Committee on Local Section Activities	LSAC	TECH-296
Committee on Minority Affairs	CMA	TECH-296
Committee on Patents and Related Matters	CPRM	TECH-297
Committee on Science	COMSCI	TECH-297
Committee on Technician Affairs	CTA	TECH-297
International Activities Committee	IAC	TECH-297
Society Committee on Education	SOCED	TECH-298
Women Chemists Committee	WCC	TECH-299
Younger Chemists Committee	YCC	TECH-300

## PRES

## Presidential Events

D. Nelson and D. Crans, *Program Chairs*

## BUSINESS MEETINGS:

Poster Session on Employment, Diversity & Organic Chemistry Education, 8:00 PM: Sun

## SUNDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 2

## Discussions with the President's Task Force on Employment

Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

D. Nelson, *Organizer, Presiding*D. Crans, *Organizer*A. E. Pavlath, *Presiding*

1:30 PRES 1. Purpose of Task Force and future plans. D. Nelson, A. Pavlath

1:45 PRES 2. Evolving nature of supply and demand factors in the chemical workforce. T. Hoerter, B. Balazs

2:00 PRES 3. It's not in the job title. Realities of the chemical industries: Career opportunities for undergraduate professionals. M. Engelman, S.B. Butts

2:15 PRES 4. Can professional certificates enhance your career opportunities? Case studies and lessons learned. A. Campbell, P. Jagodzinski

2:30 PRES 5. Do we prepare our graduates for the jobs offered by industry? K. Haider, D. Crans

2:45 PRES 6. Addressing the challenges of unemployment of young graduates and mid-career chemical professionals. P. Dorhout, W. Ewing

3:00 PRES 7. Global factors influencing employment in the U.S. W. Jones, M. Wu

3:15 Panel Discussion.

## SUNDAY EVENING

## Section A

San Diego Convention Center  
Hall D

## My Comments to the President's Task Force on Employment

Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

D. Nelson, D. Crans, *Organizers*

8:00 - 10:00

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:

[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

PRES 8. What factors determine the balance between supply and demand? D. Nelson, A. Pavlath

PRES 9. What is the employment situation for technicians? M. Engelman, S. Butts, D. Nelson, A. Pavlath

PRES 10. What are the benefits and handicaps of possible certification, licensing, and registration of chemical professionals? A. Campbell, P. Jagodzinski, D. Nelson, A. Pavlath

PRES 11. Do we prepare our graduates for jobs offered by industry? D. Crans, K. Haider, D. Nelson, A. Pavlath

PRES 12. What causes unemployment among young graduate and mid-career chemical professionals, and how can we help? P. Dorhout, W. Ewing, D. Nelson, A. Pavlath

PRES 13. What is needed to increase under-represented groups in the workforce? D. Nelson, A. Pavlath

PRES 14. What global factors influence the U.S. employment situation, and how do outsourcing and immigration contribute to this situation? M. Wu, W. Jones, D. Nelson, A. Pavlath

PRES 15. AGFD Division of Agricultural and Food Chemistry: Opportunities and advances in future chemistry. M. Appell, B. Park

PRES 16. SCHB experience helps you meet the challenges of employment in the chemical sciences sector. J. Maclachlan, A. Rahman, J. Sabol, M. Chorghade

PRES 17. Who are COMP members and where have they gone? Demographics and national meeting attendance. E. Esposito

PRES 18. Women Chemists Committee (WCC) efforts to support chemists in the workforce. K. Wozniak, A. Charlebois, L. Sremaniak, A. Nicely, C. Chow, A. Debaille, M. Rogers, M. Shultz, L. Kemp

PRES 19. Chemical Innovation and Entrepreneurship Council (CIEC): Working to enhance and highlight the impact of women in STEM worldwide. J. Bryant, J. Giordan, E. Nalley, J. Maclachlan, L. Kemp, N. LaFranzo

PRES 20. Help me get a job: the Portland Section's approach to helping new graduates and working chemists find employment in chemistry. J. Tung, M. Mackiewicz

PRES 21. Perspectives on the landscape of chemistry-related employment in the ACS Puget Sound Section. G.D. Christian, C. Fryhle, G. Milligan, M. Wicholas

PRES 22. Welcoming work environments and broadening participation for LGBTQ+ Chemists. B. Belmont, M. Crawford

PRES 23. Current career challenges in the chemical sciences- A younger chemist's perspective. W. Lawal

PRES 24. How do changes in public higher education affect career opportunities in chemistry? M. Philipp

PRES 25. Benefits of two-year institutions for employment and employers. F. Wood-Black

PRES 26. Focus on career preparation within the requirements of the ACS Certified Bachelor's Degree in Chemistry. T. Wenzel, L. Kosbar

PRES 27. Professional master program in chemistry and biochemistry technology as a tool to improve professional qualification. D. Petri

PRES 28. Increasing unemployment among Ph.D. graduates: A problem to solve or a solution to problem? S. Kostina

PRES 29. Finding your way in computational electronic structure. R. Magyar

PRES 30. Branching out from the central science. L. Schultz, M. McAfee

PRES 31. Promoting STEM disciplines in industry through hands-on applications using the biochemical excellence in science and technology (BEST) NSF grant at Milwaukee Area Technical College (MATC). S. Schlipp

PRES 32. New reality of the chemical enterprise: Traditional and non-traditional career paths. M.K. Engelman, E. Rosenberg

PRES 33. Innovation ecosystems: Technology-based economic development and workforce development. J. Curtis

PRES 34. Demand, regulation, and experience: The hindrance factors involved in American industry employment. J. Pischek, M. Reichert, L. Yet

PRES 35. Recognition of- and adaptation to- the changing career landscape for chemists. M. Windsor

PRES 36. Inside track on getting a better return on your job search investment. J. Stinson

PRES 38. Engaging the global chemistry community through partnerships and opportunity. C. LaPrade, L. Brown

PRES 39. Solving humanitarian problems leads to innovations and jobs. S. Ahuja

PRES 40. Global factors and trends influencing U.S. employment, outsourcing, and immigration as related to the science industry. N. Maceda-Johnson, N. Ledra, J. Corwin, T. McCaffrey

PRES 41. Education and employment of chemists in Germany- activities of the Gesellschaft Deutscher Chemiker (German Chemical Society, GDCh). H. Weinig, K. Schmitz

## Section B

San Diego Convention Center  
Hall D

## My Experience with &amp; Advice for Improving Diversity in Chemistry

Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

D. Nelson, D. Crans, *Organizers*

8:00 - 10:00

PRES 42. Social networking and other 21st century tools to promote the diverse job seeker in an all inclusive chemical industry. C. Supalo

PRES 43. Text-to-speech enabled organic chemistry drawing tool opens new opportunities for the blind in chemistry. C. Supalo

PRES 44. Minority student pipeline math science partnership: Recruiting under-represented minorities into science fields. D. Morgan

## Section C

San Diego Convention Center  
Hall D

## My Experiences in &amp; Advice for Organic Chemistry Courses

Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

D. Nelson, D. Crans, *Organizers*

8:00 - 10:00

PRES 45. A new milestone in chemical education at the secondary level. A. Rahman

PRES 46. Learner-centered approach to teaching undergraduate organic chemistry. A. Brown

PRES 47. Advancing graduate education in the chemical sciences with a modular curriculum. R. Halterman, M.T. Ashby

PRES 48. Identifying areas of need for the learning of organic chemistry in prerequisite classes. O. Kinney, D. Crans

PRES 49. Organic chemistry, life, the universe &amp; everything (OCLUE). M. Cooper, M. Klymkowsky

## MONDAY MORNING

## Section A

San Diego Convention Center  
Room 3

## Is There a Crisis in Organic Chemistry Education?

Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

D. Nelson, *Organizer, Presiding*D. Crans, *Organizer*M. Cooper, *Presiding*

9:00 PRES 50. Introduction: Evaluating organic chemistry textbooks. D. Nelson

9:15 PRES 51. Cengage: Is the organic chemistry course changing in reaction to the new MCAT? M. Rosener

9:30 PRES 52. Elsevier: Is there a crisis in organic chemistry education? K. Birtcher

9:45 PRES 53. McGraw-Hill: Adapting to the modern organic chemistry student. A. Pellerito

10:00 PRES 54. Macmillan: How can a publisher partner with and support faculty in times of curriculum change in organic chemistry. L. Schultz

10:15 PRES 55. Pearson: Future of teaching organic chemistry. J. Zalesky

10:30 PRES 56. Wiley: How will/does technology change the classroom. S. Hickey

10:45 Remarks and Structure - D. Nelson

10:50 Panel Discussion.

## Section B

San Diego Convention Center  
Room 5A

## How to Foster Diversity in the Chemical Sciences: Lessons Learned &amp; Taught from the Stories of Recipients of the Stanley C. Israel Award

Cosponsored by CMA and PROF

K. Bagga, C. Hobbs, *Organizers, Presiding*

8:30 Introductory Remarks by M. Jacobs and S. Israel.

8:40 PRES 57. Diversifying the STEM professional workforce by building capacity at a two-year college on the U.S.-Mexico border. D. Brown

9:00 PRES 58. Wanted! Diverse STEM professionals seek like-minded mentors, coaches, sponsors and advocates. G. Thomas

9:20 PRES 59. Diversity efforts: University of California Berkeley and other. W. Lester

9:40 PRES 60. Making education and careers in chemistry accessible and successful for deaf and hard-of-hearing students. T. Pagano

10:00 Intermission.

**10:15 PRES 61.** Instituting research at the community college level: Strategies that will secure the success of minority STEM students at the post-undergraduate level. P. Svoronos

**10:35 PRES 62.** Increasing diversity in the chemical sciences: Lessons learned. L. Colon

**10:55 PRES 63.** Empowering effect of leadership roles in undergraduate education. P. Varma-Nelson

**11:15 PRES 64.** Taking charge of the lack of diversity in STEM from graduate school to the professoriate: Developing a national, non-profit organization. C. Valdez, S.A. Lopez

**11:35** Questions and Discussion.

### New Reality of the Chemical Enterprise: Traditional & Non-traditional Career Paths

#### Chemistry Professionals Working "Outside the Box"

Sponsored by I&EC, Cosponsored by CTA, PRES and SOCED

#### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

## MONDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 3

#### Diversity-Quantification-Success?

Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

D. Nelson, D. Crans, *Organizers*

E. Nalley, *Presiding*

**1:30 PRES 65.** Introduction: Diversity strengthening STEM education. E. Nalley, D. Nelson

**1:45 PRES 66.** A decade of tracking demographics in the Top 50 Chemistry Departments via the Nelson Diversity Surveys. D. Nelson

**2:00 PRES 67.** Accelerating change: #DiversitySolutions on social media. D. Stallings, R. Hernandez

**2:15 PRES 68.** Progress made in smashing the glass ceiling. V. Kuck

**2:30 PRES 69.** Critical mass takes courage: Diversity in the chemical sciences. S. Collins

**2:45 PRES 70.** The challenges facing women in chemistry and other scientific and engineering fields. M. Jacobs

**3:00 PRES 71.** Demographics of research-active chemistry departments. R. Hernandez, D. Stallings, S. Iyer

**3:15** Panel Discussion.

### New Reality of the Chemical Enterprise: Traditional & Non-traditional Career Paths

#### Chemistry Professionals Working "Outside the Box"

Sponsored by I&EC, Cosponsored by CTA, PRES and SOCED

#### LGBT Chemists' Symposium on Chemical Biology

Sponsored by PROF, Cosponsored by BIOL‡, BIOT‡, MEDI, ORGN, PRES and WCC

### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

## MONDAY EVENING

### Section A

San Diego Convention Center  
Hall D/E

#### Sci-Mix

D. Nelson, D. Crans, *Organizers*

**8:00 - 10:00**

8-14, 16-20, 24-31, 34, 36, 38, 40, 42-49.  
See previous listings.

## TUESDAY MORNING

### Section A

San Diego Convention Center  
Room 2

#### Dreyfus Award Symposium

M. Cardillo, *Organizer*

L. Brus, M. Fox, *Presiding*

**9:00** Introductory Remarks by 2016 ACS President D. Nelson.

**9:10 PRES 72.** Innovating with evolution: Expanding the enzyme universe to make molecules and materials. F. Arnold

**9:45 PRES 73.** Instead of 2D-printing over and over again: Continuous liquid interface production of 3D objects. J. Desimone

**10:20** Intermission.

**10:35 PRES 74.** Making materials with programmable nucleic acid bonds. C. Mirkin

**11:10 PRES 75.** Science and technology of quantum dots. M. Bawendi

### New Reality of the Chemical Enterprise: Traditional & Non-traditional Career Paths

#### Chemistry Professionals Working in the Government

Sponsored by I&EC, Cosponsored by CTA, PRES and SOCED

#### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

## TUESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 2

#### Dreyfus Award Symposium

M. Cardillo, *Organizer*

M. Tirrell, R. Zare, *Presiding*

**2:00 PRES 76.** Development of new C-H bond functionalization reactions. M. Sanford

**2:35 PRES 77.** Non-canonical amino acids as tools for protein medicinal chemistry. D. Tirrell, K. Fang, S. Lieblich

**3:10** Intermission.

**3:25 PRES 78.** Combining facile synthetic strategies and simple purification techniques for the preparation of unique materials. C. Hawker

**4:00 PRES 79.** From molecules to materials: Macromolecular engineering by taming free radicals. K. Matyjaszewski

### New Reality of the Chemical Enterprise: Traditional & Non-traditional Career Paths

#### Chemistry Professionals are Entrepreneurs & More

Sponsored by I&EC, Cosponsored by CTA‡, PRES and SOCED

#### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

## TUESDAY EVENING

### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

## MPPG

### Multidisciplinary Program Planning Group

K. Merz, *Program Chair*

#### SOCIAL EVENTS:

**Reception, 3:30 PM:** Sat

#### BUSINESS MEETINGS:

**MPPG Business Meeting, 2:30 PM:** Sat

## SUNDAY MORNING

### Section A

San Diego Convention Center  
Room 3

#### Multiscales Chemistry

#### Energy

Cosponsored by ANYL, BIOL, COMP and PHYS

S. Hammes-Schiffer, R. Hernandez, *Organizers*  
L. Gagliardi, *Presiding*

**8:30 MPPG 1.** Bottom-up excitonics. A. Aspuru-Guzik

**9:00 MPPG 2.** Modeling hybrid photovoltaic cells: Insights from density functional theory. I. Ciofini

**9:30 MPPG 3.** Excited-state electron transfer in fluorescent proteins. A. Krylov

**10:00** Intermission: Café con Ordenadores.

**10:30 MPPG 4.** Structure-function relationship in materials for energy: Coupling molecular dynamics and first principles spectroscopies. G. Galli

**11:00 MPPG 5.** Multiple time step schemes for first-principles based multiscale simulations. U. Roethlisberger

**11:30 MPPG 6.** Employing simulation and experiment to evaluate and predict chemical stability of metal-organic frameworks. N. Burch, K. Walton

#### Fall 2015 InterCollegiate Cheminformatics Course

Sponsored by CHED, Cosponsored by CINF and MPPG

### Analytical & Computational Isotope Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and MPPG‡

## SUNDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 3

#### Multiscales Chemistry

#### Mini-Platform

Cosponsored by BIOL, COMP and PHYS

S. Hammes-Schiffer, R. Hernandez, *Organizers*

Q. Cui, *Presiding*

**1:00 MPPG 7.** Challenges in the computational modeling of catalysis for energy related applications. L. Gagliardi

**1:30 MPPG 8.** Osmolyte-mediated regulation of peptide structure. J. Shea

**2:00 MPPG 9.** Impact of coarse-graining upon information content and thermodynamic properties. W. Noid

### Section D

San Diego Convention Center  
Room 20A-C

#### Computers in Chemistry Plenary Session

K. Merz, *Organizer, Presiding*

**3:00 MPPG 10.** Using self-assembly to make functional materials: Computational perspectives. G. Schatz

**3:40 MPPG 11.** Proton-coupled electron transfer in catalysis and energy conversion. S. Hammes-Schiffer

**4:20 MPPG 12.** Post-evolutionary biology: Design of novel protein structures, functions and assemblies. D. Baker

**5:00 MPPG 13.** 30 years of free energy perturbation theory: From free energies of hydration to drug discovery. W. Jorgensen

#### Current Topics in Chemical Business Development & Management

Sponsored by BMGT, Cosponsored by MPPG‡

#### Environmental Interfaces

#### Surface Structures

Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡

#### Fall 2015 InterCollegiate Cheminformatics Course

Sponsored by CHED, Cosponsored by CINF and MPPG

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### Analytical & Computational Isotope Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and MPPG‡

### Molecular Modeling at the Undergraduate Level

Sponsored by CHED, Cosponsored by MPPG

## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 2

#### Multiscales Chemistry

##### Bio

Cosponsored by BIOL, COMP and PHYS

S. Hammes-Schiffer, R. Hernandez, *Organizers*

J. Shea, *Presiding*

**8:30 MPPG 15.** Experimentally-biased modelling of protein folding intermediates at high pressures. **A. Garcia**, M. Fossat, J. Roche, C. Roumestand, D. Barrick, C. Royer

**9:00 MPPG 16.** Protein folding and recognition in the cell — an in silico approach. **M. Cheung**

**9:30 MPPG 17.** Structure and dynamics of intrinsically disordered proteins from a physics-based model. **J. Mittal**

**10:00** Intermission: Café con Ordenadores.

**10:30 MPPG 18.** Probing the principles of amyloid protein aggregation. **J. Straub**, A. Panahi, L. Dominguez

**11:00 MPPG 19.** Molecular simulations of alternate frame folding in an engineered Ca<sup>2+</sup>-sensing protein switch. **A. DeGrave**, J. Ha, S. Loh, L. Chong

**11:30 MPPG 20.** Computational design of peptide therapeutics. **Y. Lin**

### Section B

San Diego Convention Center  
Room 4

#### Preparing for the Real World: Challenges Faced by Young Investigators

#### Choosing Grad Research Advisors & a Career in Academia or Industry

Cosponsored by CHED, CINP, COMP, PHYS and YCC

W. Kellett, B. Levine, K. Merz, *Organizers*

S. Riniker, D. Zgid, *Organizers, Presiding*

**8:30 MPPG 21.** Choosing your research adviser wisely. **T. Crawford**

**8:45 MPPG 22.** How to choose an academic advisor: Do's and don'ts. **A. Krylov**

**9:00 MPPG 23.** Do what you like, like what you do: Navigating the academic world after college. **F. Paesani**

**9:15 MPPG 24.** Finding advisors whose research you like the best. **T. Shiozaki**

**9:30** Panel Discussion: Choosing a Graduate and Postgraduate Advisor.

**10:00** Intermission: Café con Ordenadores.

**10:30 MPPG 25.** Research career in industry: A glass filled with life. **C. Bayly**

**10:45 MPPG 26.** Finding the perfect job: Careers for organic chemists in pharma and academia. **A. Dounay**

**11:00 MPPG 27.** From academia, to startup, to big pharma, and back again? **G. Landrum**

**11:15 MPPG 28.** Down the rabbit hole: From B3LYP to x86. **J. Hammond**

**11:30** Panel Discussion: Choosing between Careers in Academia vs. Industry.

### Environmental Interfaces

#### Redox Reactions

Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡

#### GSSPC: Resolving the Big Picture: Bringing Molecules into Focus

Sponsored by CHED, Cosponsored by ANYL‡, MPPG and PROF‡

## MONDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 2

#### Multiscales Chemistry

##### Mini-Platform

Cosponsored by BIOL, COMP and PHYS

S. Hammes-Schiffer, R. Hernandez, *Organizers*

W. Noid, *Presiding*

**1:00 MPPG 29.** Molecular simulation analysis of nanoparticle-biomolecule interactions: Challenges and developments. **Q. Cui**

**1:30 MPPG 30.** Coarse-graining solvent structure using stochastic hard collision (SHC) dynamics. **R. Hernandez**

**2:00 MPPG 31.** Polarizable force fields for condensed phase simulation. **T. Head-Gordon**

### Section B

San Diego Convention Center  
Room 4

#### Preparing for the Real World: Challenges Faced by Young Investigators

##### Research at PUI's

Cosponsored by CHED, CINP, COMP, PHYS and YCC

W. Kellett, K. Merz, S. Riniker, D. Zgid, *Organizers*

B. Levine, *Organizer, Presiding*

**1:00 MPPG 32.** Doing theory with undergraduates and having a great time. **R. Cave**

**1:15 MPPG 33.** Building an undergraduate research program at a large, comprehensive university. **M. Milletti**

**1:30 MPPG 34.** Running a productive lab where students are transformed and you actually publish. **G. Shields**

**1:45 MPPG 35.** Building a new research program in medicinal chemistry at a small liberal arts college. **A. Dounay**

**2:00** Panel Discussion: Building a Research Program at a Primarily Undergraduate Institution.

### Section C

San Diego Convention Center  
Room 5A

#### Computers in Nanoscience & Nanotechnology

H. Tierney, *Organizer*

P. Alivisatos, P. S. Weiss, *Organizers, Presiding*

**1:00 MPPG 36.** Thermodynamics of virus capsid assembly. **K.M. Merz**

**1:30 MPPG 37.** Polymers for microelectronics: A view of the future. **C.G. Willson**

**2:00 MPPG 38.** Electron transport across the Van der Waals interfaces. **P. Kim**

**2:30** Intermission.

**2:40 MPPG 39.** Fractal arrangement of atomic structures in metallic glasses. **D. Chen**, C. Shi, Q. An, Q. Zeng, W. Mao, W. Goddard, **J. Greer**

**3:10 MPPG 40.** New approaches to multimodal nanoscale imaging and analyses. **P.S. Weiss**

### Section D

San Diego Convention Center  
Room 20A-C

#### The Kavli Foundation Emerging Leader in Chemistry Lecture

D. Nelson, *Organizer, Presiding*

**4:00** Introductory Remarks.

**4:05 MPPG 41.** Computing cures: Enabling chemical discovery through the lens of a computational microscope. **R. Amaro**

**4:55** Q & A.

### Section D

San Diego Convention Center  
Room 20A-C

#### The Fred Kavli Innovations in Chemistry Lecture

D. Nelson, *Organizer, Presiding*

**5:15** Introductory Remarks.

**5:20 MPPG 42.** Quantum solutions for a sustainable energy future. **E. Carter**

**6:15** Q & A.

### Environmental Interfaces

#### Nucleation, Growth & Dissolution Processes

Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡

#### GSSPC: Resolving the Big Picture: Bringing Molecules into Focus

Sponsored by CHED, Cosponsored by ANYL‡, MPPG and PROF‡

#### Nonlinear Spectroscopy & Modeling

Sponsored by ANYL, Cosponsored by MPPG and PHYS

#### Adsorption of Metals by Geomechanical Theory & Modeling after Twenty Years

Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL

#### Communicating Chemistry Through Social Media

Sponsored by CHED, Cosponsored by MPPG

## TUESDAY MORNING

### Section A

San Diego Convention Center  
Room 3

#### Multiscales Chemistry

##### Soft Matter

Cosponsored by BIOL, COMP and PHYS

S. Hammes-Schiffer, R. Hernandez, *Organizers*

W. Noid, *Presiding*

**8:30 MPPG 43.** Multiscale characterization of macromolecular dynamics. **C. Clementi**

**9:00 MPPG 44.** Competitive adsorption of proteins on gold nanoparticles: A multiscale modeling study. **C. Hall**, Q. Shao

**9:30 MPPG 45.** Multiscale simulations for soft matter: Recent developments and applications. **K. Kremer**

**10:00** Intermission: Café con Ordenadores.

**10:30 MPPG 46.** Relative entropy information-theoretic approach to multiscale modeling. **M. Shell**

**11:00 MPPG 47.** Ultra-coarse-graining and its application to biomolecular complexes. **G. Voth**

**11:30 MPPG 48.** Novel secondary structure of biomimetic polymers enables extended two-dimensional assemblies. **S. Whitelam**

### Section B

San Diego Convention Center  
Room 4

#### Computer-Aided Drug Design

##### Free Energy Calculations

Cosponsored by BIOL, CINP, COMP, MEDI and PHYS

R. Amaro, M. Holloway, J. Jansen, *Organizers*

C. Christ, *Presiding*

**8:00 MPPG 49.** Binding affinity prediction from molecular simulations — a new standard method in structure-based drug design? **C. Christ**

**8:30 MPPG 50.** Improving and applying alchemical binding free energy calculations. **D. Mobley**

**9:00 MPPG 51.** Incorporating changes in protein-ligand hydration in free energy calculations. **J. Essex**, G. Ross

**9:40 MPPG 52.** Real-world impact of free energy perturbation. **M. Murcko**

**10:20** Intermission: Café con Ordenadores.

**10:40 MPPG 53.** Attempts to improve free-energy simulation binding-affinity estimates by quantum-mechanical methods. **U. Ryde**

**11:20 MPPG 54.** Improving kinase inhibitor selectivity with free energy perturbation molecular dynamics simulations. **B. Roux**, Y. Meng

### Section C

San Diego Convention Center  
Room 5A

#### Computer-Aided Drug Design

##### Perspectives

Cosponsored by BIOL, CINP, COMP, MEDI and PHYS

R. Amaro, J. Jansen, *Organizers*

M. Holloway, *Organizer, Presiding*

C. Reynolds, *Presiding*

**8:20 MPPG 55.** Computer-aided drug design: Successes and opportunities. **M. Holloway**, C. Reynolds

**8:50 MPPG 56.** Cheminformatics: Past, present, future. **F. Brown**, H. Wang

**9:30 MPPG 57.** Docking and scoring: A perspective on exploiting protein structures for CADD. **A. Jain**

**10:10** Intermission: Café con Ordenadores.

**10:30 MPPG 58.** Current issues with computer-aided lead optimization. **W. Jorgensen**

**11:10 MPPG 59.** Computer-aided drug design: Looking forward. **C. Peishoff**

### Environmental Interfaces

#### Surface Adsorption

Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡

**Adsorption of Metals by Geomedia****Thermodynamics & Kinetics  
Experimental Study**

Sponsored by GEOC, Cosponsored  
by ENVR, MPPG‡ and NUCL

**Advances in E-Learning**

Sponsored by CHED, Cosponsored by MPPG

**TUESDAY AFTERNOON****Section A**

San Diego Convention Center  
Room 3

**Multiscales Chemistry****Liquids**

Cosponsored by BIOL, COMP and PHYS

S. Hammes-Schiffer, R. Hernandez, *Organizers*

T. Head-Gordon, *Presiding*

**1:00 MPPG 60.** Molecular amplification in liquid crystals, from nanometer to millimeter length scales. J. De Pablo

**1:30 MPPG 61.** Multiscale modeling of condensed-phase systems: Insights and predictions from coarse-grained models. M. Guenza

**2:00 MPPG 62.** Stochastic simulations of liquid aerosol chemistry. F. Houle

**2:30** Intermission: Café con Ordenadores.

**3:00 MPPG 63.** Water-like anomalies in monatomic pair and anisotropic potentials that stabilize tetrahedral crystals. A. Bertolazzo, J. Lu, V. Molinero

**3:30 MPPG 64.** Many-body molecular dynamics: Towards chemically accurate molecular simulations from the gas to the condensed phase. F. Paesani

**4:00 MPPG 65.** Transferability challenges in atomistic and coarse grained biomolecular simulation. C. Peter

**Section B**

San Diego Convention Center  
Room 4

**The Centrality of Computing  
Across Chemistry**

M. Paley, *Organizer*

C. Bertozzi, *Organizer, Presiding*

**1:00 MPPG 66.** Modeling epoxidation of drug-like molecules with a deep machine learning network. S. Swamidass

**1:40 MPPG 67.** Promiscuity in enzyme-ligand complexation revealed at the atomistic level: Application to glutamate racemase. M. Spies

**2:20 MPPG 68.** Systematic computational and experimental investigation of lithium-ion transport mechanisms in polymer electrolytes. M. Webb, B. Savoie, N. Balsara, G. Coates, Z. Wang, T. Miller

**3:00 MPPG 69.** On the role of dynamics in understanding the properties of metal-organic frameworks. N. Lopez

**3:40 MPPG 70.** Compressing chemistry: Compressed sensing for vibrations, spectroscopy and wave function theory. A. Aspuru-Guzik

**Section C**

San Diego Convention Center  
Room 5A

**Computer-Aided Drug Design****Computational Biophysics**

Cosponsored by BIOL, CINF,  
COMP, MEDI and PHYS

R. Amaro, M. Holloway, J. Jansen, *Organizers*

V. Shanmugasundaram, *Presiding*

**1:00 MPPG 71.** Enthalpy good, entropy bad? What can we learn from protein-ligand binding thermodynamic signatures? D. Hepworth

**1:40 MPPG 72.** Plumbing the depths of entropy and enthalpy in molecular recognition. M. Gilson, A. Fenley, S. Kantonen, H. Muddana, M. Potter, S. Webb

**2:20 MPPG 73.** Ins and outs of binding: Why dynamic drug-target occupancy relationships matter in the *in vivo* setting. J. Duca, R. Pearlstein

**3:00** Intermission.

**3:20 MPPG 74.** Kinetic stability of protein-ligand complexes: Applications in virtual screening. X. Barril

**4:00 MPPG 75.** Water: A small but revolutionary molecule that together with GPCR X-ray structures enables new design approaches for kinetics, selectivity and potency. J. Mason, A. Bortolato, D. Weiss, F. DeFlorian

**Environmental Interfaces****Complex Surface Reactions**

Sponsored by GEOC, Cosponsored  
by COLL, ENVR and MPPG‡

**Adsorption of Metals by Geomedia****Thermodynamics & Kinetics  
Experimental Study**

Sponsored by GEOC, Cosponsored  
by ENVR, MPPG‡ and NUCL

**Teaching & Implementing Effective  
Data Analysis & Computational  
Approaches Across the  
Undergraduate Chemistry Program**

Sponsored by CHED, Cosponsored by MPPG

**Advances in E-Learning**

Sponsored by CHED, Cosponsored by MPPG

**WEDNESDAY MORNING****Section A**

San Diego Convention Center  
Room 3

**The History of Chemistry & Computing**

Cosponsored by COMP, HIST and PHYS

B. Shoichet, A. Tropsha, *Organizers*

G. Patterson, *Organizer, Presiding*

**8:30 MPPG 76.** Introduction to a history of computers in chemistry. G. Patterson

**9:00 MPPG 77.** Providing supercomputing capability to the scientific community: The early years. T. Weber

**9:30 MPPG 78.** Quantum chemistry and large scale computations: A parallel development. H. Schaefer

**10:00** Intermission: Café con Ordenadores.

**10:30 MPPG 79.** Computer simulations provide an understanding of the electrochemical interface. D. Henderson

**11:00 MPPG 80.** History of the use of computers in polymer science. G. Patterson

**11:30 MPPG 81.** Chemical dynamics in solution and computers. H. Kim

**Section B**

San Diego Convention Center  
Room 4

**Computational Materials  
& Nanoscience: Theory  
Meets Experiment****Forum: Materials Genome &  
Materials Informatics**

Cosponsored by COMP, ENFL,  
INOR, ORGN and POLY

A. Aspuru-Guzik, K. Merz, O. Prezhdo, S. Tretiak, *Organizers*

J. Schrier, *Presiding*

**8:20** Introductory Remarks.

**8:30 MPPG 82.** How do we combine high-throughput theory, experimentation and data science to map a material's genome in real time? J. Hatrick-Simpers, A. Kusne

**9:00 MPPG 83.** Informatics for mapping the materials genome. K. RAJAN

**9:30 MPPG 84.** Data-driven research and a rational design paradigm in the chemical and materials disciplines. M. Haghighatari, J. Hachmann

**10:00** Intermission: Café con Ordenadores.

**10:30 MPPG 85.** Panel Discussion: Materials genome and materials informatics. J. Hachmann, J. Hatrick-Simpers, K. Rajan, J. Schrier

**Section C**

San Diego Convention Center  
Room 5A

**Computer-Aided Drug Design****Real World Dynamics**

Cosponsored by BIOL, CINF,  
COMP, MEDI and PHYS

R. Amaro, M. Holloway, J. Jansen, *Organizers*

V. Pande, *Presiding*

**8:00 MPPG 86.** In silico fragment based drug discovery by molecular simulations. G. De Fabritiis

**8:40 MPPG 87.** Redesigning drug design. J. Chodera

**9:20 MPPG 88.** Can molecular dynamics simulations cure what ails ya? D. Shaw

**10:00** Intermission: Café con Ordenadores.

**10:15 MPPG 89.** Future of molecular dynamics simulation. V. Pande

**10:55 MPPG 90.** Allostery through the computational microscope: Conformational selection in a canonical signaling domain. R. Amaro, R. Malmstrom, A. Kornev, S. Taylor

**Big Data & Small Data**

Sponsored by ANYL, Cosponsored  
by CINF and MPPG

**Computer-Aided Data Analysis  
in Chemical Education  
Research (CADACER)**

Sponsored by CHED, Cosponsored by MPPG

**Environmental Interfaces****Complex Surface Reactions**

Sponsored by GEOC, Cosponsored  
by COLL, ENVR and MPPG‡

**Adsorption of Metals by Geomedia****Radionuclides: Uranium &  
Transuranium - Extension of ACS  
Garvan-Olin Medal Session**

Sponsored by GEOC, Cosponsored  
by ENVR, MPPG‡ and NUCL

**Chemical Imaging: Applications,  
Advances & Challenges**

Sponsored by ANYL, Cosponsored  
by CINF and MPPG

**Know Your Unknowns: Estimating  
the Reliability of Individual  
Activity & Property Predictions**

Sponsored by COMP, Cosponsored by MPPG

**Online Approaches in  
Chemical Education**

Sponsored by CHED, Cosponsored by MPPG

**Homework: Past, Present & Future**

Sponsored by CHED, Cosponsored by MPPG

**WEDNESDAY AFTERNOON****Section A**

San Diego Convention Center  
Room 3

**Multiscales Chemistry****Sustainable**

Cosponsored by BIOL, COMP and PHYS

S. Hammes-Schiffer, R. Hernandez, *Organizers*

Q. Cui, *Presiding*

**1:00 MPPG 91.** Multiple phase coexistence in polymer electrolytes. M. Olvera De La Cruz, J. Zwanikken, H. Kwon

**1:30 MPPG 92.** Mechanisms of singlet fission in organic chromophores: A theoretical study. N. Ananth

**2:00 MPPG 93.** MoD-QM/MM smells good: Models of olfactory receptors validated by mutagenesis and activity profiles. V. Batista, L. Ahmed

**3:00** Intermission.

**3:30 MPPG 94.** Biopolymers out-of-equilibrium: Insights from blood plugging. A. Alexander-Katz

**4:00 MPPG 95.** Development of ReaxFF reactive force fields for reactions in proteins and DNA- an alternative for QM/MM? A. Van Duin, Y. Shin, M. Gokkaram

**4:30 MPPG 96.** Large scale molecular simulation of nanoparticle-biomolecule interactions and their implications in nanomedicine. R. Zhou

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## Section B

San Diego Convention Center  
Room 4

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Powering the Future: Novel Materials for Solar Cell Technologies

*Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

A. Aspuru-Guzik, K. Merz, O. Prezhdo, S. Tretiak, *Organizers*

J. Krich, *Presiding*

1:00 Introductory Remarks.

1:10 **MPPG 97.** Joint computational-experimental studies of quantum dots, perovskites, and their union. E. Sargent

1:40 **MPPG 98.** Screening novel photovoltaic materials for bulk-carrier lifetime, stability, and manufacturability. T. Buonassisi

2:10 **MPPG 99.** Withdrawn and replaced by **133.** Rational material, interface and device engineering for high-performance polymer solar cells. A. Jen

2:40 Intermission.

3:05 **MPPG 100.** Panel Discussion: Powering the future: Novel materials for solar cell technologies. J. Krich

## Section C

San Diego Convention Center  
Room 5A

### Computer-Aided Drug Design

#### New Modalities RNA

*Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

R. Amaro, M. Holloway, J. Jansen, *Organizers*

D. York, *Presiding*

1:00 **MPPG 101.** Structure guided design of nucleic acid modifications for antisense drug discovery. P. Seth

1:40 **MPPG 102.** High-throughput platform assay technology for the discovery of pre-microRNA-selective small molecule probes. A. Garner

2:20 **MPPG 103.** Exploiting the ribosome and RNA: Small-molecule interactions for a pipeline of new antibiotics. E. Duffy

3:00 Intermission.

3:15 **MPPG 104.** DNA and RNA in multi-target drug design for the micro-satellite disease myotonic dystrophy. S. Zimmerman, L. Luu, L. Nguyen, J. Serrano, J. Lee

4:00 **MPPG 105.** Light at the end of the tunnel in modeling RNA structure, dynamics and interactions. T. Cheatham

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## Environmental Interfaces

### Complex Surface Reactions

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡*

### Big Data & Small Data

*Sponsored by ANYL, Cosponsored by CINF and MPPG*

### Computer-Aided Data Analysis in Chemical Education Research (CADACER)

*Sponsored by CHED, Cosponsored by MPPG*

### Adsorption of Metals by Geomedica

#### X-ray Spectroscopy

*Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL*

### Chemical Imaging: Applications, Advances & Challenges

*Sponsored by ANYL, Cosponsored by CINF and MPPG*

### Online Approaches in Chemical Education

*Sponsored by CHED, Cosponsored by MPPG*

### Peptide Modeling

*Sponsored by COMP, Cosponsored by MPPG*

## THURSDAY MORNING

## Section A

San Diego Convention Center  
Room 3

### Big Data Science

#### Accessing Chemical Space & Better Modeling

*Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

B. Shoichet, A. Tropsha, *Organizers*

V. Feher, J. Irwin, *Organizers, Presiding*

8:30 **MPPG 106.** Mining the chemical universe database GDB-17 for drug discovery. J. Reymond

9:00 **MPPG 107.** Enamine REAL DataBase – an instrumental and practical vehicle for charting new regions of the relevant drug discovery chemical space. Y. Moroz, A. Chuprina, D. Mykytenko

9:30 **MPPG 108.** Ligand discovery using big data with ZINC. J. Irwin

10:00 Intermission: Café con Ordenadores.

10:30 **MPPG 109.** How to use 797,834 small molecule crystal structures. E. Davis, C. Groom, S. Ward, I. Bruno, A. Sarjeant

11:00 **MPPG 110.** Small-molecule ligand/drug representation and validation in the Protein Data Bank. S. Burley

11:30 **MPPG 111.** Drug design data resource: Leveraging blinded datasets for improved docking methodologies and workflows. V. Feher, R. Amaro, M. Gilson

## Section B

San Diego Convention Center  
Room 4

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: The Future of Spectroscopies: Quantum & Classical Fields; Theoretical Perspectives

*Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

A. Aspuru-Guzik, O. Prezhdo, S. Tretiak, *Organizers*

J. Yuen Zhou, *Presiding*

8:20 Introductory Remarks.

8:30 **MPPG 112.** New directions in coherent alignment: From spinning tops to ultrafast switches. T. Seideman, J. Szekeley

9:00 **MPPG 113.** New frontiers in multidimensional spectroscopy of molecules using classical, quantum, and X-ray light. S. Mukamel

9:30 **MPPG 114.** Extracting dynamics from optimally controlled spectroscopy. P. Brumer

10:00 Intermission: Café con Ordenadores.

10:30 **MPPG 115.** Panel Discussion: The future of spectroscopies: Quantum and classical fields; theoretical perspectives. J. Yuen Zhou

## Section C

San Diego Convention Center  
Room 5A

### Computer-Aided Drug Design

#### New Modality Therapeutics

*Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

R. Amaro, M. Holloway, J. Jansen, *Organizers*

J. Duca, *Presiding*

8:00 **MPPG 116.** Withdrawn.

8:40 **MPPG 117.** Structure-based design of inhibitors of the riboflavin pathway targeting the bacterial FMN riboswitch. T. Fischmann

9:10 **MPPG 118.** Boosting antibody developability through computational protein design. Q. Chai

9:40 Intermission: Café con Ordenadores.

9:50 **MPPG 119.** Peptide drug hunter: Exploring intracellular target space and druggability. T. Sawyer

10:30 **MPPG 120.** Enhanced sampling methods in drug design. A. Roitberg

11:00 **MPPG 121.** Withdrawn

11:30 **MPPG 122.** Unnatural DNA aptamers and the potential to generate unique macromolecular targeting modalities. G. Spraggon, L. Jennings, D. Witmer, A. Kreuzsch, B. Bursulaya, J. Shaffer, D. Jones, S. Swalley, S. Clarkson, M. Knuth, S. Lesley

### Applied Geochemical Modeling

#### Carbon Storage & Environmental Protection

*Sponsored by GEOC, Cosponsored by MPPG‡*

### Adsorption of Metals by Geomedica

#### Biosorption: Metal & Bacteria

*Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL*

### Chemical Imaging: Applications, Advances & Challenges

*Sponsored by ANYL, Cosponsored by CINF and MPPG*

## THURSDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 3

### Big Data Science

#### Interpreting Pharmacology

*Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

B. Shoichet, A. Tropsha, *Organizers*

V. Feher, J. Irwin, *Organizers, Presiding*

1:30 **MPPG 124.** Influence of data curation on QSAR Modeling – examining issues of quality versus quantity of data. K. Mansouri, C. Grulke, A. Richard, A.J. Williams

2:00 **MPPG 125.** What do open databases have to offer drug discovery? A. Hersey

2:30 **MPPG 126.** Using machine learning models based on phenotypic data to discover new molecules for neglected diseases. S. Ekins

3:00 Intermission.

3:30 **MPPG 127.** Extracting actionable knowledge from large scale *in vitro* pharmacology data. E. Griffen, A.G. Leach, A. Dosssetter, L. Reid

4:00 **MPPG 128.** PubChem – A chemical information hub. J. Zhang, P. Thiessen, A. Gindulyte, E. Bolton, S. Bryant

## Section B

San Diego Convention Center  
Room 4

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Exciting Aspects of Excitation Dynamics & Dissociation at the Nanoscale

*Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

A. Aspuru-Guzik, K. Merz, O. Prezhdo, S. Tretiak, *Organizers*

D. Kilin, *Presiding*

1:00 Introductory Remarks.

1:10 **MPPG 129.** Coherent photoluminescence excitation spectroscopy of semicrystalline polymeric semiconductors. C. Silva, P. Grégoire, E. Vella

1:40 **MPPG 130.** Photo-induced dynamics of excitons in nano materials teaser talk and panel discussion. J. Parkhill

2:10 **MPPG 131.** Nanoscale electronic structure and dynamics in disordered organic conjugated systems. A. Willard

2:40 Intermission.

3:05 **MPPG 132.** Panel Discussion: Exciting aspects of excitation dynamics and dissociation at the nanoscale. D. Kilin

### Applied Geochemical Modeling

#### Energy Exploration, Metals & Metalloids

*Sponsored by GEOC, Cosponsored by MPPG‡*



## Division of Agricultural and Food Chemistry

B. Park, Program Chair

### OTHER SYMPOSIA OF INTEREST:

**Chemical, Sample & Asset Management Tools** (see CHAS, Wed)

**Cannabis: Exploring the Chemistry, History & Future** (see SCHB, Mon, Tue)

**Undergraduate Research Posters: Agricultural & Food Chemistry** (see CHED, Mon)

**Biosensing of Proteins, Peptides, DNAs & RNAs** (see ANYL, Tue, Wed)

**Sampling & Processing of Biological Particles Enabled by Micro- or Nano-Fluidics** (see ANYL, Sun)

**My Comments to the President's Task Force on Employment** (see PRES, Sun)

### SOCIAL EVENTS:

**Caribbean Cooking Program,** 12:00 PM: Tue

**Reception,** 6:30 PM: Tue

### BUSINESS MEETINGS:

**Executive Committee Meeting,** 5:00 PM: Sun

**Future Programs Planning Meeting,** 12:00 PM: Mon

## SUNDAY MORNING

### Section A

US Grant Hotel  
Celestial Ballroom

#### Bioactives & Neurodegenerative Diseases

H. Ma, N. P. Seeram, *Organizers, Presiding*

8:00 Introductory Remarks.

8:15 AGFD 1. Role of polyphenols in promotion of healthy brain aging and Alzheimer's disease preventative initiatives. G.M. Pasinetti

8:45 AGFD 2. Curcumin bioavailability and potential for prevention of neurodegenerative disease. G.M. Cole, S.A. Frautschy

9:15 AGFD 3. Neuroprotective effects of the extra-virgin olive oil component oleocanthal in Alzheimer's disease. A. Kaddoumi

9:45 Intermission.

10:00 AGFD 4. Maple syrup extract inhibits the beta-amyloid and tau oligomerization of Alzheimer's disease. D.F. Weaver, C. Hawco, Y. Wang, M. Taylor

10:30 AGFD 5. Withanamides in aswangandha botanical to treat and prevent Alzheimer's disease. M.G. Nair

11:00 AGFD 6. Blueberry fruit supplementation in human cognitive aging. R. Krikorian

### Section B

US Grant Hotel  
Grant Hall

#### Flavor Chemistry of Alcoholic Beverages

M. Granvogl, K. Tandon, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 7. Unraveling the key aroma compounds of different types of beer: Are differences in aroma profiles caused by quantitative or qualitative differences in key odorants? P.H. Schieberle

8:35 AGFD 8. Hop, the spirit of the beer. M.C. Qian

9:05 AGFD 9. Odor-active compounds in novel special flavor hop cultivars and their impact on beer aroma. M. Steinhaus, S. Nielsen

9:35 Intermission.

10:00 AGFD 10. Options to mitigate sun-struck-flavor formation in beer. S. Stingl, P.H. Schieberle

10:30 AGFD 11. Characterizing aroma components of rum. C. Ickes, K.R. Cadwallader

11:00 AGFD 12. Withdrawn.

11:30 Concluding Remarks.

### Section C

US Grant Hotel  
Crystal Ballroom

#### Undergraduate Symposium

C. J. Brine, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 13. Bioproduction and anti-inflammatory activity of delta-tocotrienol enriched extracts from hairy roots of annatto. J. Creameans, K. Vellanki, M. Dolan, F. Medina-Bolivar

8:35 AGFD 14. Quinone intermediate mediates the cytotoxicity effects of *tert*-butylhydroquinone (TBHQ). E. Sukamtoh

9:05 AGFD 15. Selectivity of separation of natural antioxidants in gradient reversed-phase liquid chromatography. M. Palmieri, P. Cesla, F. Pellati

9:35 Intermission.

9:50 AGFD 16. Effect of elemental sulfur and yeast strain on hydrogen sulfide production in wine post-bottling. E. Friedberg, G.L. Sacks

10:20 AGFD 17. Structure-property study of the selective Raman spectroscopy detection of fusaric acid and analogs. E. Martinez Rosado, M. Appell, L.E. Orellana

10:50 AGFD 18. Determination of the effect of dissolved oxygen on the rate of oxidation presented by *trans*-2-nonenal in beer. D. Kazal, W.H. Steel

11:20 Concluding Remarks.

#### Advances & Applications in Water Sensing Technologies for Drinking Water, Reuse, Agri-Tech & Research

*Sponsored by ENVR, Cosponsored by AGFD*

## SUNDAY AFTERNOON

### Section A

US Grant Hotel  
Celestial Ballroom

#### Bioactives & Neurodegenerative Diseases

H. Ma, N. P. Seeram, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 19. Actions of bioactive phytochemicals in neuropathology. R. Hartman

1:35 AGFD 20. Phenolic-enriched maple syrup extract shows neuroprotective effects in murine microglial cells and delays  $\beta$ -amyloid aggregation induced neurotoxicity and paralysis of *Caenorhabditis elegans*. H. Ma, W. Liu, P.P. Nahar, N. DaSilva, Z. Wei, P.P. Pharm, D.A. Vatter, N.P. Seeram

2:05 AGFD 21. Back to the future: Using phenotypic screening to identify Alzheimer's disease (AD) drug candidates. P. Maher

2:35 Intermission.

2:50 AGFD 22. Potential beneficial effects of a diet with walnuts in Alzheimer's disease. A. Chauhan, V. Chauhan

3:20 AGFD 23. Bioactive compounds in dairy products and their relation to neurodegenerative disease. M.H. Tunick, D.L. Van Hekken, P.M. Tomasula

3:50 AGFD 24. Assessment of the ability of dietary soy to impact age-related neurodegeneration. J. Dshane, S. Meleth, L. Wilson, S. Barnes, H. Kim

4:20 Concluding Remarks.

### Section B

US Grant Hotel  
Grant Hall

#### Flavor Chemistry of Alcoholic Beverages

M. Granvogl, *Organizer*

K. Tandon, *Organizer, Presiding*

P. H. Schieberle, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD 25. Non-volatile profiling of cask aged spirits using UHPLC/QTOF-MS. T.S. Collins

1:35 AGFD 26. Unraveling differences in key aroma compounds of a commercial American bourbon whiskey and a scotch single malt whiskey by means of the sensomics concept. V. Mall, P.H. Schieberle

2:05 AGFD 27. From the fruit to the spirit: Changes of key aroma compounds in pears and pear brandy. M. Granvogl, B. Willner, P.H. Schieberle

2:35 Intermission.

3:00 AGFD 28. Identification of compounds that contribute to trigeminal burn of alcoholic spirits. S. Kokkinidou, D.G. Peterson

3:30 AGFD 29. Grape pathogenesis related proteins (PRPs) — a factor responsible for low tannin extraction during winemaking. G.L. Sacks, L. Chen, L.F. Springer

4:00 Concluding Remarks.

### Section C

US Grant Hotel  
Crystal Ballroom

#### Graduate Student Symposium

C. J. Brine, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 30. Anti-obesity and anti-hyperlipidemic effect of *Gynostemma pentaphylla* saponins and the possible mechanisms. J. Liu, H. Shi, X. Sun, L.L. Yu

1:35 AGFD 31. Kafirin protein and its applications in nano-encapsulation, pickering emulsion and electrospinning fiber. J. Xiao, Q. Huang

2:05 AGFD 32. Physicochemical modification of an immunostimulatory gluten peptide and the potential implications for Celiac disease. C. Van Buiten

2:35 Intermission.

2:50 AGFD 33. Chemical modification of poultry feather keratin for biobased wood adhesive applications. N. Bandara, J. Wu

3:20 AGFD 34. Advanced analytical techniques for the phytochemical investigation of essential oils. R. Tardugno, F. Pellati, S. Benvenuti

3:50 AGFD 35. Colorimetric detection of *Escherichia coli* in drinking water based on bacteriophage infection. J. Chen, V.M. Rotello, S.R. Nugen

4:20 Concluding Remarks.

#### Advances & Applications in Water Sensing Technologies for Drinking Water, Reuse, Agri-Tech & Research

*Sponsored by ENVR, Cosponsored by AGFD*

## MONDAY MORNING

### Section A

US Grant Hotel  
Celestial Ballroom

#### Bioactives & Neurodegenerative Diseases

H. Ma, N. P. Seeram, *Organizers, Presiding*

8:00 Introductory Remarks.

8:15 AGFD 36. Dietary bioactives and neurocognitive function: The case for curcumin. A. Scholey, K. Cox

8:45 AGFD 37. Identifying ache inhibitors as bioactives from Chinese herbal medicine. J. Xu

9:15 AGFD 38. Evaluation of three tropical fruits on lifespan and experimentally induced neurodegeneration in *Caenorhabditis elegans*. K.C. Borges, J.C. Azevêdo, M.F. Bezerra, R. Crews, R.T. Correia, D.A. Vatter

9:45 Intermission.

10:00 AGFD 39. Experimental and theoretical studies toward the development of new amyloid inhibitors against amyloid- $\beta$  aggregation. J. Zheng

10:30 AGFD 40. Neuroprotective effects of urolithins, pomegranate ellagitannin-gut microbial derived metabolites: In silico, *in vitro*, and *in vivo* studies. D.B. Niesen, T. Yuan, H. Ma, N. Shah, W. Liu, R. Crews, D. Vatter, N.P. Seeram

11:00 AGFD 41. Metabolomics of grape seed bioactives that may have a role in postmenopausal neurodegeneration. J. Cutts, L. Wilson, S. Barnes, H. Kim

11:30 Concluding Remarks.

### Section B

US Grant Hotel  
Grant Hall

#### Flavor Chemistry of Alcoholic Beverages

K. Tandon, *Organizer*

M. Granvogl, *Organizer, Presiding*

M. Steinhaus, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD 42. Typicity of great Chardonnay wines, evidence for new potent markers. J. Gros, A. Marchal, V. Lavigne, V. Moine, P. Darriet

8:35 AGFD 43. Withdrawn.

**9:05 AGFD 44.** Synergistic effects of copper and pH - wine making variables that significantly impact reductive aromas in wines. **M.Z. Bekker, M.E. Smith, A. Mierczynska-Vasilev, P.A. Smith, E. Wilkes**

**9:35** Intermission.

**10:00 AGFD 45.** Impact of vineyard exposure to smoke on wine composition and sensory properties. **L. van der Hulst, C. Ford, R. Burton, R. Ristic, N. Lloyd, Y. Hayasaka, P. Boss, K. Wilkinson**

**10:30 AGFD 46.** Relating sensory attributes, notably 'tropical fruit' flavour, and volatile chemical composition in Chardonnay wines. **D.L. Capone, A. Barker, P. Williamson, L. Francis**

**11:00 AGFD 47.** Role of selected microbial dehydrogenases in the synthesis of flavor compounds. **S. Kermasha**

**11:30** Concluding Remarks.

### Section C

US Grant Hotel  
Crystal Ballroom

#### Cannabis: Exploring the Chemistry, History & Future

*Cosponsored by CHAS and SCHB*

R. W. Phifer, E. M. Pryor, *Organizers*

J. Marcu, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 AGFD 48.** Building a subdivision at the ACS: Sowing the seeds of change. **E.M. Pryor, J. Marcu, M.J. Wilcox**

**8:35 AGFD 49.** Potency trends in confiscated cannabis and analytical methods. **M.A. Elsohly**

**9:05 AGFD 50.** Responsible cultivation policy: Preserving personal cultivation rights while regulating commercial cultivation as agriculture. **K. Nevedal, J. Marcu**

**9:35** Intermission.

**9:55 AGFD 51.** Improving quality control methods for cannabis using flash chromatography. **J. Marcu, J.P. Kababick, M.J. Wilcox, M. Jacyno**

**10:25 AGFD 52.** Cannabis: Taxonomy and secondary metabolism. **J. Fischedick**

**10:55** Panel Discussion.

## MONDAY AFTERNOON

### Section A

US Grant Hotel  
Celestial Ballroom

#### Bioactives & Neurodegenerative Diseases

H. Ma, N. P. Seeram, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:05 AGFD 53.** Laboratory preparations of vinaxanthone and xanthofulvin, natural products enhancing CNS regeneration. **D. Siegel**

**1:35 AGFD 54.** *Salvia divinorum*: A unique CNS active plant. **T.E. Prisinzano**

**2:05 AGFD 55.** Discovery of anti-Alzheimer agents from Chinese herbal medicine. **Q. Gu, J. Xu**

**2:35** Intermission.

**2:50 AGFD 56.** Fungal metabolome as a rich resource for tau aggregation inhibitors. **S.R. Paranjape, Y. Chiang, C.C. Wang, B.R. Oakley, T.C. Gamblin**

**3:20 AGFD 57.** Disaggregation of amyloid beta peptides by tabersonine and related compounds: Biophysical, bioanalytical, and cytotoxicity studies. **T. Kai, L. Zhang, G.B. Yagnik, A. Jing, B. Zhao, F. Zhou**

**3:50 AGFD 58.** Efficient synthesis and neuroprotective activity of CN2097: A cyclic disulfide polyarginine peptidomimetic binding PDZ domain of PSD-95. **R.K. Tiwari, S.R. Kotla, J. Marshall, D.J. Goebel, K. Parang**

**4:20** Concluding Remarks.

### Section B

US Grant Hotel  
Grant Hall

#### Advances in Food Peptide & Food Protein Research: Nutrition, Functionality & Food Safety

Y. Zhang, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 AGFD 59.** Withdrawn.

**1:30 AGFD 60.** Alpha-lactalbumin-catechin conjugates improve the chemical stability of the vitamin A precursor  $\beta$ -carotene in nanoemulsions. **J. Yi, Y. Zhang, L. Zhao**

**1:55 AGFD 61.** Bioactive peptides generated from plant proteins in relation to molecular structures. **L. Chen, Z. Tian**

**2:20 AGFD 62.** Ovomucin derived peptides as anti-adhesive agents against infectious diseases. **X. Sun, M. Gänzle, J. Wu**

**2:45 AGFD 63.** New tree nut allergens. **Y. Zhang, W. Du, B. Lee, Y. Fan, S. Lyn, K. Nadeau, T.H. McHugh**

**3:10** Intermission.

**3:25 AGFD 64.** Studies on the mechanism of calcium ion on the allergenic activity of EF-hand domain food-induced allergen. **S. Han, H. Che**

**3:50 AGFD 65.** Influence of free amino acids, oligopeptides and polypeptides on the formation of pyrazines in Maillard model systems. **G. Leonardo Scalone, P. Lamichhane, T. Cucu, N. De Kimpe, B.E. De Meulenaer**

**4:15 AGFD 66.** Cold-adapted  $\beta$ -galactosidase from a psychrotrophic bacterium *Rahnella* sp. R3: Protein structure and enzymatic properties. **Y. Fan, Y. Zhang, R. Yang**

**4:40 AGFD 67.** Structural modification of an immunodominant gluten peptide upon interaction with (-)-epigallocatechin-3-gallate. **C. Van Buiten, C.N. Pacheco, E. Hatzakis, R. Elias**

**5:05** Concluding Remarks.

### Section C

US Grant Hotel  
Crystal Ballroom

#### Cannabis: Exploring the Chemistry, History & Future

*Cosponsored by CHAS and SCHB*

J. Marcu, R. W. Phifer, *Organizers*

E. M. Pryor, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 AGFD 68.** Navigating the ever changing regulations and rules of the cannabis industry. **C. Ludwig**

**1:35 AGFD 69.** Review of Bedrocan science: Patient-inspired and science-based. **A. Hazekamp**

**2:05 AGFD 70.** Consumer safety and an accredited laboratory. **S.A. Audino**

**2:35** Intermission.

**2:55 AGFD 71.** Results from auditing medical cannabis operations in the United States. **J. Marcu, S. Sherer, K. Nevedal**

**3:25 AGFD 72.** Understanding cannabis diversity in today's medical applications. **J.C. Raber**

**3:55 AGFD 73.** Beyond cannabis and anandamide. **R. Mechoulam**

**4:25** Panel Discussion.

### Undergraduate Research Posters

#### Agricultural & Food Chemistry

*Sponsored by CHED, Cosponsored by AGFD and SOCED*

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

B. Park, *Organizer*

**8:00 - 10:00**

3, 8, 49, 59, 67, 71. See previous listings.  
78, 96, 102, 110-111, 122, 136-137, 143, 158-159, 161, 166, 168, 186, 191. See subsequent listings.

## TUESDAY MORNING

### Section A

US Grant Hotel  
Celestial Ballroom

#### Applied Nanotechnology for Food & Agriculture

M. Appell, S. R. Nugen, B. Park, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 AGFD 74.** Metal oxide nanoparticles for destructing dyes and bacteria. **Y. Mao**

**8:35 AGFD 75.** Applications of nanoporous cyclodextrin polymers to prevent exposure to mycotoxins. **M. Appell, M.A. Jackson, K. Evans**

**9:05 AGFD 76.** Enzyme nanotechnology: Moving towards next-generation biocatalytic materials for food applications. **J.M. Goddard, J. Talbert**

**9:35** Intermission.

**9:50 AGFD 77.** Withdrawn.

**10:20 AGFD 78.** Colorimetric detection of *Escherichia coli* based on the enzyme-induced metallization of gold nanorods. **J. Chen, A. Jackson, V.M. Rotello, S.R. Nugen**

**10:50 AGFD 79.** Functionalization of biopolymer silver nanosubstrates for pathogen detection. **J. Chen, B. Park**

**11:20** Concluding Remarks.

### Section B

US Grant Hotel  
Grant Hall

#### Public Health Perspectives of Mycotoxins in Food

*Cosponsored by AGRO and ANYL*

L. Jackson, D. Ryu, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 AGFD 80.** Short history of mycotoxin research. **J. Pitt**

**8:55 AGFD 81.** Climate variability and mycotoxin exposure. **J. Miller**

**9:35** Intermission.

**9:50 AGFD 82.** Worldwide occurrence of mycotoxins in foods. **D. Ryu, H. Lee**

**10:20 AGFD 83.** Emerging mycotoxins: Beyond traditionally determined food contaminants. **F. Berthiller, E. Varga, M. Sulyok, R. Krska**

**10:50 AGFD 84.** Aflatoxin and child growth: The critical first 1000 days of life in underdeveloped world regions. **P.C. Turner**

**11:20** Concluding Remarks.

### Section C

US Grant Hotel  
Crystal Ballroom

#### Chemical Modification of Natural Bio-based Material: Design & Application for Value Added Products

S. Chang, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 AGFD 85.** Effects of mechanical strain on average orientation and packing of polymeric constituents in onion epidermis cell walls. **K. Kafle, Y. Park, S. Huang, D. Cosgrove, S.H. Kim**

**8:25 AGFD 86.** Swine odor removal with biochar. **O. Hwang, S. Cho, D. Han, K. Ro**

**8:45 AGFD 87.** Thermally reprocessable polylactic acid grafted cellulose nanocrystal films through reactive extrusion process. **P. Dhar, D. Tarafdar, A. Kumar, V. Katiyar**

**9:05 AGFD 88.** Chitosan-based multilayer nanocoatings that exhibit high gas barrier and flame retardant behavior. **J.C. Grunlan**

**9:25** Intermission.

**9:40 AGFD 89.** Investigation of solvent systems and potential applications of soy proteins. **G. Sun, A. Aghanouri**

**10:00 AGFD 90.** Ammonia and hydrogen sulfide removal using biochar. **K. Ro, I.M. Lima, G. Reddy**

**10:20 AGFD 91.** Effects of processing conditions on the structure of enzymatic modified soy protein isolate-based bioplastics. **E. Zadeh**

**10:40 AGFD 92.** Mountain beetle pine infestation: Characterization of the polar components for Lodge pole pine (*Pinus contorta*) acetone extractives. **R.K. Moore**

**11:00 AGFD 93.** Innovative technologies for anti-flammable cotton fabrics. **S. Chang, B.D. Condon**

**11:20** Concluding Remarks.

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:

[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## Cannabis: Exploring the Chemistry, History & Future

Sponsored by SCHB, Cosponsored by AGFD, CHAS and ORGN

## TUESDAY AFTERNOON

### Section A

US Grant Hotel  
Celestial Ballroom

### Applied Nanotechnology for Food & Agriculture

M. Appell, S. R. Nugen, B. Park, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 94. Ultra-small-angle x-ray scattering study of zein self-assembly. S. Uzun, G. Padua

1:35 AGFD 95. Isolation, characterization and anti-proliferative activities of Picroside compounds present in *Picrohiza kurroa*, (kutki) extract. B. Dayal, T. Roy, M.A. Lea, S. Patel, S. Ali, S. Li

2:05 AGFD 96. Development and characterization of functionalized TiO<sub>2</sub>/polylactic acid nanocomposite films for food packaging applications. N. Baek, S. Duncan, Y. Kim, J. Marcy, S.F. Okeefe

2:35 Intermission.

2:50 AGFD 97. Targeted delivery system based on chitosan and sulfated β-glucan for the colon. C. Yucel, J. Sotres, A. Rascon, J. Risbo, M. Cardenas

3:20 AGFD 98. Withdrawn.

3:50 Concluding Remarks.

### Section B

US Grant Hotel  
Grant Hall

### Public Health Perspectives of Mycotoxins in Food

Cosponsored by AGRO and ANYL

L. Jackson, D. Ryu, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 99. Urinary biomarkers for human multi-mycotoxin exposure. M. Solfrizzo, L. Gambacorta, A. Logrieco

1:35 AGFD 100. Risk of exposure to multiple mycotoxins from maize based complementary foods in Tanzania. A. Kamala, M. Kimanya, C. Lachat, L. Jacxsens, J. Ortiz, G. Haesaert, P. Kolsteren, B. Tiisekwa, B.E. De Meulenaer

2:05 AGFD 101. Fumonisin exposure in women linked to inhibition of an enzyme that is a key event in farm and laboratory animal diseases. R.T. Riley, K. Voss, J.L. Showker, T. Mitchell, O. Torres, J. Matute, S.G. Gregory, A.E. Ashley-Koch, J.R. Maddox, J. Gelineau-van Waes

2:35 Intermission.

2:50 AGFD 102. DNA Adduction by ochratoxin A: Insight for mechanism of action and aptasensor development for mycotoxin detection. R.A. Manderville

3:20 AGFD 103. Mycotoxins at the blood-brain barrier: Metabolism, toxicity, barrier integrity and transfer to the brain. M. Behrens, S. Hüwel, H. Galla, H. Humpf

3:50 AGFD 104. Renal gene expression changes in mice and rats exposed to dietary ochratoxin A. A. Nunnikhoven, I. Curran, A. Gannon, Z. Gillespie, L. Coady, C. Qiao, V. Liston, D. Lefebvre, N. Ross, R. Mehta, G. Bondy

4:20 Concluding Remarks.

### Section C

US Grant Hotel  
Crystal Ballroom

### Metabolomics in Agriculture & Food Chemistry: Current Status & Future Scopes

S. Chakraborty, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 AGFD 105. FlavonQ: An automated data processing tool for profiling flavone and flavonol glycosides with ultra-high-performance liquid chromatography–diode array detection–high resolution accurate mass–mass spectrometry. P. Chen, M. Zhang, J. Sun

1:55 AGFD 106. Taking metabolomics beyond primary metabolism - challenges and opportunities for capturing plant chemical diversity. B.M. Lange, S.R. Johnson

2:40 Intermission.

2:55 AGFD 107. Second-generation metabolomics in food research: Merging untargeted and targeted data acquisitions for food and exposome analysis. O. Fiehn

3:40 AGFD 108. Breast milk or infant formula: Consequences for the microbiome and metabolome. C. Slupsky

4:25 AGFD 109. Metabolomics for understanding the plant chemistry: Comparison of lipid extraction methods for lipid profiling in algae. N. Kaushik, T. Kind, O. Fiehn

4:50 Concluding Remarks.

### Section C

San Diego Convention Center  
Halls B/C

### General Posters

B. Park, *Organizer*

3:00 - 5:00

AGFD 110. Comparison of volatile compounds in fermented rice broths. H. Lim, S. Lee, Y. Roh, J. Lee, B. Eum, J. Chang, Y. Kim

AGFD 111. Crystal structure and catalytic mechanism proposal of cellobiose 2-epimerase from *Caldicellulosiruptor saccharolyticus* DSM 8903. Q. Shen, Y. Zhang, R. Yang, S. Pan

AGFD 112. Inhibition of formation of advanced glycation end-products by an oligosaccharide-enriched fraction purified from cranberry (*Vaccinium macrocarpon*). J. Sun, H. Ma, W. Liu, J. Dain, D.C. Rowley, N.P. Seeram

AGFD 113. Advanced glycation endproducts inhibitory compounds from amla (*Phyllanthus emblica*). K.N. Rose, C. Wan, H. Ma, W. Liu, N.P. Seeram

AGFD 114. Antibacterial properties of common herbs and spices. B. Lipinski, D.F. Moriarty

AGFD 115. Withdrawn.

AGFD 116. New approaches to the preparation and characterization of tormentic acid. E.J. Parish, H. Honda, T. Wei, J. Wu, H. Ho

AGFD 117. Novel approaches to the chemical synthesis and biological activity of 24-ketolanosterol an inhibitor of HMG-CoA reductase. E.J. Parish, J. Yin, H. Honda, T. Wei, H. Yin

AGFD 118. Facile synthesis and carbon-13 nuclear magnetic resonance spectral properties of cholest-4-en-3,6-dione. E.J. Parish, H. Honda, T. Wei, H. Shyu

AGFD 119. Novel approaches to the chemical synthesis and spectral characterization of hydroxysterols. Y. Lo, H. Shyu, W. Huang, H. Honda, T. Wei

AGFD 120. Chemical synthesis and characterization of lanosterol derivatives, inhibitor of cholesterol biosynthesis. E.J. Parish, W. Huang, H. Honda, T. Wei, H. Shyu

AGFD 121. Novel preparation and characterization of kinsenoside. E.J. Parish, J. Wu, H. Ho, H. Honda, T. Wei

AGFD 122. Elucidation of changes in non-volatile metabolites of amylolytic yeast, *Saccharomyces fibuligera*, according to the cultivation times. J. Jeong, N. Lee, Y. Kim

AGFD 123. Microbial synthesis of myrcene by metabolically engineered *Escherichia coli*. E. Kim, J. Eom, Y. Um, Y. Kim, H. Woo

AGFD 124. Structure activity related, mechanistic, and modeling studies of galactanins containing a glucitol-core and a glucosidase. H. Ma, L. Wang, D.B. Niesen, W. Tan, Q. Gu, J. Xu, N.P. Seeram

AGFD 125. Anti-glycative, reactive carbonyl scavenging and anti-amyloid fibrillation effects of ayurvedic medicinal plants. W. Liu, H. Ma, L. Zhang, C. Wan, J. Dain, N.P. Seeram

AGFD 126. Vapor-Infusion of wine flavor volatiles in specialty dark chocolate and analysis via GC-MS. S. Richards, R. MacFarland, P.J. Iles, L.D. Giddings, M. Alvarez, R.V. Valcarce, R. Holcomb, N.R. Bastian

AGFD 127. Pesticide mobility in soils: An initial characterization comparing productive vs non-productive soils. G.A. Querejeta, E.P. Beiguel, E.A. Hughes, J. Montserrat, A. Zalts

AGFD 128. Evaluation of immunogenicity of hepatitis B vaccine referred to the clinic. E. Rezaei

AGFD 129. Effect of pH and xanthan-locust bean mixtures on the physicochemical properties of whey protein-stabilized oil-in-water emulsions. C. Owens, H. Khouryieh, K. Williams

AGFD 130. Comparison of a brewer's water analysis kit to standardized methods and implications for brewing. N.O. Flynn, D. Reasoner, J. Read, P.T. Baumgardner

AGFD 131. Survey of amino acid composition in cider apples grown in Virginia by UPLC-PDA. S. Ma, G. Peck, A. Stewart

AGFD 132. Physicochemical properties of amorphous granular starches prepared from corn, tapioca and non-waxy rice starches using high hydrostatic pressure. J. Choi, M. Song, B. Kim, M. Baik

AGFD 133. Effects of processing and storage temperature on browning index, furosine, and HMF in aseptic cold break tomato paste during storage time. H. Yeom, J. Conte, R. Mohammed, S. DeMuri

AGFD 134. Effects of storage and heating on serum viscosity of hot break tomato paste. H. Yeom, A. Janosko, M. Ramirez, S. DeMuri

AGFD 135. Determination of ceftiofur and its metabolites in plasma using reverse-phase liquid chromatography. S. Cox, M. White, K. Gordon, J. Bailey

AGFD 136. Reversed-phase high performance liquid chromatography (HPLC) studies of the sweet diterpene glycosides isolated from *Stevia rebaudiana* bertoni. V. Chaturvedula, S. Meneni

AGFD 137. Analysis of volatile flavor components of steamed rice and identification of key odorants causing old rice smell. H. Takemitsu, Y. Sako, K. Shibakusa, S. Kitamura, H. Inui

AGFD 138. Comparison between traditional-SERS and RCA-SERS assays for 35S promoter gene detection. B. Guven, I.H. Boyaci, U. Tamer, E. Acar-Soykut

AGFD 139. Exposure estimate for semicarbazide from the use of azodicarbonamide in bread for the U.S. population. S. Bhagan, D.L. Doell, H. Lee, T. Croce, S.E. Carberry

AGFD 140. Determination of total dietary fiber in extruded food products containing grape pomace. L. Hordge, J. Yu

AGFD 141. Preparation of gelatin films incorporated with tea polyphenol nanoparticles for enhancing controlled-release antioxidant properties. F. Liu, W. Yokoyama, F. Zhong, Y. Li

AGFD 142. Rapid front end cleanup of cannabis-infused edibles using automated flash column chromatography. M.J. Wilcox, J. Marcu, J.P. Kababick, M. Jacyno

AGFD 143. Fatty acid profiles of marine fishes from Rhode Island coastal waters. M. Yurkevicius, J. Jacques, N.E. Breen, D.L. Taylor

AGFD 144. Synthesis and fungicidal activity study of 2-(thiophen-2-yl)pyridine derivatives. Y. Xie, Y. Xu, Y.L. Chen, C.L. Liu

AGFD 145. Design, synthesis, and biological activities of novel carboxylic ether derivatives containing oxime. Q. Wu, J. Yang, J. Zhang, G. Aiying, H. Ma, C.L. Liu

AGFD 146. Herbicidal properties of substituted 3-(pyridin-2-yl)benzenesulfonamide derivatives. Y. Xie, H.W. Chi, G. Aiying, C.L. Liu, H. Ma

AGFD 147. Synthesis and characterization of novel luminescent sodium carboxymethyl cellulose nanocomposites for potential safety inspection of food applications. M. Zhang, L. Qingyong, J. Ye, X. Jian

AGFD 148. Characterization of pepsin-solubilized collagens and the hydrolysates from sea cucumber species. M. Saito

AGFD 149. Red shortening: Characterization and utilization in formulating novel functional biscuits. H. Abou Gharbia, M.M. Youssef, M. Abd-El-Aal, N. Nabil

AGFD 150. Presence of *Protostrongylus stilesi* in Rocky Mountain goats and the effects of infestation. C. Dunlap

AGFD 151. Polyphenol-aluminum complex formation: Implications for aluminum tolerance in plants. A.E. Hagerman, L. Zhang

AGFD 152. Natural soil benign bacterium with an insecticidal activity. S. Stark

AGFD 153. Chemical and supramolecular structural modifications in lignin during acid catalyzed ionic liquid pretreatment: A case study of *Arundo donax* linn. T. You, L. Zhang, F. Xu

AGFD 154. Seed-specific phosphate allocation with coordinated expression of genes involved in phosphate transport function during wheat grain development. V.K. Shukla, M. Kaur, S. Aggarwal, K. Bhati, S. Sharma, S. Mantri, A. Pandey

AGFD 155. Detection of pesticides in edible oil using LC-MS analysis. S. Bhattacharya

AGFD 156. Heated headspace solid phase microextraction of marijuana for chemical testing. A. Brown, J. Sweet, C.C. Yu

- AGFD **157.** Nutritional value and total phenolics of tortillas obtained by extrusion cooking of red pigmented creole maize. **A.K. Milan**, C. Reyes-Moreno, J. Milan Carrillo
- AGFD **158.** Evaluating Raman spectroscopic data by using principal component analysis to determine the freshness of fish samples. **H. Temiz**, H. Velioglu, I.H. Boyaci
- AGFD **159.** Withdrawn.
- AGFD **160.** Dolabella-3,7,18-triene: The main constituent of *Nymphaea lotus* essential oil. **D.M. Navarro**, M. Pottier, B.N. Albuquerque, A.C. Maia, F. Hallwass, A. Navarro-Vazquez
- AGFD **161.** Molecularly imprinted polymers with desorption electrospray ionization mass spectrometry for high throughput analysis of neonicotinoids pesticides in water and food. **C.S. Bottaro**, J. Gauthier, S. Egli
- AGFD **162.** Chemical compositions of essential oils of *Psidium guajava* and *Syzygium sp.* and their *in vitro* antiviral activities. **N. Mohamed**, A.A. Abdalsalam, H. Osman, E.E. Kamarulzaman, H. Wahab
- AGFD **163.** Detecting delta-9-tetrahydrocannabinol ( $\Delta^9$ -THC) and delta-8-tetrahydrocannabinol ( $\Delta^8$ -THC) by UV-HPLC. **K. Tseng**, T. Ono, T. Hirose, K. Kimata
- AGFD **164.** Nutritional variation and antioxidant properties of wild fruits revealed through a fluorescence-based method. **S. Smith**, F. Ulerio Nunez, M. Bida, T.E. Pagano
- AGFD **165.** Using dietary preferences of wildlife to discover bioactive polyphenols in plants. **D. Conner**, H. Hoang, M. Fremgen, J.S. Forbey, C. Dadabay
- AGFD **166.** Antimicrobial activity of extracts from seaweeds of northeast Brazil. **P.C. Bezerra-Silva**, B.N. Albuquerque, B.S. Santos, T.N. Reis, P.M. Paiva, M.V. Silva, D.M. Navarro
- AGFD **167.** In situ analysis of interrelation between topochemistry and cellulose accessibility in poplar cell walls. **X. Zhou**, F. Xu, D. Ding
- AGFD **168.** Bioassay-guided isolation of secondary metabolite inhibitors of *Xylella fastidiosa* produced by endophytic fungi. **M. Papineau**, L. D'Elia, P.E. Rolshausen, C. Roper, K.N. Maloney
- AGFD **169.** Chemistry and mass spectral characterization of methylglyoxal adducts formed with metformin, aminoguanidine and okra seed extract: Relevance to diabetic complications. **B. Dayal**, R. Gohil, P. O'Connor, M.A. Lea
- AGFD **170.** LC/MS metabolomic profiling of an amber ale fermented with four different yeast strains. **C.A. Hughey**, K.M. Foss, K. Fortmann
- AGFD **171.** Antimicrobial spectrum and toxicology of a natural food grade additive obtained from avocado seed. **A. Pacheco**, R.C. Chávez, D.G. Rodriguez-Sanchez, R. Villarreal-Lara, M.I. Garcia-Cruz, C. Hernandez-Brenes

Technical program information known at press time.  
The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## WEDNESDAY MORNING

### Section A

- US Grant Hotel  
Celestial Ballroom
- Natural & Modified Carbohydrate Polymers Effects on Obesity Related Metabolic Diseases**  
M. Kale, *Organizer*
- M. Turowski, W. H. Yokoyama, *Organizers, Presiding*
- 8:00** Introductory Remarks.
- 8:05 AGFD 172.** Functional role of fiber in the diet: Prebiotics, metabolic benefits and beyond. **C. Slupsky**
- 8:30 AGFD 173.** Effects of indigestible polysaccharides on obesity related metabolic diseases and inflammation. **Y. Egashira**
- 8:55 AGFD 174.** Anti-obesity properties of mushroom polysaccharides: A review. **M. Friedman**
- 9:20** Intermission.
- 9:40 AGFD 175.** Polysaccharide structure and physiological effect: Glycemic and non-glycemic carbohydrates. **M. Kale**, B. Hamaker
- 10:05 AGFD 176.** Yeast  $\beta$ -glucan down-regulates blood glucose level in obesity/type 2 diabetes. **X. Xu**, Y. Cao, L. Zhang
- 10:30 AGFD 177.** Digestibility and health benefits of native and modified resistant starch. **J. Jane**, Y. Ai, M. Reed, H. Jiang, J. Hasjim, D. Birt
- 10:55** Concluding Remarks.

### Section B

- US Grant Hotel  
Grant Hall
- Public Health Perspectives of Mycotoxins in Food**  
*Cosponsored by AGRO and ANYL*
- L. Jackson, D. Ryu, *Organizers, Presiding*
- 8:00** Introductory Remarks.
- 8:05 AGFD 178.** New strategy for the biocontrol of *Fusarium verticillioides* in corn based on endophytic bacterial-fungal interactions. **C.W. Bacon**, D.M. Hinton, T. Mitchell
- 8:35 AGFD 179.** Bioplastic formulation of beneficial microbes to control agricultural pests. **H.K. Abbas**
- 9:05 AGFD 180.** Reduction of fumonisin toxicity by extrusion and nixtamalization (alkaline cooking). **K. Voss**, D. Ryu, L. Jackson, R.T. Riley, J. Gelineau-van Waes
- 9:35** Intermission.
- 9:50 AGFD 181.** Mycotoxin deactivation strategies – past, presence and future. **G. Schatzmayr**
- 10:20 AGFD 182.** Molecular approaches for enhancing host resistance against *Aspergillus flavus* infection and aflatoxin contamination in corn and cottonseed. **D. Bhatnagar**, R. Brown, K. Rajasekaran, J. Cary, M. Gilbert
- 10:50 AGFD 183.** Tools to determine the identity, occurrence and toxicity of conjugated mycotoxins. **V. Nagl**, G. Adam, R. Schuhmacher, R. Krska, F. Berthiller
- 11:20** Concluding Remarks.

### Section C

- US Grant Hotel  
Crystal Ballroom
- General Papers**  
B. Park, *Organizer, Presiding*
- 8:00** Introductory Remarks.
- 8:05 AGFD 184.** Making synthetic starch (amylose and amylopectin) from nonfood biomass. **Y. Zhang**
- 8:30 AGFD 185.** Effect of sulfite on the reactivity of exogenous acetaldehyde with wine flavonoids. **M.K. Sheridan**, R. Elias
- 8:55 AGFD 186.** Dietary flavonoid luteolin chemosensitizes ovarian cancer cells by inhibiting FAK-mediated epithelial-to-mesenchymal transition. **V.P. Dia**, P. Pangloli
- 9:20 AGFD 187.** Effect of cooking on saponins content in pigmented chickpea. **A.K. Milan**, J. Gutierrez-Urbe, S. Serna-Saldívar
- 9:45** Intermission.
- 10:05 AGFD 188.** Hydrophobically-modified nanoporous silica aerogel: Novel food-contact surface inhibiting adhesion of gram-negative and gram-positive bacteria. **J. Oh**, L. Cisneros-Zevallos, M. Akbulut
- 10:30 AGFD 189.** Bioavailability of cranberry flavonoid glycosides and flavan-3-ols in healthy female adults. **Y. Wang**, T. Wilson, A.P. Singh, N. Vorsra
- 10:55 AGFD 190.** Inhibitory effect of *Gynostemma pentaphyllum saponin* on adipogenesis of 3T3-L1 cells through modulating Wnt/ $\beta$ -catenin pathway and cell cycle in mitotic clonal expansion. **J. Liu**, P. Yang, H. Shi, X. Sun, L.L. Yu
- 11:20 AGFD 191.** Development of graphene based room temperature gas sensors for agricultural applications. **H. Park**
- 11:45** Concluding Remarks.

## WEDNESDAY AFTERNOON

### Section A

- US Grant Hotel  
Celestial Ballroom
- Natural & Modified Carbohydrate Polymers Effects on Obesity Related Metabolic Diseases**  
M. Turowski, *Organizer*
- M. Kale, W. H. Yokoyama, *Organizers, Presiding*
- 1:00** Introductory Remarks.
- 1:05 AGFD 192.** Bioactive pectic oligosaccharides and obesity. **A.T. Hotchkiss**
- 1:30 AGFD 193.** Prevention of metabolic diseases by HPMC, a non-fermentable fiber. **M. Turowski**, W.H. Yokoyama
- 1:55 AGFD 194.** Impact of processing on physicochemical properties and nutritional function of dietary fibers: Balancing consumer taste and tangible health effects. **N. Bordenave**
- 2:20** Intermission.
- 2:40 AGFD 195.** Characteristics of EGCG loaded modified starch during digestion. **Y. Li**, F. Wang, F. Zhong
- 3:05 AGFD 196.** Bioactive polysaccharides and gut microbiome. **W.H. Yokoyama**, M. Turowski
- 3:30** Concluding Remarks.

### Section B

- US Grant Hotel  
Grant Hall
- Public Health Perspectives of Mycotoxins in Food**  
*Cosponsored by AGRO and ANYL*
- L. Jackson, D. Ryu, *Organizers, Presiding*
- 1:00** Introductory Remarks.
- 1:05 AGFD 197.** Immunochemical methods for rapid screening of (multi)mycotoxins. **S. De Saeger**, N. Beloglazova, I.Y. Goryacheva
- 1:35 AGFD 198.** Application of nanobodies, sensors and other immunochemical techniques for the analysis of mycotoxins and other small molecules. **C.S. Bever**, S.J. Gee, B.D. Hammock
- 2:05 AGFD 199.** Waveguide optical immunosensors for the simultaneous detection of melamine and aflatoxin M1 and kinetic analysis. **H. Guo**, X. Zhou, H. Shi
- 2:35** Intermission.
- 2:50 AGFD 200.** Development and evaluation of multi-mycotoxin analysis in foods by liquid chromatography-mass spectrometry (LC-MS/MS and LC-HRMS). **K. Zhang**, J.W. Wong, C. Liao, A.J. Krynski, M. Trucksess
- 3:20 AGFD 201.** FDA regulatory program for mycotoxins in food. **H. Kim**
- 3:50 AGFD 202.** Regulation of mycotoxins in Canada. **E. Elliot**, L. Pelletier, **G. Bondy**
- 4:20** Concluding Remarks.

### Section C

- US Grant Hotel  
Crystal Ballroom
- General Papers**  
B. Park, *Organizer*
- B. D. Guthrie, *Presiding*
- 1:00** Introductory Remarks.
- 1:05 AGFD 203.** Withdrawn.
- 1:30 AGFD 204.** Synthesis of 1,2,4,5-tetraoxanes derived from naphthaleneacetic acid with potential herbicide activity. **T.D. Silva**, I. Antolinez, A. Silva, L. Barbosa, J. Boukouvalas
- 1:55 AGFD 205.** Effect of organic matter on phosphorus recovery in dairy waste. **A. Silchuk**, S.J. Parikh, K.M. Scow, S. Kim
- 2:20 AGFD 206.** Understanding flavor in California almonds. **S. Charoenprasert**, G. Huang, P. Wylie, **A.E. Mitchell**
- 2:45** Intermission.
- 3:05 AGFD 207.** Towards understanding induced resistance of ash (*Fraxinus spp.*) against emerald ash borer using proteomics and metabolomics. **S. Chakraborty**, S.O. Opiyo, A.L. Hill, D. Cipollini, D.A. Herms, P. Bonello
- 3:30 AGFD 208.** Formation of 3-MCPD fatty acid esters from monostearin and thermal decomposition of 3-MCPD mono-fatty acid ester. **Y. Zhao**, Y. Zhang, Z. Zhang, B. Gao, H. Shi, L.L. Yu
- 3:55 AGFD 209.** Tuning mechanical, barrier and thermal properties of poly(lactic acid) using polymorphic cellulose nanocrystals. **P. Dhar**, D. Tarafdar, A. Kumar, V. Katiyar
- 4:20 AGFD 210.** When *in silico* meets *in vitro*: Molecular basis of function of an anion-permeable efflux transporter from barley (*Hordeum vulgare* L.). **A. Singh**, Y. Nagarajan, M. Hrmova, Y.G. Yingling
- 4:45** Concluding Remarks.

## AGRO

## Division of Agrochemicals

J. Gan, Program Chair

## SUNDAY MORNING

## Wolfrom Award

Sponsored by CARB, Cosponsored by AGRO

## TUESDAY MORNING

## Public Health Perspectives of Mycotoxins in Food

Sponsored by AGFD, Cosponsored by AGRO and ANYL

## TUESDAY AFTERNOON

## Public Health Perspectives of Mycotoxins in Food

Sponsored by AGFD, Cosponsored by AGRO and ANYL

## WEDNESDAY MORNING

## Public Health Perspectives of Mycotoxins in Food

Sponsored by AGFD, Cosponsored by AGRO and ANYL

## WEDNESDAY AFTERNOON

## Public Health Perspectives of Mycotoxins in Food

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## ANYL

## Division of Analytical Chemistry

J. Harris and L. Baker, Program Chairs

## SUNDAY MORNING

## Section A

Wyndham San Diego Bayfront  
East Coast

## Luminescent Proteins, Dyes &amp; Sensors

H. Ai, Organizer, Presiding

**8:10 ANYL 1.** Radioisotope-responsive polystyrene-silica core-shell nanoparticles used in scintillation proximity assay for tritium. **I. Calderon, C. Janczak, E. Noviana, C.A. Aspinwall**

**8:30 ANYL 2.** New strategy of colorimetric and fluorescent dual probe for hypochlorite based on stimuli-responsive infinite coordination polymer nanoparticles. **X. Zhang, J. Deng, T. Zhou**

**8:50 ANYL 3.** Single fluorescent protein-based indicators for zinc ion ( $Zn^{2+}$ ). **Z. Chen, H. Ai**

**9:10 ANYL 4.** Evolving fluorescent proteins for enhanced photostability and brightness. **M. Wiens, F. Hoffman, R.E. Campbell**

**9:30** Intermission.

**9:45 ANYL 5.** Molecular engineering for imaging and reprogramming in live cells. **Y.P. Wang**

**10:10 ANYL 6.** Quantitative real-time imaging of glutathione dynamics. **J. Wang**

**10:35 ANYL 7.** Rationally-designed fluorogenic protease reporter visualizes spatiotemporal dynamics of apoptosis *in vivo*. **X. Shu**

**11:00 ANYL 8.** Imaging cell-cell contacts with bioluminescent proteins. **J.A. Prescher**

**11:25 ANYL 9.** Molecular probes for redox signaling and oxidative stress. **H. Ai**

## Section B

Wyndham San Diego Bayfront  
West Coast

## Sampling &amp; Processing of Biological Particles Enabled by Micro- or Nano-Fluidics

W. Zhong, Organizer, Presiding

**8:30** Introductory Remarks.

**8:35 ANYL 10.** Discovery of new therapies and diagnostics while studying blood-stream components with 3D-printed fluidic devices. **D. Spence**

**9:05 ANYL 11.** Use of integrated comprehensive droplet digital detection technology for single bacterial cell detection in blood. **W. Zhao**

**9:35 ANYL 12.** Exosome separation using electrical field flow fractionation and a new continuous SPLIT/FFF approach. **B. Gale, K. Petersen, M. Ornthai, J. Hood**

**10:05** Intermission.

**10:15 ANYL 13.** Replica molding of 3D printed structures into functional materials and its applications in tissue engineering and microfluidics. **H. Wu, H. Chan, Y. Chen**

**10:45 ANYL 14.** On-chip extraction of circulating microRNAs from various carriers. **W. Zhong, K. Flack, L. Jimenez**

**11:15 ANYL 15.** Modular microfluidic device for processing whole blood: Sorting, staining, and single cell analysis. **W. Shields, J. Wang, K. Ohiri, D. Murdoch, A. Armstrong, B. Yellen, G. Lopez**

**11:35 ANYL 16.** Bioinspired polydopamine-graphene oxide nano-interface enables ultrasensitive microfluidic analysis of exosomes. **P. Zhang, Y. Zeng, M. He**

## Multiscales Chemistry Energy

Sponsored by MPPG, Cosponsored by ANYL, BIOL, COMP and PHYS

## SUNDAY AFTERNOON

## Section A

Wyndham San Diego Bayfront  
East Coast

## Luminescent Proteins, Dyes &amp; Sensors

H. Ai, Organizer, Presiding

**1:15 ANYL 17.** Fluorescent probes for identification of enzymes in cells and tissues. **R.L. McCarley**

**1:40 ANYL 18.** Copolymerized fluorescent silica nanoparticles as reporters and sensors. **G. Patonay, M. Henary, G. Chapman, K. Emer**

**2:05 ANYL 19.** Photo-triggered and photo-calibrated release of nitric oxide and peroxyxynitrite. **Y. Yang**

**2:30 ANYL 20.** Triggered energy transfer chemiluminescence for *in vivo* imaging. **A.R. Lippert**

**2:55** Intermission.

**3:10 ANYL 21.** Fluorescent proteins: New uses in voltage sensing and molecular imaging. **M.Z. Lin**

**3:35 ANYL 22.** Redox-sensitive red fluorescent proteins for imaging redox dynamics in cellular compartments. **Y. Fan, H. Ai**

**3:55 ANYL 23.** Detection of arsenic in aqueous solution by an enzymatic catalysis system. **Y. Liu, W.C. Trogler**

**4:15 ANYL 24.** Novel ratiometric fluorescent probe for Ag<sub>2</sub> using thioflavin T-based organic/inorganic hybrid supraparticles. **Y. Li, M. Zhang, G. Shi**

**4:35 ANYL 25.** Withdrawn.

## Section B

Wyndham San Diego Bayfront  
West Coast

## Capillary Electrophoresis Applied to Bioanalysis

C. Harrison, Organizer, Presiding

**1:00** Introductory Remarks.

**1:05 ANYL 26.** Versatile capillary surface modifications for protein separation. **C. Harrison, S. Wells, E. De La Toba, J. Torres**

**1:25 ANYL 27.** Analysis of intracellular thiol metabolites in response to HNO using capillary electrophoresis. **N. Ke, G.M. Johnson, E.S. Gallagher, K.M. Miranda, C.A. Aspinwall**

**1:55 ANYL 28.** Capillary and microchip electrophoresis of pre-term birth biomarkers. **A. Woolley, A.V. Nielsen, V. Sahore, R. Knob**

**2:25** Intermission.

**2:40 ANYL 29.** In-line separation by capillary electrophoresis prior to analysis by top-down mass spectrometry for characterization of protein complexes. **J.K. Diedrich, X. Han, Y. Wang, M. Lavallee-Adam, J. Moresco, J.R. Yates**

**3:10 ANYL 30.** New diagnostic paradigms enabled by hyperresolution separations. **M.A. Hayes, C. Crowther, S. Hilton, P. Jones**

**3:40 ANYL 31.** Development of microchip electrophoresis methods and instrumentation for chiral amino acid analysis on future spaceflight missions. **P. Willis, J. Creamer, M.F. Mora**

**4:10 ANYL 32.** Postcapillary electrophoresis sample separation and encapsulation through microfluidic droplet formation. **C. Harrison, A.L. Vo, E. De La Toba, N. Kokiashvili**

## Section C

Wyndham San Diego Bayfront  
Bay Room

## XRF: Cutting Edge Elemental Spectrometry

G. J. Havrilla, Organizer, Presiding

**1:10** Introductory Remarks.

**1:20 ANYL 33.** Overcoming the self-shading problem in TXRF: Diagnostics and solutions using pL-printing and a color x-ray camera. **U.E. Fittschen, M. Menzel, S. Nowak, M. Radtke, K. McIntosh, O. Scharf, C. Strelli, V. Lopez, G.J. Havrilla**

**2:00 ANYL 34.** Imaging of hierarchical structures with x-rays. **P. Pianetta**

**2:40** Intermission.

**2:55 ANYL 35.** X-ray based spectro-imaging at the micro- and macroscopic scale: Looking at and below the surface of (painted) materials. **K.H. Janssens, F. Vanmeert, P. Ricciardi, S. Legrand, J. Caen, G. Van der Snickt**

**3:35 ANYL 36.** Mapping trace metals with x-ray fluorescence microscopy: Advances, applications, and unique opportunities. **S. Vogt**

**4:15 ANYL 37.** High resolution elemental imaging using advanced x-ray sources in environmental, earth and planetary science. **L. Vincze**

**4:55** Concluding Remarks.

## Global Initiatives in Research Data Management &amp; Discovery

## Global Landscape

Sponsored by CLINF, Cosponsored by ANYL, COMP, MED and PHYS

## SUNDAY EVENING

## Section A

San Diego Convention Center  
Sails Pavilion

## Analytical Division Poster Session

J. M. Harris, Organizer

**7:00 - 9:00**

**ANYL 38.** Imaging and spectroscopic analysis of portrait miniatures. **K.M. Passannante, R.R. Hark, J.L. Streb, E.F. Campbell**

**ANYL 39.** Application of Raman spectroscopy for revealing hidden texts and *in-situ* studies of inks, pigments and palimpsests in manuscripts. **F. Cappa, M. Schreiner, J. Hofner, P. Engel, B. Lendl**

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- ANYL 40.** Structural analysis of lead carboxylates and lead pigments found in traditional oil paintings by multinuclear NMR. **A. Murphy**, J. Catalano, Y. Yao, N. Zumbulyadis, S. Centeno, C.R. Dybowski
- ANYL 41.** Multitechnique characterization of white pigments on pre-Columbian Caribbean ceramic sherds. **A. Martnez**, I. Narganes, M. Rodriguez, I. Mendez, L. Chanlatte
- ANYL 42.** AFM-sampling-L2MS on painting cross-sections. **J. Berenbeim**, S. Owens, F. Siouri, S. Boldissar, E. Dillon, J. Brauer, C.M. Schmidt Patterson, M.S. Devries
- ANYL 43.** Quartz crystal microbalance and microkinetic modeling as complementary, non-destructive methods for tracking the physical and chemical stability of oil-based paints. **L.H. Oakley**, **L. Sturdy**, F. Casadio, K. Shull, L.J. Broadbelt
- ANYL 44.** Iron gall ink analysis of 15th century illuminated book of hours by Raman microscopy and x-ray fluorescence. **C.R. Sullivan**, A.M. Fleschman, B. Tilghman
- ANYL 45.** Microfluidic immunosensor arrays based on multi-labeled PEG-coated magnetic beads for detection of 2 cancer biomarker proteins in serum. **B.S. Munge**, K. Gamez, C. Morganti, D. DiBiase
- ANYL 46.** Multichannel impedance-based biosensing using virus-polyethyleneimine films for bladder cancer detection. **A. Ogata**, C. Eggers, R.M. Penner, G.A. Weiss
- ANYL 47.** Using microfluidic platforms to develop a model of cell-cell communication in cancer. **E. Cliff**, X. Wu, C.L. Haynes
- ANYL 48.** Development of a novel immunosorbent homogeneous assay system using luciferase-antibody complex and dye for luminescence absorption. **A. Mori**, T. Ojima-Kato, S. Fuchi, T. Kojima, H. Nakano
- ANYL 49.** Diagnosis of neuromyelitis optica using aquaporin-4 extracellular loop-based carbon nanotube biosensor. **T. Park**
- ANYL 50.** Enzyme immobilization by polydimethylsiloxane stamping for biosensor fabrication. **B. Wang**, B. Koo, H. Monbouquette
- ANYL 51.** Segmentally stratified differences in metabolite profiles along the rat colon. **M.M. Dinges**, C. Lytle, C.K. Larive
- ANYL 52.** Stabilizing enzymes in microfluidic paper analytical devices ( $\mu$ PAD) for diagnostic assays. **S. Wang**, M. Debela, N. Rehmeyer, K. Frederick
- ANYL 53.** Analysis of alpha-1 antitrypsin concentrations in serum samples using surface plasmon resonance. **S. Kim**, H.J. Lee
- ANYL 54.** Genetically encoded FRET sensor for the study of prolyl hydroxylase enzyme activity. **S. Youssef**
- ANYL 55.** Near-infrared, wavelength-shiftable, turn-on fluorescent probe for the detection and imaging of an intracellular enzyme upregulated in cancer cells. **Z. Shen**, B. Prasai, S.U. Hettiarachchi, R.L. McCarty
- ANYL 56.** Quantitative investigation of the effects of glucose on stored red blood cells. **R. Mu**, D.M. Spence
- ANYL 57.** Simultaneous microfluidic assays for quantitation of CD-62L and IL-6 protein biomarkers for metastatic bladder cancer. **G.S. Phadke**, J. Satterwhite, D. Choudhary, J. Taylor, J.F. Rusling
- ANYL 58.** 3D-printed, automated and low cost ECL arrays for detection of multiple prostate cancer biomarkers. **K. Kadimisetty**, S. Malla, J.F. Rusling
- ANYL 59.** Using open source hardware to construct diagnostic devices for the developing world. **K. Cantwell**, J. Bryant, K. Frederick
- ANYL 60.** Development of a paper microfluidic analytical device ( $\mu$ PAD) for detection of D-lactate in urine. **N. Rehmeyer**, S. Wang, M. Debela, K. Frederick
- ANYL 61.** Towards a fluorogenic enzyme complementation assay that uses an endogenous substrate. **L.C. Zarowny**
- ANYL 62.** Insight into proteolytic digestion. **L. Downer**
- ANYL 63.** Application of microwave-assisted extraction of oleandrin from *Nerium oleander* coupled with purification with using divalent metal ion-loaded cation exchange resins. **L.M. Jablonski**, D.B. Green
- ANYL 64.** Design of experiment optimization for on-column trypsin digestion of apolipoproteins and selection of target peptides with maximum cleavage rate. **C. Toth**, Z. Kuklenyik, J. Jones, B.H. Parks, M. Gardner, J. Rees, D. Schieltz
- ANYL 65.** Optimizing preparation conditions of live MDV infected samples for transmission electron microscopy. **A.L. Dolley**, Z.M. Fritz, H.H. Stenzel, K.W. Jarosinski, J.G. Nguyen
- ANYL 66.** Direct detection of microRNAs based on magnetic beads and enzyme label-released chemiluminescence assay. **H. Yang**, N. He, Z. Li, A. deMello
- ANYL 67.** Direct sensing of microRNAs based on magnetic bead-chemiluminescence platform and duplex-specific nuclease signal amplification. **H. Yang**, N. He, Z. Li, A. deMello
- ANYL 68.** Sensitivity of a multiplex PCR high resolution melt assay for food-borne pathogens *Salmonella enterica*, *Escherichia coli* and *Shigella flexneri*. **K.M. Elkins**, K.C. Sweetin
- ANYL 69.** Triplexed paper-based nucleic acid hybridization bioassay using upconverting nanoparticles as donors and quantum dots as acceptors for luminescence resonance energy transfer. **S. Doughan**, U.J. Krull
- ANYL 70.** Towards assays using intrinsically labeled oligonucleotide probes on QDs for detection of selective hybridization. **A. Shahmuradyan**, U.J. Krull
- ANYL 71.** Single-molecule kinetics study of a small-molecule-dependent split aptamer assembly. **F. Morris**, E.M. Peterson, M. Manhart, J.M. Heemstra, J.M. Harris
- ANYL 72.** Fluorescent perylene monoimide and cucurbit[8]uril complexes in water. **G. Aryal**, L. Huang, K.W. Hunter
- ANYL 73.** Efficient host-guest energy transfer in quantum dot-peryene diimides complexes in water. **G. Aryal**, L. Huang, K.W. Hunter
- ANYL 74.** Withdrawn.
- ANYL 75.** New NIR fluorescent probe for iridium(III) and its application for the highly selective detection of glutathione. **H. Chen**, F. Li, X. Bao
- ANYL 76.** Novel rhodamine B based thiol chemosensor with fluorescence enhancement. **H. Shu**, X. Bao
- ANYL 77.** Design and synthesis of a novel GSH fluorescent chemosensor based on rhodamine B and its application in living-cell imaging. **X. Wu**, X. Bao
- ANYL 78.** Fluorescent sensor based on BINOL for recognition of cysteine, homocysteine, and glutathione. **R. Peng**, X. Feng
- ANYL 79.** Determination of physicochemical parameters of chemical warfare nerve agents via potentiometric titrations. **J.M. McGuire**
- ANYL 80.** Alternative strategies for the fabrication of disk-shaped carbon fiber microelectrodes for fast-scan cyclic voltammetry measurements. **R.B. Keithley**, T.W. Beger, D.R. Miller
- ANYL 81.** Electrochemical studies of diamond microelectrode arrays: Application for the detection of pyocyanin. **A.D. Alica**, G. Swain
- ANYL 82.** Electrochemical analysis of silver nanowires fabricated in solution phase. **W. Sanders**, P.J. Iles, E. Staker, G. Glass, R. Holcomb, C.R. Thurman, M. Alvarez, N.R. Bastian, L.D. Giddings, R.V. Valcaro
- ANYL 83.** Detection of iron-rich protein binding to tau by electrochemical impedance spectroscopy. **A. Jahshan**, J.O. Esteves-Villanueva, S. Martic
- ANYL 84.** Withdrawn.
- ANYL 85.** Real-time monitoring the redox reaction between hydroquinone and silver ion at single-particle level. **M. Li**, T. Xie, Y. Long
- ANYL 86.** Laminar-flow based microfluidic microbial three-electrode cell for biosensing. **Z. Li**
- ANYL 87.** New analytical method for the measurement of sub ppb levels of inorganic arsenic in drinking water and fruit juices by HG/GC/PID. **J.N. Driscoll**, J.L. MacLachlan
- ANYL 88.** Quantification of aqueous pollutant phototoxicity: Singlet oxygen production of polycyclic aromatic hydrocarbons in octanol. **M. Rifkin**, J.K. Hartman, B. Huynh, M. Wang, S.L. Neal
- ANYL 89.** Fully automated dispersive liquid-liquid microextraction and on-column derivatization combined with gas chromatography: Mass spectrometric analysis for the determination of carbamate pesticides in environmental water samples. **L. Guo**, H. Lee
- ANYL 90.** Probing the effect of glyphosate on *Artemia salina*: An environmental metabolomics approach. **M. Morgan**, C.K. Larive
- ANYL 91.** Determination of fatty acid concentrations in algae. **D. White**, A.L. Williams
- ANYL 92.** Toxic effects of a once thought bioinactive chromium species. **J. Arroyo**, M. Malham, R. Dale, M. Schmeling
- ANYL 93.** Selective removal of strontium ions from simulated wastewater. **S. Selem**, M. Ndao, H. Ghassemi
- ANYL 94.** Investigation of the binding of potentially toxic heavy metal ions (Hg(II), Cd(II), As(III), and Cr(VI)) with human serum albumin by use of UV-visible absorption spectroscopy. **N. Whitehead**, E. Ampiah, S.O. Fakayode
- ANYL 95.** Simultaneous and multicomponent analyses of Hg (II), As (III), Cr (VI), Cd (II), and Pb (II) ion concentrations in human serum albumin by steady state fluorescence spectroscopy and multivariate regression analysis. **E. Ampiah**, S.O. Fakayode
- ANYL 96.** Investigation of the deposition of lead in zebrafish eyes. **K. Niaz**, J. Arroyo, M. Schmeling
- ANYL 97.** Structure and behavior of alkylphenols in humic acid. **I. Larraza**, E. Mordan, A. Vazquez
- ANYL 98.** Recovery of malathion from soil. **M. Potter**, C.A. Burkhardt
- ANYL 99.** Quantification of chromium in biological matrices. **J. Batycki**, J. Arroyo, M. Schmeling
- ANYL 100.** Analysis of fluoride and pH, in Utah waters and drinks. **P.J. Iles**, S. Moore, R. Holcomb, A. Rihm, A. Abbainanti, W. Ballard, T. Fullmer, L.D. Giddings, M. Alvarez, N.R. Bastian, R.V. Valcaro
- ANYL 101.** Investigation of the use of transition metal ions to remove chloride interference from nitrate ISEs. **P.J. Iles**, S. Moore, R. Holcomb, A. Rihm, L. Peralta, K. Jones, A. Abbainanti, T. Fullmer, W. Ballard, P. Schofield, L.D. Giddings, M. Alvarez, N.R. Bastian, R.V. Valcaro
- ANYL 102.** Determination of perfluorinated compounds in influents/effluents from wastewater treatment plants using ion chromatography. **I. Gavilan**, E. Becerril, E. Santos, J. Olmos
- ANYL 103.** Continued identification of pharmaceuticals in Utah's Jordan River. **N. Elmore**, H. Capps, S. Quintero, H. Hsieh, A. Teler, P.J. Iles, L.D. Giddings, M. Alvarez, N.R. Bastian, R. Holcomb, R.V. Valcaro
- ANYL 104.** Atrazine detection using GC-FID in the Macomb watershed. **S.L. Crawford**, B.J. Bellott
- ANYL 105.** Field evaluation of gold based nanosensor in a local sheep farm. **K. Weghorst**, S. Saranathan, A. Zambre, S. Prayaga, A. Upendran, R. Kannan, Z. Afrasabi
- ANYL 106.** Determination of steroid hormones in aqueous solution using high performance liquid chromatography. **P. Maldonado Pereira**, D. Román
- ANYL 107.** Developing a safer, optimized method for determining Pb in paint. **S. Lowery**, M.J. Crawford
- ANYL 108.** Determination of dibutyl phthalate in infant formula. **D. Lewis**, J.M. Bowen
- ANYL 109.** Leaching of phthalate esters into tap water with time from a commercially obtained PVC water hose using SPME-GC-MS. **M. Weems**, E. Brooks, M. Jezercak, J.M. Bowen
- ANYL 110.** Simultaneous toxicological screening of multiple drugs in human urine by on-line SPE-LC-Qq-MS analysis. **V. Linero**, L.E. Arroyo-Mora, A. De Caprio
- ANYL 111.** Investigating the LC-MS method for enzyme catalyzed reactions in biological samples. **Y. Lu**, C. Jeffries, L. Yang, T. Moriyama, J. Yang, C.J. Neely, P.J. Murray
- ANYL 112.** Profiling protein phosphatase activity using peptide arrays and mass spectrometry. **J. Su**, C. Kalinich, R. Seltor, M. Mirksich
- ANYL 113.** Revealing the effect of zeta potential in cell secreted extracellular matrix with time-of-flight secondary ion mass spectrometry. **W. Kao**, H. Chang, J. Shyue
- ANYL 114.** Development of a liquid chromatography-mass spectrometry method for the determination of aromatic amines in azo pigments used in tattoo inks. **M. Perez-Gonzalez**, J.N. Barrows, L.M. Diaz-Vazquez, O. Rosario, B. Petigara Harp
- ANYL 115.** Investigation of biomarkers indicative of laser-induced retinal damage by using mass spectrometric imaging. **M.J. Swanson**, F.J. Schaffer, R. Reich

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

- ANYL 116.** Identification of biomarkers indicative of neurological effects due to jet fuel exposure in rats using mass spectrometric imaging. F.J. Schaffer, M.J. Swanson, R. Reich
- ANYL 117.** Determination of dimethyl trisulfide (DMTS) in rabbit blood by using stir bar sorptive extraction (SBSE): Gas chromatography-mass spectrometry (GC-MS). E. Manandhar, B.A. Logue
- ANYL 118.** Coupling of paper-based microfluidic separation devices and time-of-flight secondary ion mass spectrometry for analyzing molecular mixtures. C. Wu, J. Shyue
- ANYL 119.** Headspace GC-MS vapor pressure measurement of volatile organic compounds over ionic liquid solutions. A.T. Tran, P.H. Lam, L. Yu
- ANYL 120.** Calibrating a matrix-assisted laser desorption/ionization reflectron time-of-flight mass spectrometer. M. Patterson, K.A. Reyes, K. King, C.J. Van Leeuwen, H. Hamilton, L. Barnes, P.M. Kirkconnell, K. Molek
- ANYL 121.** UPLC-MS to assist in improving the transparency of a Dow adhesive product. J. Qi, J. Bush
- ANYL 122.** Direct analysis from TLC plate using matrix assisted ionization (MAI). K. Hoang
- ANYL 123.** Effect of cluster size and energy of argon gas cluster sputter yields on the depth profiling of organic light-emitting devices. Y. You, Y. Lee
- ANYL 124.** SAMDI: Mass spectrometry for characterizations of lipoid acid derivatives on coated gold substrates. H. Yang, Q.J. Cheng
- ANYL 125.** Determination of tissue specific cancer of chemical/metabolites based on sequence specific DNA damage across the exons of P53 gene fragments using LC-MS/MS and Magnetic Bio-colloid technology. S. Malla, K. Kadimisetty, J.F. Rusling
- ANYL 126.** Determination of trace organic constituents in the color additives FD&C Yellow No. 5 and FD&C Yellow No. 6 using LC-MS/MS. N. Belai, A. Baldo
- ANYL 127.** Surface assisted laser desorption/ionization of asphaltenes using transition metal oxide nanoparticles. K.A. Reyes, K. King, M. Patterson, H. Hamilton, L.F. Barnes, P.M. Kirkconnell, K.S. Molek
- ANYL 128.** Rapid detection of endotoxin contamination in ophthalmic medical device materials using direct analysis in real time mass spectrometry. H. Li, V. Hitchins, S.I. Wickramasekara
- ANYL 129.** Influence of proton mobility, glycopeptide composition and charge carrier on energy-resolved collision-induced dissociation of tryptic N-glycopeptides. F. Aboufazel, V. Kolli, E.D. Dodds
- ANYL 130.** Utilizing volatile organic compounds to differentiate between methicillin resistant and sensitive strains of staphylococcus aureus using solid phase micro extraction (SPME) and gas chromatography-mass spectrometry (GC-MS). G. Dressler, J.M. Bowen, R. Brennan, D.L. Von Minden
- ANYL 131.** Towards a better understanding of spectral similarity between structurally related compounds. J. Schollee, R. Gulde, E.L. Schymanski, J. Hollender
- ANYL 132.** Hydrogen/deuterium exchange mass spectrometry in the drug discovery scene: Application to protein-protein interactions. A. Espada, H. Broughton, J.A. Dodge, S. Jones, S. Afshar, M. Grogan, M. Chalmers
- ANYL 133.** Synthesis, characterization and adsorption performance of molecularly imprinted nanoparticles for ursolic acid by precipitation polymerization. J. Lei
- ANYL 134.** Investigation of silver nanoparticle interactions with manganese dioxide using x-ray spectroscopic and microscopic techniques. S.R. Kanel, B.A. Manning, S. Brittle, I.E. Pavel Sizemore
- ANYL 135.** Nanopore analysis of low molecular weight poly(ethylene glycol) with enhanced resolution. C. Cao, Y. Ying, Z. Gu, H. Zhang, Y. Long
- ANYL 136.** Gold-silver alloy nanoparticles synthesis and influence on fluorescent properties. T.R. Brewer, C. Mac, R. Kondaveeti, R. Sullivan
- ANYL 137.** Graphene oxide derivatives as nanocarriers for delivery of anti-tumor agents into hela cells. P. Shanta, Q.J. Cheng
- ANYL 138.** Separation of photoluminescent carbon dots via capillary electrophoresis coupled to laser induced fluorescence detection. L. Saint-Fort, K.M. Tirado, Z. Xue, L.A. Colon
- ANYL 139.** ROS scavenging ability of graphene-based water splitting catalyst scaffolds optically sensed with DNA-encased single-walled carbon nanotubes. B. Ergul, J. Kuang-Nguyen, W. Zhao
- ANYL 140.** Assessment of ROS scavenging ability of water splitting catalysts molybdenum disulfide and tungsten disulfide. K. Wong, M. Simmons, W. Zhao
- ANYL 141.** Fabrication, characterization, and application of carbon nanoparticles for detection of heavy metal ions in aqueous media. A. Simpson, R.V. Aaryasomayajula, A. Wanekaya
- ANYL 142.** Smart optical sensor for amyloid  $\beta$  detection and fibrillation evaluation on the basis of nanoparticle assemblies. Z. Qu, M. Zhang, G. Shi
- ANYL 143.** pH and surface charge study of the adsorption behavior of silver nanoparticles to corundum mineral. K.A. O'Neil, S. Brittle, S.R. Higgins, I.E. Pavel Sizemore
- ANYL 144.** Analysis and characterization of mesembrine type alkaloids obtained from *Scelotium tortuosum*. D. Schrum, J.L. Krstenansky, R. Hendry, D. Santeliz
- ANYL 145.** Determination of trace elements, essential oils, and pharmacologically active components of Arabian annona natural products. A. Alzahrani, H. Kumakli, T. Mehari, E. Amphah, C. Babyak, S.O. Fakayode
- ANYL 146.** Synthesis, characterization, and validation of base-mediated degradation product of betamethasone-17-benzoate. D. Biswas, F. Tadjimukhamedov, D. Tran, S. Tan, J. Belsky, J.T. Simpson
- ANYL 147.** Withdrawn.
- ANYL 148.** Isolation and structural elucidation of tetracyclic diterpenoids from marine soft coral *Briareum asbestinum*. L. Zhang, D. Minond, L. West
- ANYL 149.** Detection of quercetin, gallic acid, and ferulic in ebony tree seeds by means of column chromatography including RP-HPLC. J. Lara
- ANYL 150.** Analysis of quercetin and resveratrol in Chinese fruit using HPLC. Q. Jin, J. Liu, J.M. Bowen
- ANYL 151.** Characterization of the cephalopod structural protein reflectin. K.L. Naughton
- ANYL 152.** CRAFT beer: Quantitation of the major components of commercially available sour beers using time-domain CRAFT analysis of  $^1\text{H}$  NMR spectra. D.P. Soulsby
- ANYL 153.** Generic applications of  $^{13}\text{C}$  detected NMR diffusion to formulated systems with suppression of thermal convection. J. Hou, Y. He, P. Sabatino, L. Yuan, D. Redwine
- ANYL 154.** Theoretical study of partition-layer enhanced SERS sensors for polychlorinated biphenyls. E.O. Fetisov, J.I. Siepmann
- ANYL 155.** Indirect detection of metals in ammonium nitrate using handheld Raman spectroscopy. E. Boyle, O. Primera-Pedrozo, C. Fraga
- ANYL 156.** Determination of adulterated lemon eucalyptus oil compositions by fourier transform infrared spectroscopy and multivariate partial-least-regression analysis. B. Elzey, D. Pollard, S.O. Fakayode
- ANYL 157.** Novel SERS-based approach to detect o-phenylenediamine by using drop coating deposition Raman technique. W. Qian, X. Pan, J. Dong, C. Yuan
- ANYL 158.** Vibrational and thermal analysis of the interactions between the peptide jellein-1 and model membranes. N. Andijani, N. Phambu
- ANYL 159.** Atomic force microscopy (AFM) and Raman spectroscopy of a binary lipid mixture containing cardiolipin. A. Alwadai, N. Phambu, A. Sunda-Meya
- ANYL 160.** Spurious quantum beats at the low photon-flux level. R. Leon-Montiel, J. Yuen Zhou
- ANYL 161.** Analysis of crystalline hydrates using near-infrared spectroscopy to differentiate between polymorphic structures and quantitatively determine water content. E. Towns, J. Li, J. Stults, P. Yehl
- ANYL 162.** Investigation of partitioning kinetics into individual chromatographic particles by confocal Raman microscopy. D. Bryce, J.P. Kitt, J.M. Harris
- ANYL 163.** Chiral separations in CE using cationic cyclodextrins as a buffer additive. S. Markiewicz, J. Greenspan, T.J. Wenzel, K. Frederick
- ANYL 164.** Evaluation of an L-phenylalanine-based ionic liquid for its GC stationary phase ability. I. Kimaru, A. Russo
- ANYL 165.** Capillary electrophoretic isolation of aptamers that selectively bind cancerous glycoforms of thrombospondin-1. E.D. Berggren, E.G. Carlson, M.A. Ueno, N.W. May, S.W. Suljak
- ANYL 166.** Direct fluorination of fused silica capillary surfaces. C. Lumba, C. Harrison
- ANYL 167.** Combining capillary electrophoresis and microfluidic droplets to separate and detect fluorescent biomolecules. E. De La Toba, A.L. Vo, N. Kokiashvili, C. Harrison
- ANYL 168.** Metal cations to control electroosmotic flow and phospholipid stability in capillary electrophoresis. S. Wells, E. De La Toba, C. Harrison
- ANYL 169.** Analyte concentration distribution in a silica separation column. J.A. Spies, A. Gates, D. Poerio, B.H. Milosavljevic
- ANYL 170.** Efficiency study of porous polymer monoliths with different mobile phase and stationary phase compositions using capillary electrochromatography (CEC) and scanning electron microscope (SEM). T. Tian, M.M. Bushey
- ANYL 171.** Simple but powerful headspace extraction methods using a commercial capillary electrophoresis instrument. S. Cho, H. Lee, J. Kim, D. Chung
- ANYL 172.** Stability indicating liquid chromatographic method development for the estimation of atorvastatin in bulk drug and pharmaceutical formulation. M. Semreen
- ANYL 173.** Development of a fully automated HPLC system (ASAPrep™) designed for multiple compound purifications. K. Miwa, C. Kushibe, H. Terada, Y. Katsuyama
- ANYL 174.** Application of static headspace gas chromatography-flame ionization detection in determination of chlorobenzenes and benzene series in aqueous environment. H. Hu, X. Zhang
- ANYL 175.** Qualitative and quantitative examination of volatile organic compounds using evolved gas analysis (EGA). A.M. Wilson, M.J. Samide, K. Ferguson, C. Schmicker, T. Schenck, D.L. Shinholt, J. Smith, S. Pate
- ANYL 176.** Development and optimization of an ion-exchange HPLC method for quantification of succinic acid in cerebral tissue. A. Siegel, A. Ferro, S. Lagalwar, K. Frederick
- ANYL 177.** Determination of aminothiols in blood and tissue by high performance liquid chromatography coupled with post-column derivatization and fluorescence detection. M.B. Blayney, S.E. Helm, D.B. Green
- ANYL 178.** Determination of p-toluene-sulfonic acid in biodiesel sample by reverse phase high performance liquid chromatography. C. Maldonado Figueroa, F.R. Roman
- ANYL 179.** Forensic analysis of lipstick samples by three different analytical techniques. B. Esterlen, B.J. Bellott

## MONDAY MORNING

### Section A

Wyndham San Diego Bayfront  
East Coast

### Protein Structure & Folding: From Solution to the Gas Phase

Cosponsored by PHYS

D. E. Clemmer, D. H. Russell, *Organizers, Presiding*

8:20 Introductory Remarks.

8:40 ANYL 180. Pumps, pores and channels: Out of the membrane into the gas phase. C.V. Robinson

9:20 Discussion.

9:25 ANYL 181. Insights into protein complex structure from surface-induced dissociation MS coupled to ion mobility or high resolution analysis. V.H. Wysocki

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9:55 Intermission.

10:10 ANYL 182. Collisional unfolding of gas-phase proteins: Enabling technology for protein engineering, drug discovery, and the development of biotherapeutics. B.T. Ruotolo

10:40 Discussion.

10:45 ANYL 183. Towards biophysical characterization of individual lipid binding events to membrane proteins. X. Cong, Y. Liu, W. Liu, Z. Talley, D.H. Russell, A. Laganowsky

11:15 Discussion.

11:20 ANYL 184. Charge detection mass spectrometry: Applications to virus analysis and assembly. M. Jarrold

11:50 Discussion.

## Section B

Wyndham San Diego Bayfront  
West Coast

### Electrochemical Measurements at Biological Interfaces

L. A. Baker, *Organizer, Presiding*

8:10 ANYL 185. Neuropeptide-induced mast cell degranulation and characterization of signaling modulation in response to IgE conditioning. S.M. Gruba, B. Manning, A.F. Meyer, C.L. Haynes

8:30 ANYL 186. All-printed wearable electrochemical sensors and biofuel cells. A.J. Bandojar, J. Wang

8:50 ANYL 187. Wearable salivary uric acid mouthguard biosensor with integrated wireless electronics. J. Kim, J. Wang

9:10 ANYL 188. Molecular smart surface for spatio-temporal studies of cell mobility. M.N. Yousaf

9:30 ANYL 189. Experimental measurement of the thermodynamics underlying the surface-induced structural changes of nucleic acids and proteins. M. Kurnik, N. Arroyo-Currás, H. Li, D. Kang, K. Plaxco

9:50 Intermission.

10:00 ANYL 190. Electrochemical detection of metal coordination to tau peptides/protein and evaluation of hydrogen peroxide formation. S. Martic

10:20 ANYL 191. Plasmonic imaging of cellular processes. N. Tao

10:45 ANYL 192. Direct investigation of metabolomics at single-cell level with nanopipettes. E. Ozel, N. Pourmand

11:05 ANYL 193. High resolution imaging of live cell dynamics using scanning ion conductance microscopy (SICM). M. Choi, G. Jung, Y. Cho, S. Park, S. Cho

11:25 ANYL 194. Scanning electrospray microscopy: Nontraditional electrochemical imaging. L.A. Baker

## Section C

Wyndham San Diego Bayfront  
Bay Room

### XRF: Cutting Edge Elemental Spectrometry

G. J. Havrilla, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 ANYL 195. Revolutionary x-ray microbeam delivery system for MicroXRF. W. Yun

8:40 ANYL 196. 3D elemental identification and quantification using confocal x-ray fluorescence. J. Mertens, B.M. Patterson, N. Cordes, K. Henderson, J. Griego, T. Day, D. Schmidt, G.J. Havrilla

9:05 ANYL 197. Overview of the Mars 2020 mission micro-XRF instrument PIXL. L. Wade, A. Allwood, M. Foote, D. Dawson, C. Liebe, E. Ek, M. Schein, S. Pootrakul, B. Hernandez, R. Sharrow, S. Battel, K. Arnett, K. Kozaczek, T. Parker, N. Gao, J. Hurowitz, T. Elam, E. Hertzberg

9:30 ANYL 198. Development of hiRX for measurement of plutonium in spent nuclear fuel. G.J. Havrilla, K. McIntosh, M. Holland, R. Gilmore

9:55 Intermission.

10:10 ANYL 199. Role of portable energy dispersive XRF instrumentation in state public health laboratories. P.J. Parsons, D. Guimarães

10:35 ANYL 200. Tracking architectural ceramic provenance using trace element analysis with handheld XRF. A. Uebel, S. Crette

11:00 ANYL 201. Mapping of the spatial distribution of thin coatings using x-ray fluorescence (XRF). D.A. Summa, K.J. Hollis, V.M. Lopez, G.J. Havrilla

11:25 ANYL 202. Harvesting the benefits of high count rates in modern ED-XRF. J. Heckel, D. Sachtler, D. Wissmann, M. Daniel-Prowse, M. DeLeon

11:50 Concluding Remarks.

### Global Initiatives in Research Data Management & Discovery

#### Role of Community & Standards

Sponsored by CINF, Cosponsored by ANYL, COMP, MEDI and PHYS

#### GSSPC: Resolving the Big Picture: Bringing Molecules into Focus

Sponsored by CHED, Cosponsored by ANYL+, MPPG and PROF+

#### Advances in Chemical Imaging: Ultra-Resolution to Single Molecules

Sponsored by SOCED, Cosponsored by ANYL and PHYS

## MONDAY AFTERNOON

### Section A

Wyndham San Diego Bayfront  
East Coast

#### Protein Structure & Folding: From Solution to the Gas Phase

Cosponsored by PHYS

D. E. Clemmer, D. H. Russell, *Organizers, Presiding*

1:30 ANYL 203. Probing the early stages of aggregation of intrinsically disordered peptides. J.E. Shea

2:10 Discussion.

2:15 ANYL 204. Evolution of protein structure in electrospray ionization: From solution into the gas phase. E.R. Williams, D. Mortensen, Z. Xia, C. Goings

2:45 Discussion.

2:50 ANYL 205. Mass spectrometry and structural biology: Ion mobility-mass spectrometry studies of water and water-mediated conformational preferences of peptides and proteins. D.H. Russell

3:20 Discussion.

3:25 ANYL 206. Resonance Raman and fluorescence investigations of membrane protein folding. J.E. Kim, G. Kang, D.K. Asamoto, I. Kozachenko

3:55 Discussion.

4:00 ANYL 207. Amino acid and peptide assembly. M.T. Bowers

4:30 Discussion.

4:35 Concluding Remarks.

## Section B

Wyndham San Diego Bayfront  
West Coast

### Nonlinear Spectroscopy & Modeling

Cosponsored by MPPG and PHYS

M. C. Thielges, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 ANYL 208. Probing and understanding quantum beating signals in rigid heterodimers with 2D spectroscopy. G.S. Engel

1:45 ANYL 209. Dissecting the molecular structure of the air/water interface from many-body simulations of sum-frequency generation spectra. F. Paesani

2:10 ANYL 210. Light, electrons, protons: From their interplay in model systems to applications. J. Dawlaty, S.A. Sorenson, E. Driscoll, A. Rury, S. Haghighat, J. Patrow, S. Ostresh

2:35 ANYL 211. Harnessing shared vibrations for energy transfer. P. Foster, A. Carollo, D.M. Jonas

3:00 Intermission.

3:15 ANYL 212. How is momentum conserved in charge separation in 2D crystal heterostructure? J. Zheng

3:40 ANYL 213. Calculating multidimensional vibrational spectra from classical trajectories. R.F. Loring

4:05 ANYL 214. Site-specific dynamics of protein molecular recognition via 2D IR spectroscopy. M.C. Thielges

4:30 Concluding Remarks.

## Section C

Wyndham San Diego Bayfront  
Bay Room

### Analytical Methodologies & Research Partnerships at the Interface of Chemistry & Art/Archeology

M. S. Devries, C. M. Schmidt Patterson, *Organizers*

K. A. Trentelman, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 215. Sustainable preservation of cultural heritage: An interdisciplinary effort in partnership. S. Simon

1:35 ANYL 216. Nanoscale chemical analysis using AFM based IR spectroscopy and mass spectrometry. K. Kjoller, Q. Hu, E. Dillon, C. Prater

1:55 ANYL 217. 3D chemical imaging of historic artworks and cultural heritage materials. T.E. Villafana, B. Brown, J. Delaney, M. Fischer, W.S. Warren, S. Stranick

2:15 ANYL 218. Colorimetric sensor arrays for monitoring pollutant exposure of artwork. K.S. Suslick, M. LaGasse, K. McCormick, H. Khanjian, M. Schilling

2:45 ANYL 219. Clean & check method for the simultaneous recognition of albumen and yolk by biosensing: Application in cultural heritage conservation. E. Carretti, S. Scarano, L. Dei, M. Minunni, P. Baglioni

3:05 Intermission.

3:20 ANYL 220. Deciphering ancient materials heterogeneity at the sub-microscale with synchrotron deep UV imaging.

M. Thoury, T. Séverin-Fabiani, M. Refregiers, U. Bergmann, L. Bertrand

3:40 ANYL 221. Comparison of terahertz and multispectral images of a Tando painting. J. Jackson, M. Melis, D. Giovannacci, G. Walker, D. Martos-Leviv, J. Bowen, V. Detalle

4:00 ANYL 222. Infrared imaging of art objects: Is it as easy as it sounds? T.J. Tague

4:20 ANYL Withdrawn.

4:40 ANYL 224. Withdrawn.

### Global Initiatives in Research Data Management & Discovery

#### Technical Infrastructures: Enabling Cultural Shifts

Sponsored by CINF, Cosponsored by ANYL, COMP, MEDI and PHYS

#### GSSPC: Resolving the Big Picture: Bringing Molecules into Focus

Sponsored by CHED, Cosponsored by ANYL+, MPPG and PROF+

### Undergraduate Research Posters

#### Analytical Chemistry

Sponsored by CHED, Cosponsored by ANYL and SOCED

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

L. A. Baker, J. M. Harris, *Organizers*

8:00 - 10:00

1, 12, 14, 17, 30, 38, 43, 45, 47-48, 57-58, 61, 69, 71, 84, 112, 125, 132, 159, 162, 177, 183, 211, 214, 217. See previous listings.

246, 267, 275-276, 279, 315, 317-318, 321, 359. See subsequent listings.

## TUESDAY MORNING

### Section A

Wyndham San Diego Bayfront  
East Coast

#### Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Symposium in honor of Albert J. R. Heck

Cosponsored by PHYS

D. E. Clemmer, *Organizer, Presiding*

8:10 Introductory Remarks.

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- 8:20 ANYL 225.** Ultraviolet photodissociation mass spectrometry for biological applications. **J. Brodbelt**
- 8:50 ANYL 226.** Pathways and thermodynamics of polyproline helix formation in solution from measurements of ions in the gas phase. **D.E. Clemmer**
- 9:20 ANYL 227.** Determination and quantitation of site-specific protein glycosylation. **C. Lebrilla**
- 9:50 ANYL 228.** Integrative methods for elucidating the structure and function of cellular machines. **B.T. Chait**
- 10:20** Intermission.
- 10:35 ANYL 229.** Using mass spectrometry to identify short-lived electrochemical reaction intermediates. **R.N. Zare**
- 11:05 ANYL 230.** Using mass spectrometry to understand cystic fibrosis as a protein misfolding disease. **J.R. Yates, S. Pankow, C. Bamberger, M. Lavallee-Adam, S. Martinez de Bartolome Izquierdo**
- 11:35 ANYL 231. Award Address** (Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry sponsored by Waters Corporation). Exploiting electron impact phenomena on gaseous ions to create hybrid peptide fragmentation methods of usage in structural proteomics and signaling. **A.J. Heck**

## Section B

Wyndham San Diego Bayfront  
West Coast

### Biosensing of Proteins, Peptides, DNAs & RNAs

Q. J. Cheng, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:10 ANYL 232.** Single nanoparticle SPRI for detecting single microRNA and monitoring peptide uptake into hydrogel nanoparticles. **A. Maley, H. Fung, R.M. Corn**
- 8:40 ANYL 233.** Detecting small molecule-membrane protein binding kinetics with optical fibers. **N. Tao**
- 9:10 ANYL 234.** Magnetic nanoparticles as dispersible electrodes. **J.J. Gooding, K. Chuah, E. Morago, R. Tavallaie, S.M. Silva, D. Hibbert**
- 9:40 ANYL 235.** Achieving room temperature DNA detection with lesion-induced DNA amplification (LIDA). **J. Gibbs-Davis, B.S. Alladin-Mustan, C.J. Mitran**
- 10:00** Intermission.
- 10:20 ANYL 236.** LSPR based portable sensor for quantitative cardiac troponin T detection in human fluids. **R. Sardar, T. Liyanage**
- 10:40 ANYL 237.** Super-resolution single-molecule fluorescence imaging of DNA hybridization. **E.M. Peterson, J.M. Harris**
- 11:00 ANYL 238.** Biodetection in high ionic strength solutions with polymer modified nanoscale field-effect transistors. **N. Gao, T. Gao, W. Zhou, X. Dai, X. Yang, C.M. Lieber**
- 11:20 ANYL 239.** Phage-PEI disposable urine assay for the purpose of early cancer detection. **C. Eggers, A. Ogata, K. Mohan, R.K. Dutta, R.M. Penner, G.A. Weiss**
- 11:40 ANYL 240.** Nanocluster beacons for detection of a single  $N^6$ -methyladenine epigenetic modification. **Y. Chen, J. Obliosca, Y. Liu, C. Liu, M. Gwozdz, T. Yeh**

## Section C

Wyndham San Diego Bayfront  
Bay Room

### Analytical Methodologies & Research Partnerships at the Interface of Chemistry & Art/Archeology

C. M. Schmidt Patterson, K. A. Trentelman, *Organizers*

M. S. Devries, *Organizer, Presiding*

- 8:00 ANYL 241.** Watching paint dry: Assessing the curing and aging of modern oil-based paints. **K. Faber, L. Sturdy, M. Wright, K.R. Shull, F. Casadio, K. Muir**
- 8:30 ANYL 242.** Anionic effects in the acid-induced hydrolysis of cellulose. **M. McGath**
- 8:50 ANYL 243.** Multi-analytical approach for studying the accelerated sunlight ageing of synthetic organic binders used in modern and contemporary art. **V. Pintus, M. Schreiner**
- 9:10** Intermission.
- 9:20 ANYL 244.** Art & industry: Cleaning efficacy and residual studies for novel microemulsions tailored for acrylic dispersion paints and other unvarnished works of art. **M.H. Keefe, M.B. Clark, B. Ormsby, E. Willneff, A. Phenix, T. Learner**
- 9:50 ANYL 245.** Characterization of museum materials both ancient and modern using secondary ion mass spectrometry (SIMS) and focused ion beam (FIB) approaches. **D. McPhail, A. Fricker, B. Pretzel, B. Keneghan**
- 10:10 ANYL 246.** MeV-ToF-SIMS: A novel method for the analysis of modern and contemporary art paints. **D. Jembrih-Simburger, N. Marković, Z. Siketić, M. Anghelone, I. Bogdanović Radović**
- 10:30** Intermission.
- 10:40 ANYL 247.** Daguerreotype research at the University of Rochester: Leveraging a collaborative National Science Foundation grant for extended cultural heritage materials research. **R.S. Wiegandt, N. Bigelow, B. McIntyre**
- 11:00 ANYL 248.** Technical investigation of Josef Albers's "Casa" series by x-ray fluorescence spectroscopy and imaging studies. **R.E. Bachman, G.D. Smith**
- 11:20 ANYL 249.** Instrumental analysis and characterization of candle wax and pump grease recovered from the *H.L. Hunley* submarine. **L.M. Kasprzak, S. Boussett, J. Rivera-Diaz, V. Ternisien, S. Crette**
- 11:40 ANYL 250.** Withdrawn.

### Public Health Perspectives of Mycotoxins in Food

Sponsored by AGFD, Cosponsored by AGRO and ANYL

## TUESDAY AFTERNOON

### Section A

Wyndham San Diego Bayfront  
East Coast

### Approaches for Engaging Students in Analytical Chemistry Courses

Cosponsored by CHED

C. K. Larive, *Organizer*

C. Harrison, *Organizer, Presiding*

- 1:10** Introductory Remarks.
- 1:15 ANYL 251.** Turning the analytical lab into a research method development service. **K. Frederick, L. Quimby**

- 1:35 ANYL 252.** Student-driven analytical methods in the marine microcosm laboratory. **L. Hawkins, H. Van Ryswyk**
- 1:55 ANYL 253.** Skill-oriented instrumental analysis laboratory. **K. Slowinska**
- 2:15 ANYL 254.** Design of flipped classroom with a lab component for a chromatography-mass spectrometry course. **A. Kubatova**
- 2:35 ANYL 255.** Active learning in the classroom and laboratory of undergraduate analytical chemistry courses. **T.J. Wenzel**
- 2:55** Intermission.
- 3:10 ANYL 256.** Determination of stress in university students by monitoring saliva cortisol and zinc in hair. **D. Montalvo, J. Liu, S. Gamagadara, I. Noor-Mohamadi, J. Olson, B.K. Lavine, J.M. Bowen**
- 3:30 ANYL 257.** Rolling the dice on chromatography role-playing board games. **B.M. Canfield**
- 3:50 ANYL 258.** Development and use of a cyclic voltammetry simulator to introduce undergraduate students to electrochemical simulations. **J. Brown**
- 4:10 ANYL 259.** Detection limit and limit of quantitation: An instrumental analysis exercise with statistics. **R.D. Foust, C.A. Hughey, D. Ralston**
- 4:30 ANYL 260.** Computational chemistry activities in the undergraduate chemistry laboratory. **T. Thomas Smith**

## Section B

Wyndham San Diego Bayfront  
West Coast

### Biosensing of Proteins, Peptides, DNAs & RNAs

Q. J. Cheng, *Organizer, Presiding*

R. M. Corn, *Presiding*

- 1:00 ANYL 261.** Single molecule analysis by biological nanopores. **C. Cao, Y. Ying, Z. Hu, Y. Hu, Z. Gu, Y. Long**
- 1:30 ANYL 262.** New biosensing concepts: Mologyraphy, plasmonic particle based single cell analytics and miniaturized immunofiltration. **J. Vörös**
- 2:00 ANYL 263.** Biomimetic nanosponges for detection and removal of protein toxins. **L. Zhang**
- 2:30 ANYL 264.** Multiplexed detection on microfluidic paper-based analytical devices ( $\mu$ PADS) by immunoassays. **D. Christodouleas, J. Milette, G.M. Whitesides**
- 2:50** Intermission.
- 3:00 ANYL 265.** Phage-enabled ultrasensitive detection of disease biomarker. **C. Mao**
- 3:20 ANYL 266.** Electrochemical DNA hybridization detection based on reporter strands and primers labeled with osmium tetroxide. **G. Flechsig**
- 3:40 ANYL 267.** Microarray imaging with scanning electrochemical microscopy and combination of scanning electrochemical microscopy with surface plasmon resonance. **T. Kai, S. Chen, E. Monterosso, J. Xiang, F. Zhou**
- 4:00 ANYL 268.** Diagnostic challenge in blood tests for tuberculosis: Importance of sample pretreatment in overcoming analyte complexation. **L. Laurentius, A. Crawford, R.E. Robinson, N.A. Owens, J.H. Granger, D. Chatterjee, M.D. Porter**
- 4:20 ANYL 269.** Templated biosynthesis of unnatural and natural proteins for surface plasmon resonance imaging (SPRI). **G. Manuel, A. Luptak, R.M. Corn**

- 4:40 ANYL 270.** Multiplexed neurochips as screening platforms for neurotransmitter-specific high-affinity aptamers. **N. Nakatsuka, H. Cao, S. Deshayes, A.M. Kasko, P.S. Weiss, A.M. Andrews**

## Section C

Wyndham San Diego Bayfront  
Bay Room

### Analytical Methodologies & Research Partnerships at the Interface of Chemistry & Art/Archeology

M. S. Devries, K. A. Trentelman, *Organizers*

C. M. Schmidt Patterson, *Organizer, Presiding*

- 1:10 ANYL 271.** Identification of forgery in proteinaceous cultural heritage objects by comparing the biomarkers of natural and artificial aging. **M. Moini, C.M. Rollman, M. Floyd**
- 1:40 ANYL 272.** Characterizing the age of ancient Egyptian manuscripts through micro-Raman spectroscopy. **S. Goler, J.T. Yardley, A. Cacciola, A. Hagadorn, D. Ratzan, R. Bagnall**
- 2:00 ANYL 273.** Degradation of minium ( $Pb_3O_4$ ) on the long and short term in material originating from a Red-Shroud Mummy. **F. Vanmeert, J. Jaroszewicz, K.H. Janssens, K.A. Trentelman**
- 2:20 ANYL 274.** Instrumentation for studying time-lapse *in situ* chemical change in heritage systems. **R.A. Grayburn, M. Dowsett, P. Thompson, A. Adriaens**
- 2:40 ANYL 275.** Potential of time-lapse measurements in metal degradation studies and the benefit for cultural heritage conservation. **R. Wiesinger, C. Kleber, M. Schreiner**
- 3:00** Intermission.
- 3:15 ANYL 276.** Reverse engineering ancient Athenian pottery: A collaboration between cultural heritage, industry, and academia. **K.A. Trentelman, I. Cianchetta, M. Walton, A. Mehta, P. Pianetta, B. Foran, D. Saunders, J. Maish**
- 3:35 ANYL 277.** Reverse engineering ancient Greek ceramics: Education and research through replication. **S. Balachandran**
- 3:55 ANYL 278.** Archaeological chemists & chemical archaeologists: Working together in the Lower Pecos Canyonlands, TX. **K.L. Steelman, C.E. Boyd**
- 4:15 ANYL 279.** Integrated SEM-EDS- $\mu$ RS system for the analysis of material culture. **S. Prikhodko, A. King, I. Kakoulli**
- 4:35 ANYL 280.** Exploring the potential of advanced magnetic resonance techniques for the characterization of cultural heritage materials. **N. Zumbulyadis, F. Perras, T. Kobayashi, A. Murphy, Y. Yao, J. Catalano, M. Pruski, S. Centeno, C.R. Dybowski, L. Switala, J.P. Hornak**
- 4:55** Concluding Remarks.

### Public Health Perspectives of Mycotoxins in Food

Sponsored by AGFD, Cosponsored by AGRO and ANYL

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## WEDNESDAY MORNING

## Section A

Wyndham San Diego Bayfront  
East Coast

## Big Data &amp; Small Data

Cosponsored by CINF and MPPG

B. K. Lavine, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 ANYL 281. Classification and geospatial estimation of titanium dioxide polymorphs using multivariate exploratory methods. J.P. Smith, F.C. Smith, B.P. Glass, K.S. Booksh

8:40 ANYL 282. Infrared imaging and multivariate curve resolution for the forensic examination of automotive paint chips. B.K. Lavine, M.D. Allen, N.T. Perera, K. Nishikida

9:05 ANYL 283. Quality assessments for organically-complex botanical extracts. B. Rohrbach, S. Ramos, P. Gibson

9:30 ANYL 284. Pattern recognition assisted infrared library searching of automotive paints for forensic analysis. B.K. Lavine, M.D. Allen, C. White, A. Fasasi

10:10 Intermission.

10:30 ANYL 285. Withdrawn.

10:55 ANYL 286. Withdrawn.

11:20 ANYL 287. Data processing challenges in single neuron whole genome sequencing. S. Rohrbach, J. Chun

11:45 Concluding Remarks.

## Section B

Wyndham San Diego Bayfront  
West Coast

## Biosensing of Proteins, Peptides, DNAs &amp; RNAs

Q. J. Cheng, *Organizer*

Y. Long, J. Vörös, *Presiding*

8:00 ANYL 288. Nanoparticle enhanced biosensing platforms for proteins in biological fluids. H.J. Lee

8:30 ANYL 289. Self-assembled fluorescent probes based on cyclodextrin polymer via host-guest interaction. X. Yang

9:00 ANYL 290. Probing protein folding at nano-scale interface. K. Yokoyama

9:20 ANYL 291. All solid-phase immunoassays are not created equal: A closer look at what determines signal generation. N.A. Owens, A. Crawford, L. Laurentius, N.E. Schlotter, A. Skuratovsky, M.D. Porter

9:40 ANYL 292. Selection of HBsAg-specific DNA aptamers based on carboxylated magnetic nanoparticles and their application. N. He

10:00 Intermission.

10:20 ANYL 293. Single molecule tracking across polymer scaffolded black lipid membranes. C. Fronczek, L.K. Bright, C.A. Aspinwall, S. Saavedra

10:40 ANYL 294. Monitoring extracellular glucose oxidase activity of *Aspigoillus flavus* during germination using scanning probe microscopy. H. Anteneh, T. Kai, E. Monterroso, F. Zhou

11:00 ANYL 295. Detection of progesterone and estradiol using poly (N-isopropylacrylamide) microgel-based biosensors. Y. Jiang, M. Colazo, M. Serpe

11:20 ANYL 296. Monitoring uptake of small molecules into NIPAm-based nanoparticles using single nanoparticle surface plasmon resonance imaging microscopy. H.M. Fung, A. Maley, Y. Terada, R.M. Corn

11:40 ANYL 297. Hexavalent chromium as an electrocatalyst in DNA sensing. H. Lotfi Zadeh Zhad, R.Y. Lai

## Section C

Wyndham San Diego Bayfront  
Bay Room

## Chemical Imaging: Applications, Advances &amp; Challenges

Cosponsored by CINF and MPPG

R. M. Burks, *Organizer*

J. H. Terry, *Organizer, Presiding*

8:10 ANYL 298. Nanoscience approaches to heterogeneity in biological systems. P.S. Weiss

8:50 ANYL 299. Rapid-target bio-imaging of tumors through specific biosynthesis of fluorescent probes. J. Ye, J. Wang, S. Gao, X. Wang

9:10 Intermission.

9:30 ANYL 300. High-throughput screening method for creating and assessing ionic liquid/porous silicon microarrays. S. Trivedi, F.V. Bright

9:50 ANYL 301. Micro-Raman analysis of crayfish exoskeleton mineralization using a newly released spectroscopic imaging software. S. Brittle, D. Foose, K.A. O'Neil, Z. Gagnon, I.E. Pavel Sizemore

10:10 ANYL 302. Raman microspectroscopic mapping with multivariate curve resolution-alternating least squares (MCR-ALS) applied to a high-pressure polymorph of titanium dioxide, TiO<sub>2</sub>-II. J.P. Smith, F.C. Smith, B.P. Glass, K.S. Booksh

10:30 Intermission.

10:50 ANYL 303. Multidimensional imaging and computational approaches to understanding tissue morphogenesis. K. Kwan, Y. Wan, C. Hansen, H. Gordon, S. Stringham, B. Froelich

11:30 ANYL 304. Nanospectral imaging and nanospectroscopy via photo-induced force. D. Nowak, W. Morrison, S. Park

## Public Health Perspectives of Mycotoxins in Food

Sponsored by AGFD, Cosponsored by AGRO and ANYL

## WEDNESDAY AFTERNOON

## Section A

Wyndham San Diego Bayfront  
East Coast

## Big Data &amp; Small Data

Cosponsored by CINF and MPPG

B. K. Lavine, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 ANYL 305. Ranking multivariate calibration models formed from multiple tuning parameters: Model penalties. J.H. Kalivas, A. Tencate

1:40 ANYL 306. Adaptive regression via subspace elimination: A novel algorithm for predicting in the presence of uncalibrated interferents. J. Ottaway, K.S. Booksh

2:05 ANYL 307. Compensating for the effects of unusual samples and variables in data for multivariate calibrations. S.D. Brown, C. Giglio

2:30 Intermission.

2:50 ANYL 308. Development of a predictive screening method for selection of two-dimensional liquid chromatography column pair combinations. R.K. Lindsey, D.R. Stoll, P. Carr, J.I. Siepmann

3:15 ANYL 309. Discovery-based analysis of GC x GC - TOFMS data using tile-based Fisher ratio software and combinatorial threshold determination. R.E. Synovec, B.A. Parsons, N.E. Watson, B.C. Reaser, C.E. Freye, D.K. Pinkerton

3:40 ANYL 310. Using multidimensional data to simplify the analysis of individual lipoprotein and cholesterol distributions. M.K. Eagleburger, J.W. Cooley, R.D. Jiji

4:05 ANYL 311. Surface-enhanced Raman spectroscopy study of the interaction between colloidal silver nanoparticles and *Dengue virus* virions: Unsupervised automated peak detection and quantification using a newly released spectroscopic imaging software. D.P. Foose, S.L. Paluri, K.J. Williams, K.M. Dorney, C. Anders, N.J. Bigely, I.E. Pavel Sizemore

## Section B

Wyndham San Diego Bayfront  
West Coast

## Biosensing of Proteins, Peptides, DNAs &amp; RNAs

Q. J. Cheng, *Organizer*

S. Hinman, H. J. Lee, *Presiding*

1:00 ANYL 312. General chemiluminescence strategy for biosensing of proteins, peptides, DNAs and small molecules. H. Cui, L. Gao, S. Li

1:30 ANYL 313. Ultrasensitive nanopore-based sensor for the detection of ATP. S. Cai, Y. Zheng, S. Cao, X. Cai, Y. Li

1:50 ANYL 314. Single-molecule detection of single-nucleotide polymorphisms (SNPs) in DNA hybridization kinetics. M. Manhart, E.M. Peterson, J.M. Harris

2:10 ANYL 315. Plasmonic microarrays for enhanced SPR imaging analysis of bacterial toxins. S. Hinman, Q.J. Cheng

2:30 ANYL 316. Single nanoparticle SPRI microscopy for the enzymatic detection of single microRNA molecules. A. Maley, H.M. Fung, R.M. Corn

2:50 Intermission.

3:00 ANYL 317. Single oligonucleotide discrimination with aerolysin nanopore. C. Cao, Y. Ying, H. Tian, Y. Long

3:20 ANYL 318. Precise determination of molecular mechanical forces in biological systems. T. Tsai, Y. Wang, S. Xu

3:40 ANYL 319. Prototype microfluidic immunological biosensor for point-of-care diagnostics. M. Tappert, J. Jarshaw, N. Shaffer, R. Brennan, W. Wilson, J.M. Bowen

4:00 ANYL 320. Oligonucleotide microarray-based molecular prediction of common *Salmonella* serotypes. H. Shin, B. Hwang, H.J. Cha

4:20 ANYL 321. Factors influencing RAGE lateral diffusion in the cell membrane. A. Syed, Q. Zhu, E.A. Smith

4:40 ANYL 322. Antibiotic resistance-based differentiation and separation by dielectrophoresis. S.H. Hilton, M.A. Hayes

## Section C

Wyndham San Diego Bayfront  
Bay Room

## Chemical Imaging: Applications, Advances &amp; Challenges

Cosponsored by CINF and MPPG

J. H. Terry, *Organizer*

R. M. Burks, *Organizer, Presiding*

1:00 ANYL 323. Emergent structure and dynamics of patchy coarse-grained nanoparticles. R. Hernandez

1:40 ANYL 324. Highly sensitive detection and bio-imaging of cancers based on new supramolecular probes and multifunctional nano-interface. X. Wang

2:00 ANYL 325. Investigation of surface morphology and conductance of multi-acid side chain membranes by atomic force microscopy. A. Barnes, N. Economou, S.K. Buratto

2:20 Intermission.

2:40 ANYL 326. Withdrawn.

3:00 ANYL 327. Plasmonic nanofocusing NSOM-Raman tip for high resolution chemical imaging. R. Yan

3:20 ANYL 328. Tip enhanced Raman scattering: New nanoscale chemical imaging method. A. Kravayev, M. Chaigneau

3:40 Intermission.

4:00 ANYL 329. Evaluating small molecule histone inhibitors with high resolution mass spectrometry and 3D cell cultures. A.B. Hummon, B.A. Garcia, S. Sidoli, M. Schroll, X. Liu, P. Feist

4:20 ANYL 330. Human islet amyloid polypeptide N-terminus fragment self-assembly: Effect of conserved disulfide bond on aggregation propensity. M. Giammona, A. Iltchev, T. Do, J.E. Shea, D.P. Raleigh, M.T. Bowers, S.K. Buratto

4:40 ANYL 331. Nanoscale chemical mapping of polymer matrix composites. D. Nepal

## Public Health Perspectives of Mycotoxins in Food

Sponsored by AGFD, Cosponsored by AGRO and ANYL

## THURSDAY MORNING

## Section A

Wyndham San Diego Bayfront  
East Coast

## Advances in Analytical Separations

J. L. MacLachlan, *Organizer, Presiding*

8:00 Introductory Remarks.

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**8:05 ANYL 332.** Residue analysis of anthraquinone in soybeans by GC-MS/MS. **B.G. Abbo**

**8:30 ANYL 333.** Analytical method development for toxic compounds with a field portable GC/PID. **J.N. Driscoll, J.L. Maclachlan**

**8:55 ANYL 334.** Analyzing 16 harmful and potentially harmful polycyclic aromatic hydrocarbons in tobacco products and tobacco smoke. **O. Motorykin, Y.S. Ding, B.A. Hearn, C. Watson**

**9:20 ANYL 335.** Onsite real-time analysis of fumigants via GC-PID/TCID. **J.N. Driscoll, J.L. Maclachlan**

**9:45 Intermission.**

**10:00 ANYL 336.** From monomers to polymers across the oligomeric region: Advanced biorefinery analytics. **J.T. Oberlacher, S. Boehmdorfer, T. Zwickmair, T. Rosenau, A. Pottthast**

**10:25 ANYL 337.** Improvements in solid-core particle technologies. **B. Okandeji, B.A. Alden, C.A. Boissel, M.A. Lauber, D.P. Walsh, J.T. Cook, S.A. McCall, K. Wyndham, T. Walter, J.N. Fairchild**

**10:50 ANYL 338.** Supercritical fluid chromatography as the technique of choice for small molecules analysis and separation. **G. Rosse**

**11:15 ANYL 339.** Transfer of method between conventional HPLC and UHPLC for the size-exclusion chromatographic analysis of proteins, including monoclonal antibodies: A comparison of a 5  $\mu$ m conventional HPLC column with a new silica based, 2  $\mu$ m UHPLC column. **C. Benner, A. Chakrabarti**

**11:40 Concluding Remarks.**

## Section B

Wyndham San Diego Bayfront  
West Coast

### Chemical Imaging: Applications, Advances & Challenges

*Cosponsored by CINF and MPPG*

**J. H. Terry, Organizer**

**R. M. Burks, Organizer, Presiding**

**8:30 ANYL 340.** Imaging the mobility of Ag films encapsulated in 3C-SiC as a function of annealing temperature. **D. Velazquez**

**9:10 ANYL 341.** Open plans of a low cost fluorescence and imaging ellipsometry microscope. **V. Nguyen, J. Rizzo, J. Zehner, W. Cook, B. Sani**

**9:30 ANYL 342.** In-cell fluorogenic tag-probe system for protein localization and dynamics imaging. **W. Nomura, N. Ohashi, H. Tamamura**

**9:50 Intermission.**

**10:10 ANYL 343.** 3D imaging of cells with soft x-rays. **C. Larabell, G. McDermott, M. LeGros**

**10:50 ANYL 344.** PCA-based method for identifying spectra of different wood cell wall layers in Raman imaging data set and its applications. **X. Zhang, F. Xu**

**11:10 ANYL 345.** Early brain tumor detection by chemical imaging of deoxyhemoglobin. **C. Wang, C. Hsu, Z. Li, Y. Lin**

**11:30 ANYL 346.** Deep and high-resolution three-dimensional tracking of single particles using nonlinear and multiplexed illumination. **E. Perillo, Y. Liu, C. Liu, A. Dunn, T. Yeh**

## THURSDAY AFTERNOON

### Section A

Wyndham San Diego Bayfront  
East Coast

#### Advances in Analytical Separations

**J. L. Maclachlan, Organizer, Presiding**

**1:00** Introductory Remarks.

**1:05 ANYL 347.** Proteomic applications of a simple protein fractionation strategy. **J. Moresco, J. Diedrich, M. Lavallee-Adam, J.R. Yates**

**1:30 ANYL 348.** Flow field-flow fractionation hyphenations for liposome-antimicrobial peptide interaction. **P. Iavicoli, P. Urban, A. Bella, M. Ryadnov, F. Rossi, L. Calzolari**

**1:55 ANYL 349.** Models of refined separations using insulator-based dielectrophoresis. **C.V. Crowther, M.A. Hayes**

**2:20 ANYL 350.** Peptide-conjugated elastomeric particles for acoustic isolation of biomarkers from whole blood. **W. Shields, A. Li, J. Huang, A. Zhang, K. Ohiri, A. Chilkoti, G. Lopez**

**2:45 Intermission.**

**3:00 ANYL 351.** High throughput single cell analysis using multilayer microfluidic devices. **D. Ediriweera, C.T. Culbertson, T. Mickleburgh**

**3:25 ANYL 352.** Novel sample preparation technique for ultratrace analysis: ICE concentration linked with extractive stir bar (ICECLES). **N. Maslamani, Z. Zhang, J. Dzisam, B.A. Logue**

**3:50 ANYL 353.** Spectroscopic analysis of tunable, stimuli responsive polymeric materials. **C. Daniels, A. Gasper, J. Church**

**4:15 ANYL 354.** Surface enhanced Raman spectroscopy coupled with extraction. **J. Zhan, M. Zhang, Y. Shi**

**4:40 Concluding Remarks.**

### Section B

Wyndham San Diego Bayfront  
West Coast

#### Advances in Structural Mass Spectrometry

**S. J. Valentine, Organizer, Presiding**

**1:00 ANYL 355.** Ultraviolet photodissociation mass spectrometry for top down characterization of proteins. **J. Brodbelt**

**1:40 ANYL 356.** Hydrogen exchange mass spectrometry: An enabling tool for therapeutic protein development. **D.D. Weis**

**2:20 ANYL 357.** Probing gas phase biomolecular structure via excitation energy transfer. **R. Julian, N. Hendricks**

**3:00 Intermission.**

**3:15 ANYL 358.** Photodissociation on the nanosecond timescale: Fundamental insights and analytical applications. **N.C. Polfer, N. Zhao, L.S. Bailey, A.L. Patrick, M.R. Bell, A. Cismesia, L.F. Tesler**

**3:55 ANYL 359.** Devil is in the details: Applications of emerging mass spectrometry tools for investigating biological activities. **C.E. Costello**

## BIOT

### Division of Biochemical Technology

**S. Tobler and P. Tessier, Program Chairs**

#### OTHER SYMPOSIA OF INTEREST:

**ACS Award in Colloid & Surface Chemistry: Honoring Nicholas L. Abbott** (see *COLL, Sun, Mon, Tue*)

**Frontiers in Biomolecular Recognition: From Materials to Cells** (see *BIOL, Mon*)

**Undergraduate Research Posters** (see *CHED, Mon*)

**Advances in Computer-Aided Biologics Design** (see *COMP, Wed*)

#### SOCIAL EVENTS:

**Membership Desk, 8:00 AM:**  
Sun, Mon, Tue, Wed, Thu

**Company Seminars, 12:30 PM:** Sun, Mon

**Reception, 6:30 PM:** Sun

**Poster Session, 6:00 PM:** Tue

**Program Chair's Lunch, 12:30 PM:** Wed

**Networking/Mentoring Session, 8:00 PM:** Wed

#### BIUSINESS MEETINGS:

**BIOT Executive Committee Meeting, 7:00 PM:** Mon

**Future Programming Meeting, 12:30 PM:** Tue

## SUNDAY MORNING

### Section A

Westin San Diego  
Crystal I

#### Upstream Processes

#### Disruptive Bioprocessing: Upstream Processing

**M. R. Antoniewicz, M. A. Blenner, V. Roy, Organizers**

**M. J. Betenbaugh, A. E. Schmelzer, Organizers, Presiding**

**8:30 BIOT 1.** Understanding and mitigating raw material variability in an intensified, integrated perfusion cell culture process. **M. Hollenbach, J. Wang, N. Shah, J. Walther, C. Hwang**

**8:50 BIOT 2.** Debottlenecking manufacturing capacity: Initiating cell culture manufacturing campaigns using seed train cryopreserved in a disposable bag. **S. Rameez, S. Gopalakrishnan, K. Zhang, S.S. Mostafa, A.A. Shukla**

**9:10 BIOT 3.** Single-use membrane bioreactor for culturing therapeutic T-cells. **S. Yoo, J. Bramson, R. Ghosh**

**9:30 BIOT 4.** Development of a CHO cell-free synthetic platform for production of monoclonal antibodies. **N. Majewska, R. Martin, K. Moore, A. Schmelzer, M. Jewett, V. Roy**

**9:50 Intermission.**

**10:10 BIOT 5.** Continuous processing for pre-clinical and clinical manufacturing. **J.L. Coffman**

**10:30 BIOT 6.** Development of a high performance integrated and disposable clarification solution for continuous bioprocessing. **M. Collins, E. Ayturk, R. Gantier**

**10:50 BIOT 7.** Acoustic wave separation, an alternative cell clarification technology: Optimization and applications. **J. Armando, J.P. Pieracci, P. Haberman, J. Rozembersky, C. Leidel, J. King, D. Bianchi**

**11:10 BIOT 8.** Glycoengineering in CHO cells for biomanufacturing. **Q. Wang**

### Section B

Westin San Diego  
Emerald Ballroom

#### Downstream Processes

#### Downstream Processing for Vaccines, Gene Therapy Vectors & Non-Protein Biological Products

**J. Neville, A. Noyes, T. M. Przybycien, Organizers**

**C. Heldt, J. G. Stout, Organizers, Presiding**

**8:30 BIOT 9.** Leveraging design of experiments to characterize the effects of formaldehyde concentration, incubation temperature and time on influenza A/WSN/33 (H1N1) inactivation and process analytics. **S. Patel, L. Mullin, M. Bruce, K. Cunningham, J. Caron, C. Gillespie**

**8:50 BIOT 10.** Development of a cGMP-compatible purification process for adenovirus purification. **M.A. Snyder**

**9:10 BIOT 11.** Residual DNA removal by Benzonase® endonuclease in influenza feedstreams. **L. Mullin, S. Patel, M. Bruce, K. Cunningham, J. Caron, C. Gillespie**

**9:30 BIOT 12.** Viral particle purification with osmolyte flocculation. **C. Heldt, A. Saksule**

**9:50 Intermission.**

**10:10 BIOT 13.** Use of preconditioning to control membrane fouling and enhance performance during ultrafiltration of plasmid DNA. **Y. Li, A.L. Zydny**

**10:30 BIOT 14.** Aggressive development of two recombinant protein production processes to generate a bivalent vaccine. **R. Krishnan, A. Berrill, B. Huffman, J. Cundy, S. Cook, W. Wellborn, J. Martin, K. Sunasara**

**10:50 BIOT 15.** Upstream and downstream solutions for MSCs animal origin-free processing. **L. Savary, A. Schnitzler, D. Kehoe, M. Aysola, A. Verma, T. Lawson, S. Rigby, T. Hood, S. Punreddy, S. Luther, J. Murrell, M. Rook, M. Pease, M. Bulpin**

**11:10 BIOT 16.** Ultrafiltration for purification of polysaccharide-based vaccines. **M. Hadidi, J.J. Buckley, A.L. Zydny**

### Section C

Westin San Diego  
Diamond I

#### Biomolecular & Biophysical Processes

#### Imaging, Sensing & Bioactuation

**B. Hackel, J. Kaar, H. Samra, Organizers**

**G. M. Thurber, T. Wellman, Organizers, Presiding**

**8:30 BIOT 17.** PET imaging of growth factor receptor expression in cancer using the 45-amino acid Gp2 scaffold. **M. Kruziki, E. Zudock, B. Case, B. Hackel**

**8:50 BIOT 18.** Binary aptamer for instant fluorescent analysis of specific nucleic acids *in vitro*. **N. Kikuchi, D. Kolpashchikov**

**9:10 BIOT 19.** Imaging the oxidation state of peroxiredoxin-2 in living cells. **T.F. Langford, H. Sikes**

**9:30 BIOT 20.** Development of transient induced molecular electronic spectroscopy (TIMES) for protein-ligand interactions. **T. Zhang, H. Ma, I. Lian, T. Wei, Y. Lo**

**9:50 Intermission.**

- 10:10 BIOT 21.** Engineering a novel diagnostic test for tuberculosis using nanoparticle-based detection of a whole blood gene expression signature. **H. Gliddon**, P.D. Howes, E. Kim, M. Kaforou, M. Levin, M. Stevens
- 10:30 BIOT 22.** Improving the durability of graphene composite sensors for robust biosensors. **S. Tuntithavornwat**, J. King, C. Heldt
- 10:50 BIOT 23.** Micromachined multielectrode microprobes for choline sensing with an on-probe iridium oxide reference. **L. Feng**, H. Monbouquette
- 11:10 BIOT 24.** Directed evolution of yeast peptide receptors: A new platform for low-cost healthcare diagnostic. **A. Adeniran**, S. Stainbrook, **K.E. Tyo**

## Section D

Westin San Diego

Opal

### Biofuel & Biobased Chemical Production

#### Synthetic Biology Approaches to Engineer Production of Fuels & Energy Molecules

- K. Brandon Sutton**, M. A. O'Malley, *Organizers*
- C. A. Eckert**, T. Moon, *Organizers, Presiding*
- 8:30 BIOT 25.** GPCR-based chemical biosensor for advanced biofuels. **P. Peralta Yahya**
- 8:50 BIOT 26.** Rapid construction of metabolite biosensors using domain insertion profiling. **D. Savage**
- 9:10 BIOT 27.** Synthetic extracellular sensing circuit by intein-mediated reconstitution of yeast mating factor. **K. Siu**, W. Chen
- 9:30 BIOT 28.** Deep sequencing-guided assessment and computational design of synthetic metabolic pathways. **J. Klesmith**, T. Whitehead
- 9:50 Intermission.**
- 10:10 BIOT 29.** PIACE: Parallel integration and chromosomal expansion of biofuels pathways in *E. coli*. **G. Goyal**, J. Alonso Gutierrez, J.D. Keasling, **T. Lee**, N. Hillson
- 10:30 BIOT 30.** Synthetic regulon in *Saccharomyces cerevisiae* for efficient xylose assimilation. **V. Endalur Gopinarayanan**, N. U. Nair
- 10:50 BIOT 31.** Engineering anaerobic methanogenic pathway and methyl-coenzyme M reductase in *Methanosarcina acetivorans*. **M. Raeeszadeh Sarmazdeh**, J. Gonzalez, W. Chen
- 11:10 BIOT 32.** Novel gut fungal transporters for improved fuel and energy production. **K. Solomon**, J. Henske, S.P. Gilmore, S. Seppala, M. Rite, M.A. O'Malley

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## Section A

Westin San Diego

Emerald Ballroom

### David Perlman Memorial Lectureship & Van Lanen Service Award Presentation

**T. M. Przybycien**, P. M. Tessier, S. A. Tobler, *Organizers, Presiding*

- 11:30 BIOT 33.** From bench to bedside: Developing molecules into therapies. **A. Lee**

### ACS Award in Separations Science & Technology: Symposium in honor of Steven M. Cramer

*Sponsored by I&EC, Cosponsored by BIOT*

## SUNDAY AFTERNOON

## Section A

Westin San Diego

Crystal II

### Upstream Processes

#### Mammalian Cell Culture Process Development

- M. R. Antoniewicz**, P. Apostolidis, M. A. Blenner, C. Metallo, V. Roy, *Organizers*
- N. Lewis**, B. Mulukutla, *Organizers, Presiding*
- 2:00 BIOT 34.** Identification and optimization of small molecule inhibitors of epigenetic modifying enzymes for enhancing transient protein production in mammalian cells. **M. Christensen**, K. Rege
- 2:20 BIOT 35.** Enabling use of sugar-based detergents as a shear protectant in CHO cell culture medium. **J. Lakkyreddy**, J. Wu, S. Meier
- 2:40 BIOT 36.** Fine tuning and coarse tuning of protein glycosylation profiles through novel media supplementation strategies. **C. Racicot**, S. McDermott, J. Matuck, C. Chumsae, P. Hossler
- 3:00 BIOT 37.** High-throughput microbioreactors for CHO cell transfection process development. **C. Hsu**, H. Jain, J. Wang, K.A. Brorson
- 3:20 Intermission.**
- 3:40 BIOT 38.** Influenza vaccine production using cell culture with microcarriers. **M. McGlothlen**, L. Mullin, P. Hatch, D. Asher, C. Gillespie
- 4:00 BIOT 39.** Case study on the production of live virus vaccine on platforms supporting anchorage dependent cell substrate. **D. Spatafore**, S. Christanti, S. Fox, J.C. Gercke, C.D. Jan, K. Hamaker
- 4:20 BIOT 40.** Development of a high-productivity cell culture process and implementation at large scale. **E. Ward**, W. Yang, A. Doane, W. Hu
- 4:40 BIOT 41.** Development run case study for a monoclonal antibody NS0 cell culture process. **E. Hodgman**, S. Agastin, C. Lucini, J. Shiminsky, I. Pla

## Section B

Westin San Diego

Emerald Ballroom

### Downstream Processes

#### Disruptive BioProcessing: Downstream Processing

**J. Neville**, A. Noyes, T. M. Przybycien, *Organizers*

- K. Brower**, J. P. Pieracci, *Organizers, Presiding*
- 2:00 BIOT 42.** Investigation of single pass tangential flow filtration as an inline concentration step during cell culture harvest. **M. Peck**, A. Arunkumar, N. Singh
- 2:20 BIOT 43.** Withdrawn.
- 2:40 BIOT 44.** Technical considerations for an affinity resin discovery and development platform to rapidly address complex separations of diverse therapeutics and vaccines. **W. Kett**
- 3:00 BIOT 45.** Split intein-mediated self-cleaving tag for recombinant protein purification in a mammalian cell expression system. **T. Han**, D.W. Wood
- 3:20 Intermission.**
- 3:40 BIOT 46.** Enabling continuous low pH viral inactivation with integrated in-line conditioning of protein A streams. **M. Fiadeiro**, J.A. Kubbleck, R. Fahrner, J. Salm
- 4:00 BIOT 47.** Optimized continuous mAb polishing via coupled unit operations. **X. Gjoka**, K. Rogler, M. Bisschops, R. Gantier, **M. Schofield**
- 4:20 BIOT 48.** Efficient devices for high-resolution membrane chromatography. **R. Ghosh**, P. Madadkar, R. Sadavarte
- 4:40 BIOT 49.** PD scale realization of an integrated continuous bioprocessing platform. **E. Ayturk**, R. Gantier

## Section C

Westin San Diego

Diamond I

### Biomolecular & Biophysical Processes

#### Controlling the Interface of Proteins, Cells & Materials

- B. Hackel**, H. Samra, *Organizers*
- J. Kaar**, M. Kastantin, *Organizers, Presiding*
- 2:00 BIOT 50.** Spheroid and tissue assembly via click chemistry in microfluidic flow. **M.N. Yousaf**
- 2:20 BIOT 51.** Plasma membrane imaging and cancer therapy based on cell surface engineering. **F. Wu**, H. Wang, H. Jia, X. Hua, Y. Li, J. Sun, Z. Chen
- 2:40 BIOT 52.** Dense poly(ethylene glycol) brushes reduce protein adsorption and promote unfolding. **D. Maruecos**, M. Kastantin, D.K. Schwartz, J. Kaar
- 3:00 BIOT 53.** Thermodynamics of biomolecule adsorption on calcium oxalate monohydrate crystals. **J. Kwak**, P. Karande
- 3:20 Intermission.**
- 3:40 BIOT 54.** Modification of bicelles with peptoids to alter edge chemistry. **H. Najafi**, S.L. Servoss
- 4:00 BIOT 55.** Dopa-Fe<sup>3+</sup> complexation of mussel adhesive proteins at plaque-substrate interface. **B. Yang**, C. Lim, B. Choi, D. Hwang, H.J. Cha
- 4:20 BIOT 56.** Characterization of protein-functionalized surfaces created by sortase-mediated ligation. **S. Williamson**, L. Parks, R. Le, M. Raeeszadeh Sarmazdeh, P. Frymier, E.T. Bodor

- 4:40 BIOT 57.** Adsorption and electron transfer of deca-heme cytochrome (MtrF) studied with atomistic simulations and kinetic Monte Carlo simulation. **H. Ma**, M. Sajib, T. Wei

## Section D

Westin San Diego

Opal

### Biofuel & Biobased Chemical Production

#### Synthetic Biology & -OMICS Approaches to Engineer Microbial Communities

- K. Brandon Sutton**, M. A. O'Malley, *Organizers*
- K. Solomon**, H. Tseng, *Organizers, Presiding*
- 2:00 BIOT 58.** Engineering recombinant microbial communities for cellulose degradation. **K.Z. Kalbarczyk**, M. Koffas, C.H. Collins
- 2:20 BIOT 59.** Bottom-up construction of synthetic microbial pairs inspired by nature. **S. Gilmore**, J.A. Sexton, J. Henske, K. Solomon, M.K. Theodorou, M.A. O'Malley
- 2:40 BIOT 60.** Multiple techniques for host and pathway engineering of tolerance and chemical production. **A.P. Arkin**
- 3:20 Intermission.**
- 3:40 BIOT 61.** Genome-scale engineering in probiotic organisms. **T. Mansell**, S. Rothstein
- 4:00 BIOT 62.** Optimization of *E. coli* co-cultures for the high-yield production of plant polyphenols. **J.A. Jones**, V.R. Vernacchio, D.M. Lachance, S.M. Collins, A.L. Sinkoe, J. Hahn, M. Koffas
- 4:20 BIOT 63.** Experimental examination of catabolite repression and diauxic growth in *Clostridium phytofermentans*. **H.W. Harris**, A. Navid, Y. Jiao, B. Stewart
- 4:40 BIOT 64.** Engineering a synthetic sugar sensing yeast strain. **K.M. Blocker**, A.S. Robinson

## Section E

Westin San Diego

Crystal I

### Computationally Enabled Biotechnology at the Molecular, Cellular & Process Scales

#### Biomolecular Design & Biophysics

- J. Reed**, *Organizer*
- D. J. Roush**, H. Salis, *Organizers, Presiding*
- 2:00 BIOT 65.** Discovery and design of novel regulatory noncoding RNA in bacteria. **J. Marcus**, S. Hassoun, **N.U. Nair**
- 2:20 BIOT 66.** Understanding and exploiting enzyme promiscuity for metabolic engineering. **D. Pertusi**, J. Jeffries, **K.E. Tyo**
- 2:40 BIOT 67.** Development and validation of computational methods for *de novo* design of antibody variable regions. **T. Li**, V. Pooarla, T.K. Wood, C. Maranas
- 3:00 BIOT 68.** Suppressed inactivation of  $\alpha$ -amylase in the presence of alcohol. **A. Khan**
- 3:20 Intermission.**
- 3:40 BIOT 69.** Molecular origins of high viscosity in solutions of monoclonal antibody mutants. **A. Vaish**, D.J. Rosenman, S. Yadav, I. Zarraga, **A.M. Lenhoff**
- 4:00 BIOT 70.** Modulation of protein biophysical properties with small molecule in purification and formulation. **F.K. Insaiddo**, H. Li, N. Tugcu, D.J. Roush

**4:20 BIOT 71.** Binding of proteins to multimodal surfaces: From fundamental molecular modeling to prediction of chromatographic retention. **S. Banerjee**, S. Parimal, K. Srinivasan, S. Garde, S.M. Cramer

**4:40 BIOT 72.** Biopharmaceutical informatics: Selection of well-behaved molecules with predictive algorithms for enhanced process and product development of biologic drugs. **S. Kumar**, D. Tomar, E. Stephens, A. Tiwari, J.C. Rouse, S.K. Singh

## SUNDAY EVENING

### Section B

Westin San Diego  
Emerald Ballroom

### Downstream Processes

#### Disruptive BioProcessing for Upstream & Downstream Processes

J. Neville, A. Noyes, T. M. Przybycien, *Organizers*

K. Brower, J. P. Pieracci, *Organizers, Presiding*  
M. J. Betenbaugh, A. E. Schmelzer, *Presiding*

5:00 Panel Discussion.

## MONDAY MORNING

### Section A

Westin San Diego  
Crystal II

### Upstream Processes

#### Mammalian Cell Culture Process Development

M. R. Antoniewicz, M. A. Blenner, N. Lewis, B. Mulukutla, V. Roy, *Organizers*

P. Apostolidis, C. Metallo, *Organizers, Presiding*

**8:30 BIOT 73.** Distinct metabolic states support pluripotent stem cell self-renewal. **M. Badur**, H. Zhang, A. Divakaruni, S. Parker, C. Jaeger, K. Hiller, A. Murphy, C. Metallo

**8:50 BIOT 74.** 3M purification solution for mycoplasma retention. **D.V. Smirnov**, N. Stepanova, G.M. Jellum

**9:10 BIOT 75.** Transcriptome analysis of Chinese hamster ovary (CHO) cell lines under low temperature conditions using RNA-seq. **Y. Gowtham**, C. Saski, S.W. Harcum

**9:30 BIOT 76.** Process intensification through integration of upstream perfusion cell culture with downstream continuous chromatography in monoclonal antibody production. **A. Castan**, T. Falkman, E. Fäldt, L. Blomqvist, A. Forss

9:50 Intermission.

**10:10 BIOT 77.** Increasing diversity of production cell lines through miniaturization, automation, and high-throughput analytics. **K. Le**, H. Victor, K. Daris, T. Munro

**10:30 BIOT 78.** Automatic bioreactor feeding: Moving forward with metabolic activity monitoring for nutrient feeding. **G. Emmerson**, S. Watts, **G. Barringer**

**10:50 BIOT 79.** Using a CFD model to better understand and optimize cell culture performance using the ambr15™ reactor. **W.J. Kelly**, X. Li, Z. Huang, E.J. Schaefer, S. Subramanian

**11:10 BIOT 80.** Cell death during production of biologics and its consequences on release of the intracellular contents. **M. Krajcovic**, S. Hutchins, K. Aron, M.C. Borys, Z. Li

### Section B

Westin San Diego  
Emerald Ballroom

### Downstream Processes

#### Advances in Chromatographic Separations

J. Neville, A. Noyes, T. M. Przybycien, *Organizers*

S. M. Cramer, J. Pollard, *Organizers, Presiding*

**8:30 BIOT 81.** Evaluation of novel adsorptive hybrid filters for impurity removal during biologics purification. **N. Singh**, A. Arunkumar, M. Peck, A. Voloshin, J.F. Hester

**8:50 BIOT 82.** Maximizing productivity with AEX membrane adsorbers: Impact on robustness and edge of failure. **W. Rayfield**, D.J. Roush, A. Gospodarek, M. Brower, C. Cutler, N. Tugcu

**9:10 BIOT 83.** Evaluation of ligand design for downstream processes: Application to aggregate removal. **J.K. Rasmussen**, C. Bothof, G. Griesbraber, A. Vail, S. Colak Atan, F. Sgolastra

**9:30 BIOT 84.** Developing high performance responsive HIC membrane adsorbers. **Z. Liu**, X. Qian, R. Wickramasinghe

9:50 Intermission.

**10:10 BIOT 85.** Breaking through the productivity barrier: Integration of a novel modular chromatography scaffold and a new resin design to achieve a hyper-productive Protein A capture process. **M. Siwak**, G. de los Reyes, R. Todd

**10:30 BIOT 86.** Insight into the profile of associated HCP with protein A resin cycle number. **K. Lintern**, M. Pathak, A.S. Rathore, D.G. Bracewell

**10:50 BIOT 87.** Evaluation of excipients and cleaning solutions to enhance the performance of Protein A media. **A. Becerra-Arteaga**, A. Gupta

**11:10 BIOT 88.** Best of both worlds: High affinity and structural stability in 3D-structured synthetic ligands for protein purification by affinity chromatography. **S. Menegatti**

### Section C

Westin San Diego  
Diamond I&II

### Biomolecular & Biophysical Processes

#### Protein Engineering & Design

B. Hackel, J. Kaar, H. Samra, *Organizers*

D. Liu, *Organizer, Presiding*

A. J. Karlsson, *Presiding*

**8:30 BIOT 89.** Systemic depletion of serum L-cyst(e)ine with an engineered human enzyme mediates potent induction of ROS and specifically sabotages tumor metabolism. **S. Cramer**, A. Saha, S. Tadi, S. Tiziani, W. Yan, K. Triplett, S. Alters, D.E. Johnson, Y. Zhang, J. DiGiovanni, G. Georgiou, E. Stone

**8:50 BIOT 90.** Lessons learned from using phage display to select for fibrin binding peptides. **J. Rice**

**9:10 BIOT 91.** New approaches for high-throughput analysis and engineering of enzymes and protein therapeutics. **J. Cochran**

9:50 Intermission.

**10:10 BIOT 92.** Computational redesign of acyl-ACP thioesterase for medium-chain fatty acid production. **M. Grisewood**, N. Hernandez-Lozada, B. Pfeleger, C. Maranas

**10:30 BIOT 93.** Engineering substrate specificity of chymotrypsin for mass spectrometry based proteomics. **S. Abnoui**, B. Ramesh, N. Varadarajan

**10:50 BIOT 94.** Peptide ligands bind to electrostatic domains of Abeta. **B. Murray**, J. Lippens, D. Fabris, G. Belfort

**11:10 BIOT 95.** Inclusion of inter-domain linkers improves the stability and function of fusion proteins in cell-based assays. **J. Cook**, A. Charlesworth

### Section D

Westin San Diego  
Opal

### Biofuel & Biobased Chemical Production

#### Engineering Microbes to Utilize Next Generation Feedstocks

K. Brandon Sutton, M. A. O'Malley, *Organizers*

T. Lee, P. Peralta Yahya, *Organizers, Presiding*

**8:30 BIOT 96.** Unveiling cryptic xylose metabolism in *Yarrowia lipolytica*. **G.M. Rodriguez**, M. Shabbir-Hussain, L. Gambill, **M.A. Blenner**

**8:50 BIOT 97.** Enzyme assembly for increased methanol utilization. **J.V. Price**, L. Chen, W. Chen

**9:10 BIOT 98.** Conversion of lignin-derived aromatic compounds into lipids by engineered *Rhodococcus opacus* strains. **W.R. Henson**, S. Kim, Y.J. Tang, M. Foston, G. Dantas, **T. Moon**

**9:30 BIOT 99.** Optimal pathway rebalancing for 3-hydroxypropionic acid production from glycerol in *Escherichia coli*. **H. Lim**, M. Noh, G. Jung

9:50 Intermission.

**10:10 BIOT 100.** Comprehensive bioconversion of algae to liquid fuels and intermediate value products. **R.W. Davis**, W. Wu, M. Tran-Gyamfi, T. Lane, R. Pate, B. Wu

**10:30 BIOT 101.** Synthetic methylotrophy: Engineering *Escherichia coli* to metabolize methanol for growth and metabolite production. **W.B. Whitaker**, **R.K. Bennett**, M. Palmer, J. Gonzalez, M.R. Antoniewicz, **E.T. Papoutsakis**

**10:50 BIOT 102.** Deciphering the regulation of biomass degradation by anaerobic fungi. **J. Henske**, K. Solomon, M.K. Theodorou, I. Grigoriev, M.A. O'Malley

**11:10 BIOT 103.** Engineering *Ralstonia eutropha* to produce fuels and chemicals from diverse biomass-derived substrates. **S. Singer**

### Section E

Westin San Diego  
Crystal I

### Computationally Enabled Biotechnology at the Molecular, Cellular & Process Scales

#### Bio-Design & Systems Analyses at the Cellular Scale

J. Reed, D. J. Roush, *Organizers*

A. P. Burgard, J. Varner, *Organizers, Presiding*

**8:30 BIOT 104.** Genome-scale models can compute proteome allocation. **B.O. Palsson**

**9:10 BIOT 105.** Development and analysis of precursor production strains for chemical production. **X. Zhang**, C. Tervo, J. Reed

**9:30 BIOT 106.** Detection of novel metabolites and enzyme functions through in silico expansion of metabolic models. **J. Jeffries**, C. Lerma-Ortiz, A.J. Cooper, T. Niehaus, A. Thamm, O. Frelin, T. Kind, L.J. Broadbelt, O. Fiehn, A. Hanson, K.E. Tyo, C. Henry

9:50 Intermission.

**10:10 BIOT 107.** iSCHRUNK: In silico approach to characterization and reduction of uncertainty in the kinetic models of genome-scale metabolic networks. **S. Andreatti**, **L. Miskovic**, V. Hatzimanikatis

**10:30 BIOT 108.** System-level analysis of phototrophic metabolism of aromatic compounds in *Rhodospseudomonas palustris*. **A. Navid**, Y. Jiao, J. Pett-ridge

**10:50 BIOT 109.** Modeling of cell-free glycoprotein production in *Escherichia coli*. **N. Horvath**, J. Wayman, M.C. Jewett, M.P. DeLisa, J. Varner

**11:10 BIOT 110.** Enabling selection in directed evolution of enzymes via cellular engineering. **N. Hassanpour**, E. Ullah, M. Yousofshahi, **N.U. Nair**, S. Hassoun

### Section F

Westin San Diego  
Pearl Room

### Biomolecular & Biophysical Processes Biocatalysis & Biotransformations

B. Hackel, J. Kaar, H. Samra, *Organizers*

K. Brower, P. Cirino, *Organizers, Presiding*

**8:30 BIOT 111.** Influence of the intracellular metabolite profile on outcomes in protein engineering. **C. Cooper**

**8:50 BIOT 112.** Role of redundancy in metabolic networks and its implications in metabolic engineering. **E.C. Brunk**, J. Monk, A. Sastry, B. Palsson

**9:10 BIOT 113.** Designing custom subcellular organelles in bacteria. **C. Jakobson**, M. Siininger, E. Kim, J. Glasgow, M. Asensio, Y. Chen, D.T. Ercek

**9:30 BIOT 114.** HaloTag mediated artificial cellulosome assembly on DNA template for efficient cellulose hydrolysis. **Q. Sun**, W. Chen

9:50 Intermission.

**10:10 BIOT 115.** Biosynthesis of high-value inositol via *in vitro* synthetic enzymatic pathways. **Y. Zhang**, C. You

**10:30 BIOT 116.** Understanding short and medium chain volatile ester biosynthesis by AATase activity in yeast. **J. Zhu**, J. Lin, I.R. Wheeldon

**10:50 BIOT 117.** Discovery, expression and characterization of novel extremozymes from the deep Red-Sea brine pools. **S. Grootzinger**, E. Strillinger, A. Frank, M. Groll, D. Weuster-Botz, J. Eppinger

**11:10 BIOT 118.** Extreme thermoacidophiles as biocatalysts for heavy metal recovery: A delicate balance between biooxidation and resistance. **G. Wheaton**, A. Mukherjee, J. Counts, J. Kruh, B. Ijeomah, J. Desai, R.M. Kelly

### Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:

[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## Section A

Westin San Diego  
Emerald Ballroom

### Marvin J. Johnson Award in Microbial & Biochemical Technology

T. M. Przybycien, P. M. Tessier, S. A. Tobler,  
*Organizers, Presiding*

**11:30 BIOT 119.** Directed evolution of new viruses for therapeutic gene delivery. D.V. Schaffer

## MONDAY AFTERNOON

## Section A

Westin San Diego  
Crystal II

## Upstream Processes

## Microbial Process Development

M. R. Antoniewicz, M. A. Blenner, V. Roy,  
*Organizers*

M. C. Jewett, J. Latone, *Organizers, Presiding*

**2:00 BIOT 120.** Strategies for developing industrial microbial strains for chemicals production. S. Lee

**2:40 BIOT 121.** Strain engineering for robust *E. coli* fermentation processes. K. Veeravalli, T. Schindler, M. Yamada, R. Hamilton, K. Bodner, M. Laird

**3:00 BIOT 122.** Metabolic engineering with a dual-acting small RNA molecule for improved biofuels fermentations. A. Lahiry, S.D. Stimple, R. Lease, D.W. Wood

**3:20** Intermission.

**3:40 BIOT 123.** Rapid production and characterization of membrane-bound oligosaccharyltransferases with the aid of cell-free protein synthesis. J. Schoborg, J. Hershewe, J. Techner, M. Mkrsich, M. Jewett

**4:00 BIOT 124.** Bioprocess development of a natural product: An integrated strain improvement and fermentation process development program to accelerate process improvement. M.R. Mikola, N. Amrhein, S. Becker, P. Bhosale, E. Blackburn, D. Brown, J. Brunson, S. Casada, M. Chase, N. Clark, U. Galm, R. Garrison, K. Hill, E. Ibwe, H. Jones, J. Jones, P. Ketterer, P. Lewer, A. Lutocka, P. Maddipati, L. Marcun, J. Marty, E. Miller, E. Miller, N. Mouncey, N. Pollack, B. Raman, T. Ramseier, P. Reifel, R. Roberts, M. Roach, T. Schatzer, P. Speakman, C. Stowers, E. Traub, D. Tyagi, B. Ward, K. Work, S. Wensing

**4:20 BIOT 125.** Cooperation in a synthetic microbial community through engineered commensalism. E.E. Kelly, C.H. Collins

**4:40 BIOT 126.** Dynamic two-stage fermentation in *S. cerevisiae* allows for rapid and scalable strain design for microbial chemical synthesis. B. Reed, M. Lynch, J. Burg

## Section B

Westin San Diego  
Emerald Ballroom

## Downstream Processes

## Advances in Chromatographic Separations

J. Neville, A. Noyes, T. M. Przybycien,  
*Organizers*

S. M. Cramer, J. Pollard, *Organizers, Presiding*

**2:00 BIOT 127.** High capacity polishing chromatography for antibody purification processes. Y. Tao

**2:20 BIOT 128.** High throughput determination of cleaning solutions to prevent the fouling of an anion exchange resin. T. Elich, T. Iskra, W. Daniels, C.J. Morrison

**2:40 BIOT 129.** Method development for resin selectivity screening in RoboColumn® format. A. Kiesewetter, P. Menstell, L. Peock, A. Stein

**3:00 BIOT 130.** Variable surface transport modalities on functionalized chromatographic supports revealed with single molecule spectroscopy. L.J. Tausin, H. Shen, J.K. Rasmussen, C. Bothof, G. Griesbraber, A.K. McNulty, C.F. Landes

**3:20** Intermission.

**3:40 BIOT 131.** Probing nanoscale effects of ligand density in tentacular ion exchangers using x-ray scattering. R.S. Bhambure, D.G. Greene, C. Gillespie, M.W. Phillips, H. Graafls, A. Rapp, A.M. Lenhoff

**4:00 BIOT 132.** Application of mechanistic modeling for enabling PAT in process chromatography: Separation of charge variants of mAbs by ion exchange chromatography. V. Kumar, A.S. Rathore

**4:20 BIOT 133.** Spectral deconvolution of chromatograms with PLS models and calibration-free methods. M. Rüd, N. Brestrich, J. Hubbuch

**4:40 BIOT 134.** General gradients for preparative chromatography. A. Holmqvist, A. Sellberg, F. Magnusson, B. Nilsson, A. Staby

## Section C

Westin San Diego  
Diamond I&II

## Biomolecular &amp; Biophysical Processes

## Protein Engineering &amp; Design

B. Hackel, J. Kaar, H. Samra, *Organizers*

A. J. Karlsson, D. Liu, *Organizers, Presiding*

**2:00 BIOT 135.** When bad is good: Directed evolution using negative selection can result in alleles with superior properties. B. Steinberg, M. Ostermeier

**2:20 BIOT 136.** Creating catenanes with lasso peptides. C.D. Allen, A. Link

**2:40 BIOT 137.** Yeast surface display-based method for the directed evolution of optimized self-cleaving intact purification tags. S.D. Stimple, M.J. Coolbaugh, Y. Fan, K. Cochran, D.W. Wood

**3:00 BIOT 138.** Computationally de novo designed peptide-mediated hetero-oligomeric interactions for modular self-assembly of protein and lipoprotein nanostructures. M.S. Ardejani

**3:20** Intermission.

**3:40 BIOT 139.** Functional selection of full-length antibodies in the cytoplasm of living bacterial cells. M. Robinson, N. Ke, M. Berkemen, M.P. DeLisa

**4:00 BIOT 140.** Improved methods for co-evolving the affinity and stability of antibody fragments specific for amyloid-forming polypeptides. K.E. Tiller, M. Julian, C. Lee, L. Rabia, J. Young, P.M. Tessier

**4:20 BIOT 141.** Engineering antibody specificity through multi-dimensional high-throughput screens. D. Li, Y. Cho

**4:40 BIOT 142.** Evolving an intrinsically disordered peptide, the  $\beta$ -roll, for biomolecular recognition. B. Bulutoglu, K. Dooley, S. Banta

## Section D

Westin San Diego  
Opal

### Biofuel & Biobased Chemical Production

## Biomass Pretreatment &amp; Hydrolysis

K. Brandon Sutton, M. A. O'Malley, *Organizers*

M. B. Foston, M. Resch, *Organizers, Presiding*

**2:00 BIOT 143.** Multimodal characterization of industrial steam exploded biomass samples: A modelling approach to predict enzymatic digestibility. T. Auxenfans, B. Chabbert, G. Paes

**2:20 BIOT 144.** Evaluation of *In planta* transient expression of cell wall degrading enzymes as a biological pretreatment for cellulosic biomass. L. Anthony, M. Hwang, M. Phu, B.W. Falk, A.M. Dandekar, K. McDonald

**2:40 BIOT 145.** Energy analysis of algal biocude production. E. Martinez-Guerra, V. Gude

**3:00 BIOT 146.** Enhanced saccharification of biomass to aqueous soluble oligosaccharides and monosaccharides at high biomass loading in molten salt hydrate medium. N. Li, J. Kraft, X. Pan

**3:20** Intermission.

**3:40 BIOT 147.** Effect of water-soluble kraft lignin fraction on the enzymatic saccharification of pretreated poplar. Y. Jin, Y. Wang, W. Wang

**4:00 BIOT 148.** Liquid hot water pretreatment inhibitors. E. Ximenes, Y. Kim, C. Farinas, M.R. Ladisch

**4:20 BIOT 149.** Determination of lignin kinetics during organosolv pretreatment. J. Meyer, M.B. Foston

**4:40 BIOT 150.** Making room during pretreatment. A. Ragauskas, Y. Pu, M. Li, C.G. Yoo

## Section E

Westin San Diego  
Crystal I

### Computationally Enabled Biotechnology at the Molecular, Cellular & Process Scales

## Process Modeling in Biotechnology

J. Reed, D. J. Roush, *Organizers*

R. Todd, A. K. Velayudhan, *Organizers, Presiding*

**2:00 BIOT 151.** Using a Monte Carlo simulation model to predict process performance during scale-up. R. Ashton, A. Gates, J. Moscariello

**2:20 BIOT 152.** Advanced multiscale metabolic modeling of a nitrogen fixing cyanobacterium. J. Gardner, B. Miller, W. Sinclair, H. North, B. Hodge, N.R. Boyle

**2:40 BIOT 153.** Bioprocess modeling of fouling phenomena in cross-flow micro-filtration of viable bacteria. X. Li, S. Ku, K. Thomas, K. Foster, E. Ximenes, H. Jaycey, X. Liu, M.R. Ladisch

**3:00 BIOT 154.** Facilitating the analysis of complex samples using data reduction techniques: Case studies in downstream processing. S. Konstantinidis, N. Field, K. Jurlewicz, A.K. Velayudhan

**3:20** Intermission.

**3:40 BIOT 155.** Designing flow-through chromatography processes for aggregate removal. S. Hasegawa, D. Itoh, Y. Isakari, N. Yoshimoto, A. Podgornik, S. Yamamoto

**4:00 BIOT 156.** Mechanistic modeling of chromatography and its application in biopharmaceutical process development. F. Stueckler, K. Doninger, J. Griesbach

**4:20 BIOT 157.** General gradients for preparative chromatography: Mechanistic modeling and practical consideration. A. Sellberg, A. Holmqvist, C. Andersson, B. Nilsson

**4:40 BIOT 158.** Ensuring long term robustness of a CEX chromatographic step for separation of charge variants with optimized yield. K. Haeringer, E. Rosenberg, S. Heppbildkier, K. Lacki, E. Brekkan, M. Ahnfeldt

### LGBT Chemists' Symposium on Chemical Biology

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## Undergraduate Research Posters

## Biotechnology

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## MONDAY EVENING

## Section A

San Diego Convention Center  
Hall D/E

## Sci-Mix

P. M. Tessier, S. A. Tobler, *Organizers*

**8:00 - 10:00**

242-244, 246-248, 250-253, 255-258, 263-264, 266, 270-271, 275, 278, 280, 287-290, 292-293, 295, 301, 304, 308, 315-319, 322-325, 330, 332, 335, 350, 353-354, 360, 378, 388, 408. See subsequent listings.

## TUESDAY MORNING

## Section A

Westin San Diego  
Diamond II

## Upstream Processes

## Engineering Non-Model Hosts for Biological Production

M. R. Antoniewicz, M. A. Blenner, V. Roy,  
*Organizers*

H. Dhamankar, D. T. Ercek, *Organizers, Presiding*

**8:30 BIOT 159.** Novel gut fungal sugar transporters for improved bioprocess efficiency. S. Seppala, K. Solomon, J. Henske, S.P. Gilmore, M.D. Rieth, M.A. O'Malley

**8:50 BIOT 160.** Metabolic engineering of the marine cyanobacterium, *Synechococcus* sp. PCC 7002 for phototrophic production of L-lysine and sugar feedstocks. A.L. Markley, B. Pfleger

**9:10 BIOT 161.** Extreme thermophile metabolic engineering platforms: Production of biofuels and bio-based chemicals at elevated temperatures. A.J. Loder, B.M. Zeldes, A. Hawkins, C.T. Straub, M.W. Keller, G.L. Lipscomb, G.J. Schut, M.W. Adams, R.M. Kelly

**9:30 BIOT 162.** *Clostridium autoethanogenum*, a chassis for low carbon fuel and commodities production at commercial scale by gas fermentation. S. Nagaraju

**9:50** Intermission.

**10:10 BIOT 163.** *Yarrowia lipolytica* as a technology platform for industrial applications. **Q.Q. Zhu**

**10:30 BIOT 164.** High efficiency genome editing in *Yarrowia lipolytica* by CRISPR/Cas9. **C.M. Schwartz**, M. Shabbir-Hussain, B. Simmons-Rowls, A. Loebis, M.A. Blenner, I.R. Wheeldon

**10:50 BIOT 165.** Rapid isolation of chromosome hubs to facilitate nonconventional yeast engineering. **Z. Shao**, M. Cao, M. Gao, C. Lopez, Y. Wu

**11:10 BIOT 166.** Programmable genetic sensors and circuits for pathway engineering. A. Hoynes-O'Connor, C. Immethun, D. DeLorenzo, K. Ng, **T. Moon**

## Section B

Westin San Diego  
Emerald Ballroom

### Downstream Processes

#### Downstream Processing for Antibodies, Drug Conjugates & Related Molecules

J. Neville, A. Noyes, T. M. Przybycien, *Organizers*

K. Mehta, N. Sanaie, *Organizers, Presiding*

**8:30 BIOT 167.** Capture resin screening for Bis-scFv purification using high throughput methodologies. **B. Thangaraj**, R. Gillespie

**8:50 BIOT 168.** Mitigating novel ADC impurity challenges through creative approaches: Check the antibody variants. **X. Lin**, J. Franklin, M. Hutchinson, J. Gorrell

**9:10 BIOT 169.** Selective on-column PEGylation of a therapeutic protein using hydroxyapatite and fluoroapatite adsorbents. **M. Bakshayeshi**, G. Bolton, J.P. Pieracci, D. Cecchini

**9:30 BIOT 170.** Development of peptide based affinity media for the purification of monoclonal antibodies: Effect of spacer arms, peptide variants and process conditions. **T. Islam**, A. Naik, Y. Hashimoto, S. Menegatti, R.G. Carbonell

**9:50 Intermission.**

**10:10 BIOT 171.** Evaluating novel harvest methods for high density mammalian cell culture processes. **M. Rohani**, C. Chase, B. Guzman, K. Mehta, N. Osei-Ovusu

**10:30 BIOT 172.** Evaluation of preparative ion exchange and multimodal chromatography for separation of charge variants in the mAb purification process. **A. Gronberg**, **T. Bjorkman**, L. Kärf, A. Ljunglöf, E. Heldin

**10:50 BIOT 173.** Eco-friendly detergent for viral inactivation. **A. Ladiwala**, S. Fisher, L. Norling, K. Abadie, G. Magill, N. Magarian, K. Skidmore, R. Shearer, M. Butler, J. Gorrell, Q. Chen, P. Lester

**11:10 BIOT 174.** Development of challenging aggregate removal step in a bi-specific antibody purification process: A case study. **S. Jain**, M. Mercaldi

## Section C

Westin San Diego  
Diamond I

### Biomolecular & Biophysical Processes

#### Protein Therapeutics: Discovery & Production

B. Hackel, J. Kaar, H. Samra, *Organizers*

N. Basse, Y. Y. Chen, *Organizers, Presiding*

**8:30 BIOT 175.** Selection of inhibitory antibodies using next generation high throughput sequencing. **T.J. Lopez**, X. Ge

**8:50 BIOT 176.** High-throughput conformational epitope mapping by deep sequencing for antibody discovery. **T. Whitehead**

**9:10 BIOT 177.** Rethinking affibody: Evolving small proteins using data-driven diversification. **D.R. Woldring**, P.V. Holec, B. Hackel

**9:30 BIOT 178.** Human G protein-coupled receptors expression and signaling in yeast: Design and optimization of the host/protein platform for therapeutic development. **A. Jain**, A.S. Robinson

**9:50 Intermission.**

**10:10 BIOT 179.** Bispecific antibody vs. binary mixture: Synergy in the treatment of pertussis. **E. Wagner**, J. Maynard

**10:30 BIOT 180.** Discovery of highly soluble antibodies prior to purification using affinity-capture self-interaction nanoparticle spectroscopy. **J. Wu**, J.S. Schultz, C.L. Weldon, S.V. Sule, Q. Chai, S.B. Geng, C.D. Dickinson, P.M. Tessier

**10:50 BIOT 181.** Withdrawn.

**11:10 BIOT 182.** Effect of air-liquid interface in monoclonal antibody aggregate formation. **T.A. Mammo**, B. Constantine, M. Zhu, D. Robbins

## Section D

Westin San Diego  
Opal

### Emerging Technologies

#### New Tools & Approaches

J. Latone, G. M. Thurber, I. R. Wheeldon, *Organizers*

B. Thronset, J. Wang, *Organizers, Presiding*

**8:30 BIOT 183.** Site-specific covalent labeling of RNA with RNA-TAG: A robust technology applicable to a variety of biologically relevant investigations. **S.C. Alexander**, N.K. Devaraj

**8:50 BIOT 184.** New synthetic chemical biology approach for the development of HIV-1 vaccine. **N. Wang**, Z. Yuan, W. Niu, Q. Li, **J. Guo**

**9:10 BIOT 185.** Mimicking protein functions with entropically constrained peptides. **B. Farrow**, A. Wang, K. Deyle, D. Bunck, J.R. Heath

**9:30 BIOT 186.** Peptoid-based microsphere coating to increase the binding efficiency in sandwich ELISA microarrays. **G.R. Perez-Bakovic**, S.L. Servoss

**9:50 Intermission.**

**10:10 BIOT 187.** Disease screening pill for breast cancer; *In vivo* demonstration of an orally available near-infrared molecular imaging agent using mouse xenografts. **S. Bhatnagar**, K. Dhingra, W. Kelley, J. Liao, A. Priluck, **G.M. Thurber**

**10:30 BIOT 188.** High-throughput production of multifunctional suspension microarrays by massive coding of dissociated elements. **J. Wang**

**10:50 BIOT 189.** Bio-orthogonal chemistry enables proteomic analysis of *Staphylococcus aureus* during mammalian infection. **S. Stone**, D.A. Tirrell

**11:10 BIOT 190.** Engineering commensal microbes to fight against pathogen. **I. Hwang**, M. Chang

## Section E

Westin San Diego  
Crystal I

### Biosimilars

#### Development & Manufacturing Considerations for Biosimilars

J. Myers, *Organizer*

O. Jaquez, K. Sampathkumar, *Organizers, Presiding*

**8:30 Introductory Remarks.**

**8:50 BIOT 191.** Considerations in the development and control of biosimilar manufacturing in the United States. **J.C. Baker**

**9:30 BIOT 192.** From process characterization to control strategy. **D. Boeth**

**9:50 Intermission.**

**10:10 BIOT 193.** Development of a biosimilar: Pooling efforts from all technical forces. **R.S. Gronke**, O. Jaquez, B. Woppmann, Y. Lyubarskaya, S. Prajapati

**10:30 BIOT 194.** Flexibility in high-throughput two column purification platforms for biosimilar mAb manufacturing. **K. Blando**, C.W. Richey, G. Winzeler, K. Dhanasekharan, V. Vinci

**10:50 BIOT 195.** FMEA based characterization of biosimilar drug product manufacturing. **S. Kamat**, B. Bernat, J. TerWee

**11:10 Panel Discussion.**

## Section F

Westin San Diego  
Crystal II

### Upstream Processes

#### Metabolic Engineering & Synthetic Biology: Pathways/Products

M. R. Antoniewicz, M. A. Blenner, V. Roy, *Organizers*

C. H. Collins, H. Le, *Organizers, Presiding*

**8:30 BIOT 196.** Exploring enhancement of 1,4-butanediol production in recombinant *E. coli* using large-scale kinetic models. **S. Andreozzi**, A. Chakrabarti, K. Soh, A.P. Burgard, T. Yang, S. Vandien, **L. Miskovic**, V. Hatzimanikatis

**8:50 BIOT 197.** Metabolic biology of *Saccharophagus degradans*, a cellulolytic biomass-digesting bacterium, as revealed by <sup>13</sup>C metabolic flux analysis. **A. Quinn**, B.D. Gastfriend, J.G. Corckran, S.W. Hutcheson, G. Siram

**9:10 BIOT 198.** Isopentenyl diphosphate (IPP)-bypass mevalonate pathways for C<sub>5</sub> alcohol production. **T. Lee**

**9:30 BIOT 199.** Using phosphoproteomic analysis to better understand gene regulatory networks. **M. Marten**, N. Ramsbramaniam, C. Chelius, L. Ribeiro, K. Boppidi, S. Li, S. Harris, R. Srivastava

**9:50 Intermission.**

**10:10 BIOT 200.** Pathway manipulations enhance acetyl-CoA supply for natural product synthesis. **J. Cardenas**, N.A. Da Silva

**10:30 BIOT 201.** Complete biosynthesis of opioids in yeast. **S. Galanie**, K. Thodey, I.J. Trenchard, M. Filsinger Interrante, C.D. Smolke

**10:50 BIOT 202.** Construction of inducible gene expression systems in *Pichia pastoris* for recombinant protein production. **J. Cao**, P. Perez-Pinera, T. Lu

**11:10 BIOT 203.** Guiding CHO cell engineering for biopharmaceutical development using genome-scale models of CHO cell metabolism. **N.E. Lewis**

## Section A

Westin San Diego  
Emerald Ballroom

### BIOT Young Investigator Award Lecture & Peterson Award Presentations

T. M. Przybycien, P. M. Tessier, S. A. Tobler, *Organizers, Presiding*

**11:30 BIOT 204.** Metabolic engineering of *Yarrowia lipolytica* for fuels and chemicals production. **H.S. Alper**

## TUESDAY AFTERNOON

## Section A

Westin San Diego  
Crystal II

### Upstream Processes

#### Metabolic Engineering & Synthetic Biology: Tools Development

M. R. Antoniewicz, M. A. Blenner, V. Roy, *Organizers*

M. Lipscomb, K. E. Tyo, *Organizers, Presiding*

**2:00 BIOT 205.** Building a biological foundry for next-generation synthetic biology. **H. Zhao**

**2:40 BIOT 206.** Development of platform-based technologies for the optimization of sustainably produced chemicals. **S.J. Culler**

**3:00 BIOT 207.** Next generation synthetic biology tools for rapid, high-throughput optimization of metabolic pathways. **S. Chandran**

**3:20 Intermission.**

**3:40 BIOT 208.** redGEM: A unbiased approach for systematic reduction of genome-scale models. **V. Hatzimanikatis**

**4:00 BIOT 209.** Co-opting uncharacterized CRISPR-Cas systems as the next generation of biomolecular tools. **R. Leenay**, K. Maksimchuk, **C. Beisel**

**4:20 BIOT 210.** Trackable genome engineering with single nucleotide resolution. **A.D. Garst**, M. Bassalo, G. Pines, S. Lynch, A. Edwards, R.T. Gill

**4:40 BIOT 211.** Transcription activator-like effectors as tools for manipulation of bacterial gene expression. **M.C. Politz**, M. Copeland, B. Pfeleger

## Section B

Westin San Diego  
Emerald Ballroom

### Downstream Processes

#### Downstream Processing for Antibodies, Drug Conjugates & Related Molecules

J. Neville, A. Noyes, T. M. Przybycien, *Organizers*

K. Mehta, N. Sanaie, *Organizers, Presiding*

**2:00 BIOT 212.** Development of efficient cation exchange (CEX) chromatography to remove low and high molecular weight species for commercial manufacturing of a mAb. **M. Mayani**, D. Yu, E. Schutsky, A.T. Lewandowski, Y. Song, S. Traylor, R. Swanson, Z. Li

**2:20 BIOT 213.** Re-oxidization of partially reduced monoclonal antibody by charged depth filters. **H. Hoang**

**2:40 BIOT 214.** Matrix HD-Sb membrane adsorber: A new high-performance purification tool for mAb purification in flowthrough mode. **D.M. Kanani**, N. Paghdal, A. Shang, R. Jacquemart, J.G. Stout

**3:00 BIOT 215.** Influence of downstream processing on the glycosylation of recombinant anthrax receptor fusion protein transiently expressed in *Nicotiana benthamiana*. **K. Karuppanan**, J.K. Muchena, S. Duhra-Gill, M. Phu, C. Lebrilla, A.M. Dandekar, S. Nandi, K. McDonald

**3:20 Intermission.**

**3:40 BIOT 216.** Enabling high-throughput downstream process development: From method screening to process characterization. **J. Gervais**

**4:00 BIOT 217.** Optimization of mAb charge and size variants separation using dual pH/salt gradient elution IEC. **Y.F. Lee**, S. Kluters, F. Wittkopp, **C. Frech**

**4:20 BIOT 218.** Evaluation of cation exchange chromatography resin lot variability and optimization of process conditions for the intermediate purification of a fusion protein. **A. Slocum**, K. Sterl, R. Wright

**4:40 BIOT 219.** Knob-hole assembly of bispecific antibodies from half-antibodies. **A.J. Williams**

### Section C

Westin San Diego

Diamond I

### Biomolecular & Biophysical Processes

#### Protein Therapeutics: Formulation & Delivery

**B. Hackel**, J. Kaar, *Organizers*

**E. Y. Chi**, H. Samra, *Organizers, Presiding*

**2:00 BIOT 220.** Characterization of highly concentrated mAb solution: One step towards the prediction of long-term stability. **M. Schermeyer**, A.K. Will, J. Hubbuch

**2:20 BIOT 221.** Predicting high-concentration antibody interactions with coarse-grained molecular modeling. **C. Calero-Rubio**, R. Ghosh, A. Saluja, C.J. Roberts

**2:40 BIOT 222.** Evaluation of pH-responsive hydrogel networks as oral delivery systems for hematologic factor IX. **S. Horava**, K. Moy, J. Liou, N. Peppas

**3:00 BIOT 223.** How predictive are protein-protein interactions of elevated viscosity for protein solutions. **M.A. Woldeyes**, C. Calero-Rubio, E.M. Furst, C.J. Roberts

**3:20 Intermission.**

**3:40 BIOT 224.** Protein-excipient interaction hotspots: *In silico* method development and Fab case study. **T.S. Barata**, P. Dalby, S. Brocchini, M. Zloh

**4:00 BIOT 225.** Electrospun nanofibers of gelatin/cyclodextrin and their potential application as hydrophobic drug delivery system. **A. Laha**, S. Majumdar, C. Sharma

**4:20 BIOT 226.** Effects of small molecule co-solutes on the viscosity and stability of highly concentrated solutions of monoclonal antibodies. **B. Dear**, J. Hung, A. Borwankar, T. Truskett, K.P. Johnston

**4:40 BIOT 227.** Accelerating pharmaceutical development: Case studies with automated approaches and formulation 'miniaturization'. **R. Rajan**, V. Razinkov, C. Ren, P. Yeh

### Section D

Westin San Diego

Opal

### Emerging Technologies

#### Stem Cells & Regenerative Medicine

**J. Latone**, G. M. Thurber, I. R. Wheeldon, *Organizers*

**P. Apostolidis**, Y. Kim, *Organizers, Presiding*

**2:00 BIOT 228.** CD264: A cell-surface marker for an aging population of mesenchymal stem cells. **S. Madsen**, K. Russell, A. Tucker, B. Bunnell, **K. O'Connor**

**2:20 BIOT 229.** Regenerative medical bio-adhesive based on photo-curable mussel adhesive protein hydrogel. **E. Jeon**, B. Choi, B. Hwang, Y. Yang, G. Jung, H.J. Cha

**2:40 BIOT 230.** Modeling the blood-brain barrier using human pluripotent stem cells. **E. Shusta**

**3:20 Intermission.**

**3:40 BIOT 231.** Cell-derived microparticles for cell & gene therapy: The case of megakaryocytic microparticles. **J. Jiang**, C. Kao, E.T. Papoutsakis

**4:00 BIOT 232.** High yield *in vitro* expansion of cancer stem cells / tumor initiating cells. **S.G. Tilson**, E.M. Haley, **Y. Kim**

**4:20 BIOT 233.** Scalable hepatic differentiation of human endodermal cells from pluripotent stem cell. **D. Chau**, K. Ortiz, W. Hu

**4:40 BIOT 234.** Extracellular matrix mimetic chemical and physical cues for promoting human mesenchymal stem cell tenogenic gene expression. **M. Rehmman**, A.M. Kloxin

### Section E

Westin San Diego

Crystal I

### Biosimilars

#### Challenges in Demonstrating Analytical Biosimilarity

**J. Myers**, K. Sampathkumar, *Organizers*

**B. Bernat**, A. Fotopoulos, *Organizers, Presiding*

**2:00 Introductory Remarks.**

**2:20 BIOT 235.** Characterization and quantitative comparison of remicade and its biosimilar remsima. **A. Schwendeman**

**2:40 BIOT 236.** Using critical quality attributes in the development of biosimilars. **B. Bernat**, J. TerWee

**3:00 BIOT 237.** Higher order structure analysis using hydrogen deuterium exchange mass spectrometry (HDX MS) and differential scanning calorimetry (DSC). **C.F. Quinn**

**3:20 Intermission.**

**3:40 BIOT 238.** Application biophysical techniques and NMR for higher order structure biosimilarity studies. **J. Qiao**, D. Tsao, R. Sridharan, J. Myers, C. Bell, J. Anderson

**4:00 BIOT 239.** Challenges and approaches in demonstrating biosimilarity at the physicochemical and biological level. **J. Myers**, V. Farutin, J. Glajch, J. Anderson

**4:20 Panel Discussion.**

## TUESDAY EVENING

### Section A

Westin San Diego

Emerald Ballroom

### BIOT Industrial Biotechnology Award

**T. M. Przybycien**, P. M. Tessier, S. A. Tobler, *Organizers, Presiding*

**5:00 BIOT 240.** Commercialization of Keytruda™: Overcoming molecular design challenges and time. **D.J. Roush**

### Section A

San Diego Convention Center

Hall E

### Poster Session

**B. Berger**, A. C. Dumetz, *Organizers*

**6:00 - 9:00**

**BIOT 241.** New approaches to the chemical synthesis and characterization of azetidione. **E.J. Parish**, Y. Lo, **H. Honda**, T. Wei, **H. Shyu**

**BIOT 242.** Efficiency in cellbanking and seed preparation through intensified perfusion. **A. Castan**, O. Larsson

**BIOT 243.** Single-pass tangential flow filtration (SPTFF) for process intermediate volume reduction. **N.E. Levy**, A.C. Szkodny, T.H. Wiley, J.R. Molek, K.E. Goklen

**BIOT 244.** Implementation of miniaturized fed-batch processes in microliter-scale vessels for the development of high performance CHO cell culture media. **M.R. Good**, M. Goldfeld, W. Ling

**BIOT 245.** Evaluating the effect of cross-flow pattern on product sieving within hollow fiber cell retention devices in CHO cell perfusion. **P. McInnis**, D. Rank, A. Dupont, C. Martin, M.W. Phillips

**BIOT 246.** Application of ambr250 mini-bioreactor platform to microcarrier cultures for high throughput vaccine development. **W. Malik**

**BIOT 247.** Feed optimization to improve productivity and product quality enabled by automated sampling system. **L. Hoshan**, S. Xu, K. O'Neill, A. Mehta, T. Seamans, H. Chen

**BIOT 248.** Characterizing oxygen kLa in bioreactors to support scale-up and scale-down of cell culture bioprocesses. **G. Yao**, S.R. Patel, Z. Ahmed, L. Marquardt, J. Lagos, K. Aron, J. Yee, M.C. Borys, Z. Li

**BIOT 249.** Gamma irradiated microcarrier-based virus production in a single-use rocking bioreactor system. **A. Magnusson**, M. Lundgren, E. Blanck, M. Berg

**BIOT 250.** Implementing automated sampling, process monitoring, and nutrient feedback control for a system of 3-L bioreactors. **K. O'Neill**, A. Mehta, L. Hoshan, S. Xu, T. Seamans

**BIOT 251.** Withdrawn.

**BIOT 252.** Evaluating the cytotoxicity of antioxidant and plasticizer additives used in single use cell culture bags. **R. Shah**, T. Linville, L. Yordy, J. Briggs, N. Chandarana, A. Whynot, C.S. Brazel

**BIOT 253.** Development of a model at home medical device using a two-step enzymatic process for the detection of hemoglobin A1c levels in human blood. **N. Ledra**, T. McCaffrey, J. Cabrera

**BIOT 254.** Effect of surfactants on the fluorescence behavior of dye-conjugated DNA for FRET enhancement. **T. Oh**, J. Choi, M. Heller

**BIOT 255.** Synthesis of CdSe/ZnS nanocrystals and their bioconjugation to DNA. **C.D. Hanson**, L. Mohr

**BIOT 256.** Simultaneous detection of *Vibrio cholerae* and cholera toxin using a hybrid chip ba double biomolecular markers. **H. Shin**, J. Seo, C. Kim, B. Hwang, H.J. Cha

**BIOT 257.** Creating a DNA thermometer: An application for DNA computation. **R.J. Karadeema**

**BIOT 258.** Micromachined multielectrode microprobes for glutamate and dopamine detection. **A. Yorita**, H. Monbouquette

**BIOT 259.** Multiplexed detection of pathogenic DNA using zinc finger proteins without DNA amplification. **J. Kim**, M. Kim

**BIOT 260.** Novel applications to the new development of amperometric biosensor for serum cholesterol level determination. **Y. Lo**, E.J. Parish, H. Honda, T. Wei

**BIOT 261.** Withdrawn.

**BIOT 262.** Novel application of scanning electron microscopes and the comparison of non-native Tephritid flies. **E.J. Parish**, Y. Lo, H. Honda, T. Wei

**BIOT 263.** Process analytical technology solutions for real-time monitoring and control of CHO bioprocesses. **E.R. Gibson**

**BIOT 264.** Withdrawn.

**BIOT 265.** Strategies for optimizing a cell culture platform to achieve high recombinant protein titer. **R. Gruver**, S.B. Varna, N. Vijayasankaran, S.J. Meier

**BIOT 266.** Improving the dynamic control of fatty acid ethyl ester production. **A. Yaguchi**, E. Arvay, G.M. Rodriguez, N. Wilson, M.A. Blenner

**BIOT 267.** Gamma-aminobutyric acid production through GABA shunt by the introduction of synthetic scaffolds in recombinant *Escherichia coli*. **S. Hong**, V. Pham, S. Somasundaram

**BIOT 268.** Genetic incorporation of unnatural amino acids biosynthesized from  $\alpha$ -keto acids by an aminotransferase. **W. Ko**, H. Lee

**BIOT 269.** Genetic incorporation of recycled unnatural amino acids. **H. Lee**, **S. Kim**

**BIOT 270.** Translating unnatural amino acids with phenotypically-diverse, engineered EF-Tu and tRNA variants. **V. Cox**, E. Gaucher

**BIOT 271.** Developing a protein-specific purification approach for osteopontin expressed in chloroplast of *Chlamydomonas reinhardtii*. **A. Ravi**, S. Guo, S. Kulkarni, B. Rasala, M. Tran, S. Mayfield, Z.L. Nikolov

**BIOT 272.** Synthetic biology based multiple approaches for coenzyme B12 production in *Escherichia coli*. **M. Noh**, H. Lim, S. Park, G. Jung

**BIOT 273.** Overcoming cellular barriers for enhancing polymer-mediated transgene expression. **M. Christensen**, J. Eimer, S. Barua, S. Eaton, L. Gonzalez-Malerva, J. Lehman, J. LaBaer, K. Haynes, K. Rege

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)



- BIOT 274.** Development of advanced genome engineering tools for a model cyanobacterium. **H.R. Aucoin, M. Sanktjohanser, N.R. Boyle**
- BIOT 275.** Functional chitosan-nanofibers fabricated by an acidic shell matrix protein for the preparation of efficient tissue engineering scaffold. **W. Song, Y. Choi**
- BIOT 276.** New approaches to optically transparent elastic materials for optical device in ophthalmology. **Y. Lo, H. Shyu, H. Honda, T. Wei**
- BIOT 277.** Particle size evaluation for improved CHO and *E. coli* harvest operations. **S. Gerekpa, J. Bill, A. Naim, J. Borrajo**
- BIOT 278.** Dendronized polymers for mRNA delivery. **N.J. Oldenhuis, Z. Guan**
- BIOT 279.** Engineering large pore mesoporous silica nanoparticles for progene delivery application. **H.W. Omar, J.G. Croissant, L. Deng, N.M. Khashab**
- BIOT 280.** Design and formulation of novel nanoemulsions that inhibit *Mycobacterium smegmatis* biofilm formation. **A. Kratzer, M. Brantley, C. Magee, W. Magilton, V. Ware, B. Berger**
- BIOT 281.** Novel preparation and characterization of Epicatechin-3-allopyranoside. **E.J. Parish, J. Wu, H. Ho, H. Honda, T. Wei**
- BIOT 282.** Novel development of a computational drug target prediction method based on chemical similarity networks. **Y. Lo, E.J. Parish, H. Honda, T. Wei**
- BIOT 283.** Determination of optimum bead size for immobilized cell fermentations for enhanced production of lovastatin by *Aspergillus terreus*. **G. Chun**
- BIOT 284.** Development of fed-batch fermentation process for enhanced production of *cis-cis* muconic acid using high-yielding mutant cells of *Corynebacterium glutamicum*. **S. Kim, G. Chun, S. Byun, S. Seo, B. Lee, S. Park, Y. Kim, W. Shin, S. Lee, E. Kim, D. Lee, S. Kim**
- BIOT 285.** Scale-down model development for a 5000-L production bioreactor process using 0.5-L shake flask and 5-L bioreactor systems. **J. Discenza, H. Graham, E. Crabbe, N.G. Dalal**
- BIOT 286.** Hydrogenolysis of biomass-derived glycerol to propanediols over Pd-Re catalyst: Influence of different Pd precursors. **Y. Li, L. Ma, D. He**
- BIOT 287.** Optimizing metabolic pathways for the improved production of natural products. **J.A. Jones, M. Koffas**
- BIOT 288.** Improving scale-down models through characterization of metabolism in a streptomyces fermentation. **J. Easson, S. Moses, M. Fieger**
- BIOT 289.** Substrate-dependent surface display of a cellulosome by *Saccharomyces cerevisiae*. **P. Botero Besada-Lombana, N.A. Da Silva**
- BIOT 290.** Succinic acid production on xylose-enriched biorefinery streams by *Actinobacillus succinogenes* in batch fermentation. **A. Mohagheghi, D. Salvachua, H. Smith, M. Bradfield, W. Nicole, B. Black, M. Biddy, N. Dowe, G. Beckham**
- BIOT 291.** Advancing modeling and simulation in the biopharmaceutical industry. **S.M. Hunt, J. Robinson, R.J. Todd**
- BIOT 292.** Developing a better scale-down model of a manufacturing scale CHO bioreactor process using targeted transcriptomics. **A.G. Lee, W.D. Croughan, A. Lewis, N.R. Abu-Absi, M.C. Borys, Z. Li**
- BIOT 293.** Influence of cell age on cell biological variability during early process development. **P. Bolisetty, G. Tremml, S. Herzer, L. Paul**
- BIOT 294.** Process analytical technology (PAT) for bioprocessing. **A. Williams, B. Chavez, C. Agarabi, K.A. Brorson**
- BIOT 295.** Development of a heroin vaccine: Accurate assessment of heroin binding to polyclonal antibodies using inhibition equilibrium dialysis (IED) combined with ultra-high performance liquid chromatography/tandem mass spectrometry (UPLC/MS/MS). **O.B. Torres, R. Jalah, F. Li, J. Antoline, A. Jacobson, C. Alving, K. Rice, G. Matyas**
- BIOT 296.** Bioglue for wet condition; dopa incorporated engineered mussel adhesive proteins. **B. Yang, N. Ayyadurai, H. Yun, Y. Choi, J. Huang, Q. Lu, H. Zeng, B. Hwang, H.J. Cha**
- BIOT 297.** Directed evolution methods for improving the affinity and stability of Alzheimer's antibody fragments. **K.E. Tiller, M. Julian, C. Lee, L. Rabia, J. Young, P.M. Tessier**
- BIOT 298.** Novel application to bioinformatics approaches of glycoprotein domain identification and functional prediction. **E.J. Parish, Y. Lo, H. Honda, T. Wei**
- BIOT 299.** New approaches to RT-PCR analysis of animal tissue mRNA expression for ChREBP gene sequence. **E.J. Parish, H. Shyu, H. Honda, T. Wei**
- BIOT 300.** Withdrawn.
- BIOT 301.** Evaluation of product antibody (mAb) heterogeneity in non-clonal cell pools for early pre-clinical development. **Y. Zhang, Z. Fang, M. Wang, L. Paul, W. Ding, J. Li, M. Gokhale, J. Valente**
- BIOT 302.** Inference of cohort-specific HIV-1 kinetics. **J. White**
- BIOT 303.** Interactions of LAH4-Lx and LAH4-Ax family of histidine-rich amphipathic peptides with biomembrane models. **B.N. Suarez-Gonzalez, L. Vermeer, E. Glattard, A. Galy, D. Fenard, B. Bechinger**
- BIOT 304.** Withdrawn.
- BIOT 305.** Decrease in transthyretin tetramer stability enhances inhibition of beta-amyloid aggregation. **P. Mangrolia, R.M. Murphy**
- BIOT 306.** Well characterized and consistent quality carbohydrates improves robustness and stability of protein formulation. **B. Thiyagarajan, M. Cox, C. Deily, N. Deorkar**
- BIOT 307.** Investigating mechanisms and levers to control trisulfide formation in mAbs produced in CHO cell culture. **B. Wong, M. Shiratori, V. Grosskopf, A. Meier, J. Wu, M. Gawlitzek, S. Meier**
- BIOT 308.** Sequence and domain architecture of minicollagen from sea anemone and their impacts on mechanical properties. **D. Jung, Y. Yang, J. Seo, Y. Choi, B. Hwang, H.J. Cha**
- BIOT 309.** Molecular design of self-assembled  $\beta$ -sheet-forming peptides as amyloid inhibitors. **B. Ren, R. Hu, H. Chen, M. Zhang, F. Yang, J. Zheng**
- BIOT 310.** Probing a potential molecular link between  $\beta$ -Amyloid and Human Islet Amyloid polypeptide via specific cross-sequence amyloid interactions. **R. Hu, M. Zhang, H. Chen, B. Ren, F. Yang, J. Ma, B. Jiang, J. Zheng**
- BIOT 311.** NMR analysis of protein-peptide interactions for in silico affinity maturation of chromatographic peptide ligands. **C. Goodwine, D. Chandra, S. Timmick, N. Vecchiarello, S.M. Cramer, P. Karande**
- BIOT 312.** Methods for discovering serum antibodies associated with diseases via bacterial display peptide libraries. **J. Bozekowski, R. Pantazes, P.S. Daugherty**
- BIOT 313.** Functional carbohydrate chip-based screening for substrate specificity of sialyltransferase. **H. Heo, C. Kim, J. Seo, H.J. Cha**
- BIOT 314.** Compressive properties of cartilage. **F. Horkay, I. Horkayne Szakaly, E.K. Dimitriadis, P.J. Basser**
- BIOT 315.** Improving resolution and migration in non-reduced CE-SDS: A tale of two desirable but antagonistic optimizations. **A. Shirke, R. Vanam, M. Marlow**
- BIOT 316.** Controlling mRNA translation in both prokaryotic and eukaryotic cells using PUF domains. **J. Cao, M. Arha, C. Sudrik, X. Wu, A. Mukherjee, R. Kane**
- BIOT 317.** Folate binding protein: Therapeutic natural nanotechnology. **R.L. Merzel, S. Boutom, J. Chen, E. Marsh, M.M. Banaszak Holl**
- BIOT 318.** Identifying solid binding polypeptides (SBP) with a high affinity for cellulose paper: Toward bio-tethering of functional devices. **T. Omokehinde, M.A. Allen**
- BIOT 319.** Probing the role of N and C-terminal regions in allosteric regulation of *Thermodesulfobivrio yellowstonii* ADP-glucose pyrophosphorylase. **C.R. Meyer, E. Yik, S. Kaur, E. Pushkarev, N. Duran, C. Diep, L. Mulato, A. Avila**
- BIOT 320.** Engineered zinc finger proteins: A diagnostic tool for the detection of methylated DNA. **A. Kini**
- BIOT 321.** Development of an analytical assay to characterize the glycosylation pattern in monoclonal antibodies. **J. DeChiara, D. Radhakrishnan, A.S. Robinson, B. Ogunnaiké**
- BIOT 322.** Characterisation of proteases in anion exchange chromatography for the bioprocess of a therapeutic enzyme. **D. Migani, M. Smales, D.G. Bracewell**
- BIOT 323.** EBA 2.0: Improving expanded bed adsorption technology for bioproduct recovery. **V. Koppejan, E. van de Sandt, G. Ferreira, M. Ottens**
- BIOT 324.** Withdrawn.
- BIOT 325.** Nanofilter scalability: A comprehensive look into viral clearance capabilities at all sizes. **A.H. Schwartz**
- BIOT 326.** Minimizing the impact of process buffer variations by optimization of the Ampsphere™ A3 Protein A resin design. **A. Naresh, B. Jeugt, G. Stroehlein, H. Shiho, M. Siwak**
- BIOT 327.** Ternary adsorption isotherms of proteins from high-throughput experiments and multivariate analysis. **N. Field, S. Konstantinidis, A.K. Velayudhan**
- BIOT 328.** Evaluation of large scale disposable pre-packed columns for use in biologics and vaccine purifications. **E. Wen, J. Konietzko, J. Jacob, F. Torres, J.G. Joyce**
- BIOT 329.** Leveraging solute surface analytics and high throughput screening to define binding mechanisms of virus particles to multimodal anion exchange resin. **M. Brown, K.A. Brorson, S. Lute, D.J. Roush, T.O. Linden**
- BIOT 330.** Increasing productivity of a mAb capture step: Alternate design approaches. **L. Madhavan, C. Gerberich, J.R. Molek, A.C. Dumetz, G.J. Terfloth**
- BIOT 331.** Withdrawn.
- BIOT 332.** Complications of accurately sizing filtration trains for the purification of a sodium carboxymethylcellulose solution. **A. Steele**
- BIOT 333.** Targeted, high-throughput assessment of the selectivity of chromatographic resins. **S. Timmick, S. Ruppel, S.M. Cramer**
- BIOT 334.** Characterization of peptide-functionalized agarose resin supports for applications in affinity chromatography. **N. Vecchiarello, S. Timmick, D. Chandra, C.A. Goodwine, P. Karande, S.M. Cramer**
- BIOT 335.** Optimal application of high area pleated devices for sterile filtration. **S. Liu, S. Giglia, D. Durie, G. Kazan, R. Sylvia**
- BIOT 336.** Purification of therapeutic proteins by affinity precipitation using peptide-conjugated smart biopolymers. **A. Mullerpatan, P. Karande, S.M. Cramer**
- BIOT 337.** Development of novel assays to predict viral hydrophobicity. **S. Johnson, M. Brown, S. Lute, K.A. Brorson**
- BIOT 338.** Chromatographic depth filters: Opportunities for turbidity reduction and process intensification. **M. Mercaldi, S. Jain, M. Shifrin, W. Olsen**
- BIOT 339.** Lean green efficiency machine: How to continuously improve your work environment. **R.C. Massiccotte**
- BIOT 340.** Optimization of ultrafiltration and diafiltration process for a shear sensitive and aggregation prone monoclonal antibody. **S. Patel, S. Rios, S. Dukleska, I. Han, H. Li, N. Tugcu**
- BIOT 341.** Evaluation of body-feed assisted cell culture clarification in single-use device. **X. Zhao, M. Shearer**
- BIOT 342.** Impact of buffer exchange and protein concentration on biologics quality during ultrafiltration and diafiltration (UF/DF). **E. Schutsky, A. Arunkumar, R.K. Swanson, D. Yu, A.T. Lewandowski, N. Singh, Z. Li**
- BIOT 343.** Withdrawn.
- BIOT 344.** Automating mAb purification workflows: Combining tandem and multi-D purification methodology with sample analysis. **J. Habel**
- BIOT 345.** Bispecific antibodies: Screening from traditional to mixed-mode chromatography modalities for a purification solution. **T. Matos, H. Karkov, G. Andersen, L. Sejergaard, H. Ahmadian, S.M. Cramer**
- BIOT 346.** Virus detection using restricted-access adsorbents. **U. Patil, S.P. Dhamane, M. Adhikari, A. Hagstrom, U. Strych, K. Kourentzi, R.C. Willson**
- BIOT 347.** Modes of controlling charge variant distribution in mAb production by upstream and downstream process parameters. **T. Bjorkman, L. Kärf, A. Ljunglöf, T. Falkman, A. Vitina**
- BIOT 348.** Investigation of the biophysics of host cell protein associations with monoclonal antibodies. **S. Ranjan, W. Chung, M. Zhu, D. Robbins, S.M. Cramer**

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- BIOT 349.** Enhancement of dynamic body feed clarification performance using chitosan treatment. **H. Kaligotia**
- BIOT 350.** Computational fluid dynamics (CFD) modeling of flow and fouling in hollow fiber tangential flow (HFTFF) and alternating tangential flow (HFATF) filtration of a perfusion bioreactor. **F. Radoniqi, S. Wang, H. Zhang, P. Shamlou, J.L. Coffman**
- BIOT 351.** Chromatographic quantification of a complex protein mixture using problem-specific deconvolution. **K. Jurlewicz, S. Konstantinidis, A.K. Velayudhan**
- BIOT 352.** Why synthesize protein-polymer conjugates? The stability and activity of chymotrypsin-polymer bioconjugates synthesized by RAFT. **S. Sloane, R. Falatach, D. Konkolewicz, J. Berberich, R.C. Page, S. Averick**
- BIOT 353.** Impact of pre-filter chemistry and operating conditions on virus filter performance. **M. Luther, J. Weaver, A. Kantardjiff, R. Alford**
- BIOT 354.** Electrical stimulation of human dermal fibroblasts and quantification of collagen, elastin, and collagenase. **E. Nguyen, K. Columa, J. Wishner, K. Stowinska**
- BIOT 355.** Multiphoton spectroscopy on thioflavin T: A nonlinear approach for amyloid detection. **J. Donnelly, F.E. Hernandez**
- BIOT 356.** Protein diffusion as an approach to characterize the stability and viscosity of concentrated protein solutions. **K.C. Bauer, M. Göbel, M. Schwab, M. Schemeyer, J. Hubbuch**
- BIOT 357.** Using rheology as an indicator of cell lysis in *E. coli* fermentation to determine optimal harvest time and prevent product loss. **J.M. Newton, Y. Zhou, J. Vlahopoulou, D. Schofield**
- BIOT 358.** Rapid discovery of peptidomimetics as antibody alternatives via epitope-targeted screening. **J. Liang, A. Nag, S. Das, D. Bunck, A. Umeda, A. McCarthy, A. Mishra, J. Heath, J.R. Heath**
- BIOT 359.** X-ray computed tomography for the representation of chromatographic structure at the individual bead and packed bed scales. **T. Johnson, P.R. Shearing, L. Peter, D.G. Bracewell**
- BIOT 360.** Engineering fatty acid responsive elements for metabolic engineering in oleaginous yeast, *Yarrowia lipolytica*. **M. Shabbir-Hussain, P. Baker, M.A. Blenner**
- BIOT 361.** Use of chromatography simulation and fundamental measurements to determine equivalent IEX loading under different bed compression conditions for a fusion protein. **X. Xu, C. Huang, S. Traylor, N. Zhang, Z. Li**
- BIOT 362.** Polyelectrolyte multilayers loaded with antifungal  $\beta$ -peptide reduce the formation of *C. albicans* biofilms in film-coated catheter segments *in vitro* and *in vivo*. **N. Raman, M. Lee, K. Marchillo, A. Rodríguez López, D. Andes, S. Palecek, D.M. Lynn**
- BIOT 363.** Design and evaluation of advanced Amsphere™ A3 protein A chromatography resin: The relationships and considerations of bead structure, pore structure, surface chemistries and ligand design on affinity resin performance targets. **A. Naresh, M. Siwak, M. Hanamura, M. Higami, T. Matsuda, S. Nakamura, Y. Okano**
- BIOT 364.** Expanded toolbox for various MAb purification challenges. **A. Gronberg, L. Kärf, K. Nilsson Välimaa, C. Brink, A. Edman Orlefers**
- BIOT 365.** Biotreatment of slaughterhouse wastewater accompanied with electricity generation in microbial fuel cell. **Z.Z. Ismail, A. Mohammed**
- BIOT 366.** Two-dimensional isobutyl acetate production pathways to improve carbon yield. **Y. Tashiro, S. Desai, S. Atsumi**
- BIOT 367.** Automated nucleic acid extraction workstation based on magnetic separation. **Y. Wu, N. He**
- BIOT 368.** Bioinformatical analysis of spider silk protein sequences: Finding relation with evolution and mechanical properties. **D. Jung, Y. Yang, H.J. Cha**
- BIOT 369.** Cross-seeding amyloid interactions between human IAPP and Rat IAPP. **M. Zhang, R. Hu, H. Chen, B. Ren, M. Yang, J. Ma, B. Jiang, J. Zheng**
- BIOT 370.** Cyclic peptide ligands for the purification of erythropoietin by affinity chromatography. **W.S. Kish, A. Naik, H. Sachi, B.G. Bobay, S. Menegatti, R.G. Carbonell**
- BIOT 371.** Molecular recognition of novel heptapeptides at Fc-binding sites from molecular dynamics simulations. **X. Sun, J. Weaver, R. Wickramasinghe, X. Qian**
- BIOT 372.** Overcoming buffer challenges in downstream processes by In-line conditioning. **K. Busson, E. Carredano, H. Martin**
- BIOT 373.** Developmental approaches for overloaded cation exchange chromatography. **Y. Yigzaw, A. Mehta, C. Williams, K. Nagpal, J. Yang**
- BIOT 374.** Integration of platform high throughput technologies in biopharmaceutical downstream process development. **G. Ma, Y. Feng, C. Gerberich, A. Dumetz, G.J. Terltoth, K.E. Goklen**
- BIOT 375.** Maximizing productivity of protein A capture. **I. Savoy, B. Kalbfuss-Zimmermann, S. Rueger, L.W. Pampel**
- BIOT 376.** Remediation of crude oil-polluted agricultural oil by *Fimbristylis littoralis*. **E.O. Nwaichi, G. Iwo, G. Attuah**
- BIOT 377.** Purification and characterization of the *Drosophila melanogaster* (Dm) IKK $\beta$ /IKK $\gamma$  complex. **W. Rogers, T. McDowell, T. Huxford**
- BIOT 378.** Withdrawn.
- BIOT 379.** Base-free aerobic oxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic acid over Pt/C-O-Mg catalyst. **X. Han, Y. Wang**
- BIOT 380.** Multiple reaction pathways and mechanisms of cellulose conversion into bio-platform molecules in water and alcohol medium. **D. Ding, Y. Wang**
- BIOT 381.** Bioactive crosslinked pepsin nanoaggregates above pH 5.0. **T. Akkas, A. Zakharyuta, A. Taralp**
- BIOT 382.** Bottom-up approach to describe protein-protein interactions in a continuum mechanics biomolecular model of fibrin. **A. Solernou, D. Read, S. Harris, O. Harlen, K.A. Smith, S.P. Muench**
- BIOT 383.** Rates of reaction of the sulphhydryl groups of some derivatives of human hemoglobin A with 5, 5-dithiobis-(2-nitrobenzoic acid). **Fu. Akhigbe**
- BIOT 384.** Rapid generation of dCas9-regulated, orthogonally repressible hybrid T7-lac promoter sets for modular, tunable control of metabolic pathway fluxes in *E. coli*. **B. Cress, J.A. Jones, D. Kim, Q. Leitz, R.J. Linhardt, M. Koffas**
- BIOT 385.** Design of two new protein A resins. **H.J. Johansson**
- BIOT 386.** Model-based process development for biopharmaceuticals. **S. Pirrung, A. Hanke, L.A. van der Wielen, P.D. Verhaert, E. van de Sandt, M. Eppink, M. Ottens**
- BIOT 387.** Impact of channel shear effects on process hydraulics and biologics quality during ultrafiltration and diafiltration (UF/DF). **A. Arunkumar, E. Schutsky, N. Singh**
- BIOT 388.** Platelet-targeting thiol reduction sensor detects protein disulfide isomerase activity on activated platelets in mouse and human blood under flow. **S. Zhu, J. Welsh, L. Brass, S. Diamond**
- BIOT 389.** Pitting rational against random: Improving light-driven P450 biocatalysts. **M. Kato, L. Baragan, L. Tang, L.E. Cheruzel**
- BIOT 390.** Simple process strategies to increase the utilization of protein A media in clinical manufacturing. **A. Becerra-Arteaga**
- BIOT 391.** Withdrawn.
- BIOT 392.** Engineering affinity, selectivity and elutability into peptides for their development as ligands for downstream bioprocessing of non-mAb biologics. **D. Chandra, S. Timmick, N. Vecchiarello, C. Goodwine, S.M. Cramer, P. Karande**
- BIOT 393.** Withdrawn.
- BIOT 394.** Tailoring continuous protein A mAb capture for facility fit and process economics. **X. Gjoka, K. Rogler, M. Bisschops, R. Gantier, M. Schofield**
- BIOT 395.** Enhanced bioadsorption of rare earth elements through cell surface display of lanthanide binding tag. **D.M. Park, M. Yung, A. Eslamimanesh, D.W. Reed, Y. Fujita, A.M. Anderko, Y. Jiao**
- BIOT 396.** QSAR models for prediction of chromatographic behavior of homologous Fab variants. **J. Robinson, H. Karkov, J. Woo, B.O. Krogh, H. Ahmadian, S.M. Cramer**
- BIOT 397.** Dynamic modeling of human coagulation cascade using reduced order effective kinetic models. **A. Sagar**
- BIOT 398.** Polymer grafting to functionalize chromatography for purification of monoclonal antibodies. **J.U. Hansson, E. Brekkan, J. Bengtsson**
- BIOT 399.** Recombinant DNA and its medical benefits: Synthesis of insulin. **B.B. Ibrahim**
- BIOT 400.** New enabling technologies for continuous final formulation of mAbs. **E. Ayturk**
- BIOT 401.** Analyzing the mechanical properties of three synthetic based biopolymers. **R. Anderson**
- BIOT 402.** Evaluation of flow-through hydrophobic interaction and hydroxyapatite chromatography steps for the removal of aggregates in the purification of monoclonal antibody TBL-mAb-01. **W. Evans, A. Chakrabarti**
- BIOT 403.** Capturing carbon dioxide in hydroxyacid-derived bio-plastics. **I.s. Al Rowaihi, S. Grotzinger, K. Dietrich, J. Eppinger**
- BIOT 404.** Single-molecule kinetics of protein adsorption on thin nylon 6,6 films. **H. Shen, L.J. Tazuin, W. Wang, B. Hoener, L. Kinsley, A. Hoggard, C.F. Landes**
- BIOT 405.** More affordable version of therapeutic protein recombinant Streptokinase to address over a million ST elevated Myocardial Infarction (STEMI) deaths in part of the world where affordability is the key. **D. Ghosh, S. Paul, R.K. Gupta**
- BIOT 406.** Improving the alkali stability of the kappa light chain-binding polypeptide from domain of peptostreptococcus protein L. **R. Palmgren, G. Rodrigo, A. Mattsson, T. Bjorkman, J. Vasic, E. Monie, M. Ander, G. Bauren**
- BIOT 407.** Keynote: Emerging technologies. **E. Shusta**
- BIOT 408.** Optimum pulse mode selection for biodiesel production using ultrasound irradiations. **E. Martinez-Guerra, V. Gude**
- BIOT 409.** Mapping the collective response of water to predict biomolecular interaction interfaces. **R.C. Remsing, J.D. Weeks**
- BIOT 410.** Molecular dynamics simulations of proteins coupled to nanoparticles. **S. Sen, P. Kral**
- BIOT 411.** Withdrawn.
- BIOT 412.** Moving towards a sterile chromatography platform for virus purification. **J. Konietzko, S. Wang, A. Kristopeit, M. Wenger, J. Joyce**
- BIOT 413.** Computational reconstruction of the protein secretion pathway in CHO cells. **J.M. Gutierrez Bugarin, A. Feizi, N.E. Lewis**
- BIOT 414.** Examination of multivariate model generation using UV-vis spectral data for mAb titer. **J. Miller, J.L. Coffman, P. Shamlou**
- BIOT 415.** Engineering the ligand affinity and specificity of the human adenosine A<sub>2A</sub> receptor. **J. Yoo, P.S. Daugherty, M.A. O'Malley**
- BIOT 416.** Computational investigation of mutational impact on terpene synthases. **L. Li, C. Pirie**
- BIOT 417.** Use of Fc gamma receptors as chromatographic ligands to enrich high affinity subclasses and glycoforms from human plasma IgG. **A. Boesch, T. Chu, H. Kappel, A. Mahan, G. Alter, M. Ackerman**

## WEDNESDAY MORNING

### Section A

Westin San Diego  
Crystal II

### Upstream Processes

#### Advances in Systems Biology

M. R. Antoniewicz, M. A. Blenner, V. Roy, *Organizers*

N. Jacob, G. Sriram, *Organizers, Presiding*

**8:30 BIOT 418.** Large scale dynamic models of metabolism as a tool for analysis and design of metabolic engineering and synthetic biology strategies. **G. Fengos, L. Miskovic, V. Hatzimanikatis**

**8:50 BIOT 419.** Characterizing strain variation in engineered *E. coli* using a multi-omics based workflow. **E.C. Brunk, K. George, J.D. Keasling, B. Palsson, T. Lee**

**9:10 BIOT 420.** Hierarchy of decisions that impact the accuracy of tissue-specific metabolic models. **S. Opdam, N.E. Lewis**

**9:30 BIOT 421.** Technical evaluation of RNA-Seq and microarray approaches in comparative transcriptomics analysis of CHO cells. **C. Chen, H. Le, C. Goudar**

**9:50 Intermession.**

**10:10 BIOT 422.** Directed evolution of *Escherichia coli* quorum sensing promoter region of the *IsrACDBFG* operon: A tool for synthetic biology systems and protein expression. **P. Hawk, R. McKay, C. Virgile, H. Ueda, M. Ostermeier, W.E. Bentley**

**10:30 BIOT 423.** Evaluation of public genome references for RNA-Seq data analysis in Chinese hamster ovary cells. **H. Le, C. Chen, C. Goudar**

**10:50 BIOT 424.** Applying adaptive laboratory evolution to engineer platform strains. **A. Feist**

**11:10 BIOT 425.** Genome-scale stoichiometric model of poplar for investigation of woody plant metabolism. N. Boruah, A. Misra, M. Simons, G. Coleman, G. Sriram

## Section B

Westin San Diego

Emerald Ballroom

### Downstream Processes

#### Leveraging Fundamentals for Accelerated Downstream Process Development

J. Neville, A. Noyes, T. M. Przybycien, *Organizers*

K. Lacki, V. Natarajan, *Organizers, Presiding*

**8:30 BIOT 426.** Ultrafiltration behavior of highly concentrated monoclonal antibodies. E. Binabaji, A.L. Zydny, J. Ma

**8:50 BIOT 427.** Thermodynamically based modelling of effects of ethanol and potassium chloride on reversed-phase chromatography. K. Johansson, S.S. Frederiksen, M.P. Breil, E. Broberg Hansen, B. Nilsson

**9:10 BIOT 428.** Mechanistic modeling of antibody transport, adsorption equilibrium, and uptake kinetics in protein A chromatography resins with PEGylated ligand. J. Weinberg, T.M. Przybycien

**9:30 BIOT 429.** Mechanistic basis for adsorptive selectivity in conventional and dextran-functionalized ion exchangers: Model and experiment. A.M. Lenhoff, C. Narambuena, I. Szeifer, J.M. Angelo

**9:50** Intermission.

**10:10 BIOT 430.** Enhancing the power of HTPD with empirical interpolation models to predict elution behavior at high protein loads. A. Creasy, J. Calzada, G. Barker, S. Herzer, L. Paul, S. Rieble, G. Carta

**10:30 BIOT 431.** Predicting cation exchange Fab purification using micro-tip chromatography and general rate modelling. S. Gerontas, S. Kong, N.J. Titchener-Hooker

**10:50 BIOT 432.** Scalability of mechanistic models for ion exchange chromatography. T. Huuk, T. Hahn, J. Griesbach, S. Hepbildikler, J. Hubbuch

**11:10 BIOT 433.** Withdrawn.

## Section C

Westin San Diego

Diamond I

### Biomolecular & Biophysical Processes

#### Protein Conjugates & Materials

B. Hackel, J. Kaar, H. Samra, *Organizers*

J. Berberich, J. A. Van Deventer, *Organizers, Presiding*

**8:30 BIOT 434.** Responsive polymer-protein conjugates: From stimulus-induced self-assembly to the treatment of accelerated bone disorders. B.S. Sumerlin, B. Tucker, J.D. Stewart, J. Aguirre

**9:10 BIOT 435.** Structure-based guidelines for increasing protein conformational stability via PEGylation. J.L. Price

**9:30 BIOT 436.** SuFEx bioconjugation. S. Li, E. Kallick, S. Averick

**9:50** Intermission.

**10:10 BIOT 437.** Densely modified chymotrypsin-polymer conjugates with increased stability to low pH. C. Cummings, A.J. Russell

**10:30 BIOT 438.** Engineered knottin peptide-drug conjugates selectively deliver small molecules to brain tumors in mice. N. Cox, J.R. Kintzing, N.V. Currier, S.E. Ackerman, S.M. DePorter, M. Smith, G.A. Grant, J. Cochran

**10:50 BIOT 439.** Self-assembly of temperature-responsive protein-polymer bioconjugates. J. Li, D. Moatsou, A. Ranji, A. Pitto-Barry, I. Ntai, R.K. O'Reilly, M. Jewett

**11:10 BIOT 440.** Novel biocompatible modifications of phage-displayed peptide libraries to generate genetically-encoded libraries of peptide derivatives. R. Derda

## Section D

Westin San Diego

Opal

### Emerging Technologies

#### New Tools & Approaches

J. Latone, B. Thronset, G. M. Thurber, J. Wang, I. R. Wheeldon, *Organizers*

N. Agarwal, A. Chatterjee, *Presiding*

**8:30 BIOT 441.** Development of a SERS-based biomolecular assay. T. Chuong, A. Pallaoro, G.D. Stucky, M. Moskovits, T. Soh

**8:50 BIOT 442.** Lysate of engineered *Escherichia coli* supports high-level conversion of glucose to 2,3-butanediol. J. Kay, M. Jewett

**9:10 BIOT 443.** Exploring alternative materials to fabricate microfluidic gradient generators to study algal growth and migration. A.T. Melvin

**9:30 BIOT 444.** Sequence-specific nucleic acid detection based on ionic current measurement through a glass nanopore. B. Koo, A. Yorita, H. Monbouquette

**9:50** Intermission.

**10:10 BIOT 445.** Construction of robust, tunable genetic circuits to prevent infectious diseases. T. Shopera, W.R. Henson, A. Ng, Y. Lee, K. Ng, C. Johnson, A. Hoynes-O'Connor, T. Moon

**10:30 BIOT 446.** Controlling cells through RNA Folding: Towards design principles for RNA engineering. J.B. Lucks

**10:50 BIOT 447.** Advances in the development of a protein catalyzed capture (PCC) agent for the L1R protein of vaccinia as an antibody alternative for biosurveillance in austere environments. M. Coppock, D. Cangelosi, S. Das, J.R. Heath, D. Stratis-Cullum

**11:10 BIOT 448.** Microfluidic gradient generator-flow cell system as a novel tool to study biofilm development and control. Y. Zhang, Y. Cohen, B. Cao

## Section E

Westin San Diego

Crystal I

### Quality by Design for Biopharmaceuticals

#### QbD Case Studies: Process Characterization

C. Torigoe, *Organizer*

S. Singh, M. Westoby, *Organizers, Presiding*

**8:30 BIOT 449.** Bioreactor scale-down model verification case study. M. Mollet, R. Patel, G. Miro-Quesada, L. Qu

**8:50 BIOT 450.** High-throughput chromatography as qualified scale-down model: Challenges and opportunities. J. Aucamp, J. Hitzler, S. Urig, L.W. Pampel, J. Shultz

**9:10 BIOT 451.** QbD six years after A-mAb: What we expected, what happened, and what now. J. Erickson

**9:50** Intermission.

**10:05 BIOT 452.** First principles modeling towards accelerated process development: Experiences and prospects of computational model-based filing. C. Undey, T. Larsen, M. Coufal, O. Kaltenbrunner, B. Kuhn, T. Mire-Sluis

**10:25 BIOT 453.** Ultrafiltration diafiltration: Process characterization and process validation. Z. Begum

**10:45 BIOT 454.** Commercial antibody formulation development using quality by design elements. M. Bhattacharya, S. Mehta, M. Dey

**11:05 BIOT 455.** Use of quality by design approach to optimize downstream cross-step operation space of an Fc fusion protein. C. Huang, X. Xu, Z. Li

## Section F

Westin San Diego

Diamond II

### Biomolecular & Biophysical Processes

#### Protein Structure & Function

B. Hackel, J. Kaar, H. Samra, *Organizers*

W. C. Pomerantz, R. St. John, *Organizers, Presiding*

**8:30 BIOT 456.** Exploring the space of sense codon reassignment in *E. coli*. J. Fisk

**8:50 BIOT 457.** Engineering leave-one-out-GFP based biosensors. K. Fraser, S. Banerjee, C. Schenkelberg, K. Zhang, D. Chan, C. Thornton, C. Lamberson, V. Jones, A. Choi, R. Altschuler, J.S. Dordick, C. Bystroff

**9:10 BIOT 458.** Solvent-free functional biofluids as a route for retained structure and improved protein stability in nonaqueous environments. A. Brogan, J.P. Hallett

**9:30 BIOT 459.** Observing structural changes in biopharmaceutical proteins as a function of concentration. C.W. Meuse

**9:50** Intermission.

**10:10 BIOT 460.** Nanobody activation immunotherapeutics that selectively destroy cancer cells. A. Ta, M. Gray, R. Tao, B. McNaughton

**10:30 BIOT 461.** Dissecting the initial steps of heme uptake between an outer membrane receptor protein of *Shigella dysenteriae* and hemoglobin by phage display. L. Meneghini, G.A. Weiss

**10:50 BIOT 462.** N- and C-terminal domains differentially contribute to the structure and function of dystrophin and utrophin tandem calponin-homology domains. S. Singh, S. Bandi, K. Mallela

**11:10 BIOT 463.** Characterization of knob-in-hole assembly variants in support of bispecific antibody development. V. Lundin

## WEDNESDAY AFTERNOON

### Section A

Westin San Diego

Crystal II

#### Upstream Processes

##### Advances in Biocatalysis

M. R. Antoniewicz, M. A. Blenner, V. Roy, N. Vishwanathan, *Organizers*

M. Bryndlisen, A. Yongky, *Organizers, Presiding*

**2:00 BIOT 464.** New yeast strain to produce fuels and chemicals instead of ethanol. J. Avalos, L. Grundy

**2:20 BIOT 465.** Carbon-efficient conversion of methanol to chemical commodities via synthetic methanol condensation cycle (MCC). C. Chen, I.W. Bogorad, T. Wu, M. Theisen, J.C. Liao

**2:40 BIOT 466.** Identifying ester biosynthesis pathways in the yeast *Kluyveromyces marxianus*. A. Loebis, I.R. Wheeldon

**3:00 BIOT 467.** Withdrawn.

**3:20** Intermission.

**3:40 BIOT 468.** Engineering thiolase enzyme specificity. Y. Tarasova, B. Bonk, B. Tidor, K.L. Jones Prather

**4:00 BIOT 469.** Accelerating biocatalysis in thin films. J. Britton, C.L. Raston, G.A. Weiss

**4:20 BIOT 470.** Integrating metabolic engineering and electrocatalysis for the production of polyamides from sugar. M. Suastegui, J. Matthiesen, J. Tessonnier, Z. Shao

**4:40 BIOT 471.** Utilizing electrochemical bioreactors for efficient biofuel and chemical applications. C.S. Morrison, R.S. Kane, J.S. Dordick, D.R. Dodds, W.B. Armiger, M. Koffas

## Section B

Westin San Diego

Emerald Ballroom

### Downstream Processes

#### Technology Transfer, Scale-up & Scale-Down

J. Neville, A. Noyes, T. M. Przybycien, *Organizers*

P. J. Alfonso, J. Cyganowski, *Organizers, Presiding*

**2:00 BIOT 472.** Downstream processes: Past, present and future. J. Myers

**2:40 BIOT 473.** Multiproduct resin reuse for biopharmaceuticals: Application to clinical and commercial manufacturing. R. Sharnez, K. Mehta, R.G. Soderquist

**3:00 BIOT 474.** Learning from small-scale process characterization studies gone wrong: A case study in chromatography resin lifetime. P.R. Smith, A. Pike, B.F. Marques, K.E. Goklen

**3:20** Intermission.

**3:40 BIOT 475.** Implementation of a single-use mixer as a point-of-use and disposable heat exchanger in cGMP downstream processing. B. Youchak, W. Bell, R. O'Keefe, M. Elsnor

**4:00 BIOT 476.** Investigation of low molecular weight species and implementation of mitigation strategies into large scale biologics manufacturing. Z. Tan, A.T. Lewandowski, V. Ehamparanathan, B. Ng, E. Schutsky, M. Mayani, D. Yu, R. Martel, S. Egan, M. Krajcovic, K. Aron, M. Peck, J. Ray, N. Singh, N. Zhang, C. Du, A. Borwankar, M. Lu, N. Hershey, Y. Huang, L. Tao, M.C. Borys, Z. Li

**4:20 BIOT 477.** Leveraging Monte Carlo simulations and mechanistic models to optimize a high concentration UDF process within facility constraints. A. Brinkmann, M. Westoby

**4:40 BIOT 478.** Optimization of bio-molecule separation by combining microscale filtration and design-of-experiment methods. A.S. Kazemi, K. Kawka, D.R. Latulippe

## Section C

Westin San Diego  
Diamond I

## Biomolecular &amp; Biophysical Processes

## Protein Conjugates &amp; Materials

B. Hackel, J. Kaar, H. Samra, *Organizers*  
J. Berberich, J. A. Van Deventer, *Organizers, Presiding*

**2:00 BIOT 479.** Protein nanoparticle conjugates for cancer immunotherapy. **M. Neek**, N. Molino, J. Tucker, E.L. Nelson, S. Wang

**2:20 BIOT 480.** Tuning the activity and stability of protein-polymer conjugates by attaching functional polymers. **M. Lucius**, D. Konkolewicz, J. Berberich, R.C. Page

**2:40 BIOT 481.** Whole animal to single cell near infrared fluorescent imaging of antibody drug conjugate metabolism. **C. Cilliers, G.M. Thurber**

**3:00 BIOT 482.** *In vivo* synthesis of nanoparticles through evolved peptide lipidation. **R. Menacho Melgar, M. Lynch**

**3:20** Intermission.

**3:40 BIOT 483.** Platform for constructing, evaluating, and screening bioconjugates on the yeast surface. **J.A. Van Deventer, D. Le, J. Zhao, R.L. Kelly**

**4:00 BIOT 484.** Point of care device for detection of myeloperoxidase as a wound infection marker. **E. Ramon, A. Francesko, T. Tzanov**

**4:20 BIOT 485.** Biofabrication of protein networks via tobacco mosaic virus-virus like particles (TMV-VLP): 3D scaffold interfaces. **N. Bhokisham, K. Wang, A. Brown, G.F. Payne, J.N. Culver, W.E. Bentley**

**4:40 BIOT 486.** Wiring of redox enzymes using a collagen heterotrimer protein. **H.F. Ozbakir, J. Brisendine, R.L. Koder, S. Banta**

## Section D

Westin San Diego  
Opal

## Emerging Technologies

## Protein &amp; Molecular Engineering

J. Latone, G. M. Thurber, I. R. Wheeldon, *Organizers*

R. Bott, M. Kim, *Organizers, Presiding*

**2:00 BIOT 487.** Artificial TCA cycle metabolism: Direct evidence for metabolon formation and substrate channeling. **K. Garcia, B. Bulutoglu, F. Wu, S.D. Minter, S. Banta**

**2:20 BIOT 488.** Osteogenic differentiation of stem cells promoted by the assemblies of genetically engineered bacteriophage. **C. Mao**

**2:40 BIOT 489.** Bacterial inner membrane display for screening a naïve antibody library to isolate antibodies that bind survivin. **P. Moghaddam-Taaheri, A.J. Karlsson**

**3:00 BIOT 490.** Rational design and development of polysialic acid-binding peptides: Implications in neural stem cell purification. **D. Shastry, P. Karande**

**3:20** Intermission.

**3:40 BIOT 491.** Constructing new bioluminescent tools with minimally perturbed luciferins. **C.M. Rathbun, R.C. Steinhardt, W.B. Porterfield, K. Jones, D. McCutcheon, M.A. Paley, J.A. Prescher**

**4:00 BIOT 492.** Circle Akt In: Macrocycles against phosphorylated Akt. **A. Nag, S. Das, J.R. Heath**

**4:20 BIOT 493.** Switchable protein sensors and enzyme reactions based on dynamic DNA assembly. **R.P. Chen, D. Blackstock, Q. Sun, W. Chen**

**4:40 BIOT 494.** RNA length affects form and function of the Type I CRISPR-Cas surveillance complex. **M. Luo, C. Beisel**

## Section E

Westin San Diego  
Crystal I

## Quality by Design for Biopharmaceuticals

## QbD Case Studies: Process Validation

S. Singh, C. Torigoe, *Organizers*

K. A. Barnhouse, M. T. Schmidt, *Organizers, Presiding*

**2:00 BIOT 495.** Manufacturability assessment tool for effective decision-making and efficient process development: Development and applications. **K. Brower, R.A. Patil, D.A. Shah, J. Walther, N.M. Troccoli, T.A. Vetter, V. Warikoo**

**2:20 BIOT 496.** Process linkage approach for establishing critical quality attribute target ranges. **S. Khoo, M. Mun, M.T. Schmidt**

**2:40 BIOT 497.** Use of relevant process history for the determination of critical process parameters. **B. Huffman, J. Cundy, K. Sunasara**

**3:00 BIOT 498.** Using characterization data to support process validation: A Monte Carlo approach. **C. Thompson, T. Linke, A. Hunter, G. Miro-Quesada, X. Wang**

**3:20** Intermission.

**3:40 BIOT 499.** Defining process design space for a therapeutic monoclonal antibody: Clearance of phospholipase B-Like 2 (PLBL2), a CHO host-cell protein impurity, by hydrophobic interaction chromatography. **A. Sanchez, J. Bill, S. Fisher**

**4:00 BIOT 500.** Multivariate process monitoring towards enhanced continued process verification. **C. Undey, S. Oruklu, B. Looze, C. Garvin**

**4:20 BIOT 501.** Designing resin end of lifetime studies and their application in the three stages of process validation. **A. Magill, E.S. Wilhelm, J. Weiss, D. Saini**

**4:40 BIOT 502.** Improving the control strategy of legacy products using quality by design principles. **D. Vu, A. Hagstrom, G. Miro-Quesada, G. Ferreira**

## WEDNESDAY EVENING

## Section A

Westin San Diego  
Emerald Ballroom

## Biotechnology &amp; Bioengineering Daniel IC Wang Award

T. M. Przybycien, P. M. Tessier, S. A. Tobler, *Organizers, Presiding*

**5:00** Biotechnology & Bioengineering Daniel IC Wang Award Presentation.

## THURSDAY MORNING

## Section A

Westin San Diego  
Crystal II

## Upstream Processes

## Engineering Natural Products Biosynthesis

M. R. Antoniewicz, M. A. Blenner, V. Roy, *Organizers*

S. Ahuja, W. Zhang, *Organizers, Presiding*

**8:30 BIOT 503.** Biosynthetic engineering of new anti-infectives and anticancer agents. **T. Mahmud**

**8:50 BIOT 504.** Engineered biosynthesis of terminal alkyne-tagged natural products. **W. Zhang**

**9:10 BIOT 505.** PqqD homolog is a stand-alone leader peptide binding protein in lasso peptide biosynthesis. **W.L. Cheung, M. Chen, M. Maksimov, A. Link**

**9:30 BIOT 506.** New technologies to understand and engineer carrier protein mediated pathways. **M.D. Burkart**

**9:50** Intermission.

**10:10 BIOT 507.** Directing biosynthesis with diversity-generating metabolism. **E.W. Schmidt**

**10:30 BIOT 508.** Heterologous microbial biosynthesis of natural product analogues using dynamic metabolic control. **Z. Ye, M. Lynch**

**10:50 BIOT 509.** Comprehensive re-engineering and synthesis of a complex biosynthetic gene cluster. **J. Kim, K. Louie, T. Northen, S. Deutsch, C. Hoover**

**11:10 BIOT 510.** Strategies toward discovering new natural products from fungal species. **Y. Tang**

## Section B

Westin San Diego  
Emerald Ballroom

## Downstream Processes

## Non-Chromatographic Separations &amp; Process Integration

J. Neville, A. Noyes, T. M. Przybycien, *Organizers*

H. Ahmadian, A. M. Lenhoff, *Organizers, Presiding*

**8:30 BIOT 511.** Investigations of alternative clarification methods to obviate protein A on-column precipitation. **K. Galipeau, J. Caron, C. Gillespie**

**8:50 BIOT 512.** Development of an affinity precipitation process using protein nanocages as a non-chromatographic alternative to platform therapeutic antibody purification. **A. Swartz, Q. Sun, W. Chen**

**9:10 BIOT 513.** Novel approach for non-chromatographic purification of monoclonal antibodies from cell culture supernatant. **R.B. Wollacott, R. Sharpe, D. Seeman, S.S. Ozturk, P.L. Dubin**

**9:30 BIOT 514.** Development of robust impurity clearance methods using chromatographic and non-chromatographic techniques. **S. Chollangi, N. Singh, M. Peck, K. Sing, Y. Li**

**9:50** Intermission.

**10:10 BIOT 515.** Benzonase® endonuclease for improved primary recovery in an *E. coli*-based process for Fab production. **A. Stein, A. Heinen-Kreuzig, A. Kiesewetter, N. Lutz**

**10:30 BIOT 516.** Purification process for heparin using the pH responsive behavior of chitosan. **U. Bhaskar, L. Fu, J.S. Dordick, R.J. Linhardt**

**10:50 BIOT 517.** Assessment of beta glucan leachables originating from cellulose based depth filtration media. **A. Gupta, D. Kinzlmair, K.M. Pizzelli, E.M. Goodrich**

**11:10 BIOT 518.** Progress in development of size exclusion filter paper material for virus removal applications. **A. Mhriyran**

## Section C

Westin San Diego  
Diamond I

## Biomolecular &amp; Biophysical Processes

## General Topics in Biomolecular &amp; Biophysical Processes

B. Hackel, J. Kaar, H. Samra, *Organizers*

A. Lajimi, H. Sikes, *Organizers, Presiding*

**8:30 BIOT 519.** Withdrawn.

**9:10 BIOT 520.** Effect of histatin-5 mutations on proteolytic degradation by *Candida albicans* secreted aspartic proteases. **S.P. Ikononova, A.J. Karlsson**

**9:30 BIOT 521.** Membrane cholesterol and the adenosine A<sub>2A</sub> receptor. **C. McGraw, K. Cooke, A.S. Robinson**

**9:50** Intermission.

**10:10 BIOT 522.** Identification of functional group characteristics and physicochemical properties of *Pseudomonas* sp. strain ADP biofilm. **V. Henry, J.L. Jessop, T.L. Peeples**

**10:30 BIOT 523.** Characterization of an engineered, ligand-induced, viral membrane fusion protein. **M. Valverde, M. Bell, E.T. Boder**

**10:50 BIOT 524.** Analyzing the effects of glycosylation on the physicochemical properties and biological activity of antibody Fc regions using a model system. **T.J. Tolbert**

**11:10 BIOT 525.** Cyclic peptide mimics of A $\beta$  binding domain on transthyretin. **X. Lu, R.M. Murphy**

## Section D

Westin San Diego  
Opal

## Emerging Technologies

## Disease &amp; Biomedical Applications

J. Latone, G. M. Thurber, I. R. Wheeldon, *Organizers*

C. Chen, S. L. Servoss, *Organizers, Presiding*

**8:30 BIOT 526.** N-terminal hypothesis for Alzheimer's disease. **B. Murray, J. Lippens, D. Fabris, S. Li, G. Belfort**

**8:50 BIOT 527.** Stem cell-based blood-brain barrier model for drug transport studies. **J. Mantle, K.H. Lee**

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**9:10 BIOT 528.** Controlling differentiation of induced pluripotent stem cells into neurons in well-defined, hydrogel-based microenvironments. **E. Ovidia**, D.W. Colby, A.M. Kloxin

**9:30 BIOT 529.** Discovery and deconstruction of oscillations in the nitric oxide stress network of *Escherichia coli*. **M. Brynildsen**, J. Robinson

**9:50** Intermission.

**10:10 BIOT 530.** Elucidating core mechanisms of dormancy regulation in breast cancer cells. **A. Das**, A. Kumar, J. Priecado, A. Aksan, **S. Azarin**

**10:30 BIOT 531.** Impact of high extracellular lactate on breast cancer metabolism. **D. Odenwelder**, A. Brodsky, S.W. Harcum

**10:50 BIOT 532.** Novel aminoglycoside-hydrogel based in-vitro models of tumor dormancy, relapse and metastases: Phenotype specific drug screening, discovery and delivery. **T. Grandhi**, T. Potta, K. Rege

**11:10 BIOT 533.** Reprogramming the local lymph node environment to promote myelin-specific tolerance. **L.H. Tostanoski**, **C. Jewell**

## Section E

Westin San Diego  
Crystal I

### Quality by Design for Biopharmaceuticals

#### Lifecycle Management

S. Singh, C. Torigoe, *Organizers*

S. Abraham, C. Agarabi, *Organizers, Presiding*

**8:30 BIOT 534.** Raw material specification lifecycle management. **L. Miller**, A. Fries

**8:50 BIOT 535.** Maximizing the value of commercial scale data: A case study. **G. Naugle**

**9:10 BIOT 536.** Analytical method evolution during biological product life cycle. **P. Lei**, Q. Qin, R. Zhang, M. Washabaugh

**9:30 BIOT 537.** Regulatory and technical considerations for life cycle management. **S. Lute**, C. Agarabi, K.A. Brorson

**9:50** Intermission.

**10:10** Panel Discussion.

## Section F

Westin San Diego  
Diamond II

### Upstream Processes

#### Control of Protein Quality Attributes

M. R. Antoniewicz, M. A. Blenner, V. Roy, *Organizers*

V. Janakiraman, T. Whitehead, *Organizers, Presiding*

**8:30 BIOT 538.** Elucidating raw material variability in mammalian cell cultures using high throughput small-scale models. **H. Barkhordarian**, J. Huang, C. Goudar

**8:50 BIOT 539.** Effects of process parameters and medium components on charge variant distribution of a human monoclonal antibody. **T. Falkman**, A. Vitina, T. Bjorkman, L. Kärf

**9:10 BIOT 540.** Impact of media components and seed conditions on cell culture productivity and quality attributes of a fusion protein. **J. Xu**, Y. Wang, X. Xu, J. Tian, C. Huang, L. You, N. Qian, Z. Li

**9:30 BIOT 541.** Achieving cell growth control and increased specific productivity in CHO cell cultures without impacting product quality. **T. Tharmalingam**, B.D. Follstad, T. Munro, C. Goudar

**9:50** Intermission.

**10:10 BIOT 542.** Understanding and controlling monoclonal antibody charge heterogeneity in cell culture. **Y. Huang**, W.C. Yang, C. Kwiatkowski

**10:30 BIOT 543.** Mechanistic elucidation of Fc glycan high mannose modulation and its application for product attribute control. **J. Huang**, P. Slade, S. Gupta, I. Liu, C. Zupke, G. Nyberg

**10:50 BIOT 544.** Effects of induction strategies on heterologous protein expression and virus-like particle assembly in *Pichia pastoris*. **B. Blaha**, T. Mukhopadhyay

**11:10 BIOT 545.** End-to-end approach to monitoring and reducing LMW Formation during mAb process development. **A. Cura**, R. Maurer, A. Shupe, S. Chollangi, K. Sing, K. McWade, J. Yee, J. Ray, M. Peck, M. Lu, R. Martin, Y. Li, Z. Li

## Section A

Westin San Diego  
Emerald Ballroom

### Biotechnology & Bioengineering Elmer Gaden Award

T. M. Przybycien, P. M. Tessier, S. A. Tobler, *Organizers, Presiding*

**11:30** Biotechnology & Bioengineering Elmer Gaden Award Presentation.

## THURSDAY AFTERNOON

## Section A

Westin San Diego  
Crystal II

### Upstream Processes

#### General Topics in Upstream Processes

M. R. Antoniewicz, M. A. Blenner, V. Roy, *Organizers*

C. Beisel, T. Tharmalingam, *Organizers, Presiding*

**2:00 BIOT 546.** Design, analysis and assessment of novel enzymatic reactions and biopathways. **N. Hadadi**, M. Ataman, J. Hafner, V. Hatzimanikatis

**2:20 BIOT 547.** Transcriptomics-guided design of regulatory elements: A workflow to create synthetic promoters for mammalian hosts. **J.K. Cheng**, H.S. Alper

**2:40 BIOT 548.** Guiding rational glycan assay development using observability analysis. **D. Radhakrishnan**, A.S. Robinson, B. Ogunnaike

**3:00 BIOT 549.** Mechanistic understanding of chromosomal rearrangements in CHO cells. **J. Baik**, K.H. Lee

**3:20** Intermission.

**3:40 BIOT 550.** Evaluation of oxidative stress on cell metabolism and product quality. **M. Handlogten**, M. Zhu, S. Ahuja

**4:00 BIOT 551.** Evaluation of advanced media / feed characterization methods for an improved understanding of media / feed variability. **S. Tummala**, T. Webster, R. Beri

**4:20 BIOT 552.** Poloxamer: Steps towards cell culture media consistency. **J. von Hagen**

**4:40 BIOT 553.** Semicontinuous bioreactor production of a recombinant therapeutic protein in metabolically regulated transgenic rice cell cultures. **J. Corbin**, B.I. Hashimoto, K. Karuppanan, Z.R. Kyser, R.L. Rodriguez, S. Nandi, B.A. Roberts, A.R. Noe, K. McDonald

## Section B

Westin San Diego  
Emerald Ballroom

### Downstream Processes

#### Non-Chromatographic Separations & Process Integration

J. Neville, A. Noyes, T. M. Przybycien, *Organizers*

H. Ahmadian, A. M. Lenhoff, *Organizers, Presiding*

**2:00 BIOT 554.** Salt tolerant tangential flow ultrafiltration membranes for protein fractionation. **A. Arunkumar**, M.R. Etzel

**2:20 BIOT 555.** Production of stable high concentration monoclonal antibody solutions with low viscosity by tangential flow ultrafiltration. **J. Hung**, A. Borwankar, B. Dear, T. Truskett, K.P. Johnston

**2:40 BIOT 556.** Continuous processing for diafiltration operations in biomanufacturing. **E. Peterson**, H. Lutz

**3:00 BIOT 557.** Development of chiral membranes for purifying chiral feed streams. **J.M. Imbrogno**, V.L. Schultz, R.J. Linhardt, G. Belfort

**3:20** Intermission.

**3:40 BIOT 558.** Enhancement of viral filtration performance by characterization of the foulant particulates and controlling factors contributing to sub-visible particle formation. **J. Woo**, R. Emery, C. Garcia, N. Sanaie

**4:00 BIOT 559.** Pre-filtration and process improvements: Enhancing virus filter performance by pre-filtration with surface modified membrane. **B. Cacace**, S. Giglia, P.M. Goddard, H. Bak, C. Cowan, C. Passno

**4:20 BIOT 560.** Effects of filtration condition on virus clearance. **R. Te**, S. Eswaranandam, R. Wickramasinghe, X. Qian

**4:40 BIOT 561.** Understanding the impacts of viral clearance artifacts in nanofiltration. **A.H. Schwartz**

## Section C

Westin San Diego  
Diamond I

### Biomolecular & Biophysical Processes

#### Prediction & Characterization of Biophysical Properties

J. Kaar, H. Samra, *Organizers*

B. Hackel, F. He, *Organizers, Presiding*

**2:00 BIOT 562.** Withdrawn.

**2:20 BIOT 563.** Unfolding thermodynamics and  $\beta$ -sheet formation of helical peptides. **C. Calero-Rubio**, B.A. Paik, X. Jia, K.L. Kluck, C.J. Roberts

**2:40 BIOT 564.** Protein conformational array as a process development tool for antibody higher order structure analysis. **D. Yu**, Y. Song, E. Schutsky, M. Mayani, A.T. Lewandowski, Z. Li

**3:00 BIOT 565.** Measurements of antibody self-association using affinity-capture self-interaction nanoparticle spectroscopy are correlated with complex biophysical properties. **S.B. Geng**, M. Wittekind, A. Vigil, P.M. Tessier

**3:20** Intermission.

**3:40 BIOT 566.** Microrheology and intrinsic viscosities of antibodies. **L. Josephson**, D.L. Leiske, W.J. Galush, E.M. Furst

**4:00 BIOT 567.** Understanding of structural factors for enzyme activity and stability and application to simultaneous enhancement of enzyme activity and organic solvent stability. **Y.J. Yoo**, C.F. Yagonia, H. Lee, S. Kang

**4:20 BIOT 568.** What effect does cleaning and sanitization in place have on protein affinity ligands? **M. Wetterhall**, E. Monie, A. Mattsson, A. Gronberg, G. Rodrigo, T. Bjorkman

**4:40 BIOT 569.** Structural flexibility, hydrophobicity and charge regulation in histidine-rich antimicrobial piscidins underpin membrane disruption examined in real time. **M. Sorci**, J. Seckute, N. Smajic, S.B. Perrin, L.K. Nicholson, J. Blazyk, R. Pastor, M. Cotten, G. Belfort

## Section D

Westin San Diego  
Opal

### Emerging Technologies

#### Disease & Biomedical Applications

C. Chen, J. Latone, S. L. Servoss, G. M. Thurber, I. R. Wheelodon, *Organizers*

N. Gupta, C. Heldt, *Presiding*

**2:00 BIOT 570.** Fourier transform infrared spectroscopic spectral feature subset selection for optimal diagnosis of oral lesion. **S. Banerjee**, J. Chakraborty, M. Pal, R. Paul, J. Chatterjee

**2:20 BIOT 571.** Highly sensitive smartphone-based point-of-care diagnostics enabled by persistent luminescence nanoparticles. **A. Paterson**, B. Raja, G. Garvey, E. Finley, J. Brgoch, R.C. Willson

**2:40 BIOT 572.** Paper microfluidics for the detection of infectious diseases. **J. Trabuco**, D.M. Prazeres, R.C. Willson

**3:00 BIOT 573.** New method of decreasing fouling and increasing gas transfer of polysulfone hollow-fiber membranes using peptoids. **N. Mahmoudi**, M. Asgharpour, L. Reed, J. Hestekin, S.L. Servoss

**3:20** Intermission.

**3:40 BIOT 574.** Therapeutic probiotics engineered to target colorectal cancer. **H.C. Loong**, M. Chang

**4:00 BIOT 575.** Rapid uptake of fluorescent peptides into intact mammalian cells using a  $\beta$ -Hairpin sequence motif. **A.T. Melvin**

**4:20 BIOT 576.** Connectosomes for direct intracellular drug delivery. **A. Gadok**, D. Busch, J. Stachowiak

**4:40 BIOT 577.** Importin-4 regulates gene delivery by enhancing nuclear retention and chromatin deposition by polyplexes. **M.O. Sullivan**, E. Munsell, N.L. Ross

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## BIOL

## Division of Biological Chemistry

V. Bandarian and L. Hedstrom, Program Chairs

## SUNDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Marina Salon D

## Young Investigators in Biological Chemistry

V. Bandarian, Organizer

J. Houglund, Presiding

**9:00 BIOL 1.** Targeting transcription factor HNF1 $\beta$  in ovarian cancer using stapled peptides. **M. Wiedmann**, D.R. Spring, J. Brenton

**9:15 BIOL 2.** *In vivo* applications of a targetable and activatable photosensitizer (TAPS). **J. He**, Y. Wang, M.P. Bruchez

**9:30 BIOL 3.** Promiscuity of terpene biosynthesis as a platform for natural product diversification. **S. Lund**, G.J. Williams

**9:45 BIOL 4.** Lysine acylation: A one-size-fits-all solution. **Z. Wang**

**10:00 BIOL 5.** Small molecule control of protein function in living cells. **J. Luo**

**10:15 BIOL 6.** Identification of a set of atypical integral membrane hydrolases that degrade bioactive FAHFs. **W.H. Parsons**, M.J. Kolar, S. Kamat, A. Saghatelian, B.F. Cravatt

**10:30 BIOL 7.** Site-selective and direct electrophilic C-F bond formation onto proteins. **A. Phanumartwivat**, M. Schombs, S. Forsback, A. Kirjavainen, O. Solin, M. Haaparanta-Solin, A.M. Dickens, D.C. Anthony, O. Boutoureira, G. Bernardes, B.G. Davis

**10:45** Intermission.

**10:55 BIOL 8.** Lipid anchors for controlled localization of protein to phospholipid membranes. **A. Rudd**, J. Valls Cuevas, N.K. Devaraj

**11:10 BIOL 9.** Unanticipated interactions for vitamin B<sub>12</sub> revealed by chemical probing. **P. Nandhikonda**, Y. Maezato, D. Rodionov, I. Rodionov, Y. Kim, V. Kodali, T. Metz, M. Romine, A.T. Wright

**11:25 BIOL 10.** Chemical probe approach to elucidate the role of MEK4 in metastasis. **K.K. Deibler**, A. Antanasijevic, R.K. Mishra, M. Clutter, M. Caffrey, K. Scheidt

**11:40 BIOL 11.** Uncovering catalytic driving forces in the hammerhead ribozyme: Binding of Mg<sup>2+</sup> promotes pK<sub>a</sub> shifting of guanine towards neutrality. **E.A. Frankel**, C.D. Keating, P.C. Bevilacqua

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**11:55 BIOL 12.** Mapping enzymatic interactions of bacterial cell wall biosynthesis with photo-affinity probes. **S. Sarkar**, E. Libby, S. Pidgeon, J. Dworkin, M.M. Pires

**12:10 BIOL 13.** Single-protein reporter for hyperpolarized xenon magnetic resonance imaging. **B.W. Roose**, Y. Wang, V. Carnevale, I.J. Dmochowski

## Section B

Marriott Marquis San Diego Marina  
Marina Salon E

## Computational Enzymology

A. Kohen, Organizer, Presiding

9:00 Introductory Remarks.

**9:05 BIOL 14.** Probing electrostatics and conformational motions along the catalytic cycle of dihydrofolate reductase. **S. Hammes-Schiffer**

**9:50 BIOL 15.** Multistate density functional theory for enzymatic and protein dynamical processes. **J. Gao**

**10:35 BIOL 16.** Theoretical studies of enzyme catalysis: Towards the design of new biocatalysts. **V. Moliner**

**11:20 BIOL 17.** Comparing Computed Findings to Experimental Data: Challenges and Opportunities. **A. Kohen**

## Multiscales Chemistry

## Energy

Sponsored by MPPG, Cosponsored by ANYL, BIOL, COMP and PHYS

## Structure &amp; Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment &amp; Theory

## Active Sites

Sponsored by PHYS, Cosponsored by BIOL

## SUNDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
Marina Salon D

## Young Investigators in Biological Chemistry

V. Bandarian, Organizer

M. E. Farkas, Presiding

**1:00 BIOL 18.** Fluorinated bromodomains: Choosing the right halogen for small molecule discovery. **W.C. Pomerantz**, C. Gee, A. Urick, N.K. Mishra, E. Schonbrunn, S. Ember, L.M. Hawk

**1:20 BIOL 19.** Simultaneous inhibition of methicillin resistant *Staphylococcus aureus* acetate kinase and phosphate acetyltransferase as potential antibacterial agents targeting energy metabolism. **C. Wu**, W. Lawrence, J. Tice, T. McCune, K. Schmidt

**1:40 BIOL 20.** Peptide ixosin uses an ATCUN motif for its oxidative antimicrobial activity and its synergy with other tick peptides. **A.M. Angeles Boza**, M.D. Libardo, V. Gorbatyuk

**2:00 BIOL 21.** Structural effects of 8-hydroxy-7,8-dihydropurines in RNA and their effects on function using the aptamers for pre-Q<sub>1</sub> and theophylline as models. **M.J. Resendiz**, K. Gibala, Y.J. Choi, K. Van Deventer

**2:20 BIOL 22.** Metal ion induced alterations in amyloid precursor protein expression and tau hyperphosphorylation via microRNA mediated pathways. **M.J. Sever**

**2:40 BIOL 23.** Characterization and development of Taq DNA polymerase mutants capable of synthesizing 2' modified DNA. **A. Leconte**

**3:00** Intermission.

**3:10 BIOL 24.** Investigation of the *glmS* ribozyme: New catalytic roles for the GlcN6P cofactor and metal ions. **J. Bingaman**, S. Zhang, S. Hammes-Schiffer, P.C. Bevilacqua

**3:25 BIOL 25.** Substrate sequestration and protein-protein interactions in pyrrole biosynthesis. **M.J. Jaremko**, D.J. Lee, V. Winslow, M.D. Burkart

**3:40 BIOL 26.** Mutations at a single active site residue in TET2 stall oxidation at 5hmC and reveal requirements for catalysis. **M. Liu**, H. Torabifard, D.J. Crawford, J.E. DeNizio, G.A. Cisneros, R.M. Kohli

**3:55 BIOL 27.** Programmable DNA origami based multi-hairpin force probes. **P.K. Dutta**

**4:10 BIOL 28.** Understanding single-molecule protein dynamics via electronic circuit. **M. Iftikhar**

**4:25 BIOL 29.** Spontaneous formation and remodeling of synthetic membranes. **R.J. Brea Fernández**, A. Rudd, N.K. Devaraj

## Section B

Marriott Marquis San Diego Marina  
Marina Salon E

## E. Bright Wilson Award in Spectroscopy: Symposium in honor of Robert G. Griffin

Cosponsored by PHYS

Financially supported by Bruker BioSpin

T. M. Swager, Organizer, Presiding

W. E. Maas, Presiding

**1:00 BIOL 30.** Applications of solid-state NMR spectroscopy to antifungal drugs, Parkinson's disease and blood coagulation. **C. Rienstra**

**1:25 BIOL 31.** Structural studies of Y145Stop prion protein amyloids. **C.P. Jaronic**

**1:50 BIOL 32.** NMR approaches to GPCRs in phospholipid bilayers. **S. Opella**

**2:15 BIOL 33.** Structural investigations on membrane proteins by MAS NMR and dynamic nuclear polarisation (DNP). **H. Oschkinat**

**2:40 BIOL 34.** Direct observation of hierarchical protein dynamics. **J.R. Lewandowski**, M. Halse, M. Blackledge, **L. Emsley**

**3:05** Intermission.

**3:15 BIOL 35.** Structural investigations of membrane proteins and plant cell walls by resolution- and sensitivity-enhanced solid-state NMR spectroscopy. **M. Hong**

**3:40 BIOL 36.** Functional studies of an ion channel by NMR in native membranes. **A.E. McDermott**

**4:05 BIOL 37.** ↑↑↑↑... and ↓ of nuclear spins. **A. Pines**, J. King

**4:30 BIOL 38.** Amyloid, membranes, microwaves and the magic angle. **R.G. Griffin**

## Multiscales Chemistry

## Mini-Platform

Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS

## Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINP, COLL, COMSCI, DAC, GEOC, I&amp;EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## Structure &amp; Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment &amp; Theory

## Conformations &amp; Dynamics

Sponsored by PHYS, Cosponsored by BIOL

## SUNDAY EVENING

## Section A

San Diego Convention Center  
Hall F

## Current Topics in Biochemistry

V. Bandarian, Organizer

7:00 - 9:00

**BIOL 39.** Heterologous expression of the human polybromo-1 protein in the methylotrophic yeast *Pichia pastoris*. **S. Hopson**, M. Thompson

**BIOL 40.** Progress in design of programmable DNA minor groove agents for recognition of mixed sequences. **A. Paul**, R.K. Nanjunda, A. Kumar, S. Laughlin-Toth, R. Nhilli, S. Depauw, Y. Chai, A. Chaudhary, M. David-Cordonnier, D.W. Boykin, W. Wilson

**BIOL 41.** Knockdown and knockout of DNMT3a affects chick eye morphogenesis. **N.G. Burns**, Z. Han, E. Grajales Esquivel, A. Madrigal, K. Del Rio-Tsonis

**BIOL 42.** Thermodynamic analysis of ATP binding in DEAD-box proteins. **C. Bardine**, Y. Xu, A. Cosgrove, I. Garcia

**BIOL 43.** Genetically induced production of secondary metabolites in *Bacillus megaterium*. **M. Foster**, J.L. Brewster, P.M. Joyner

**BIOL 44.** Expression and purification of human polyamine oxidase. **A. Arreola**, J.R. Tormos

**BIOL 45.** Free energies of interaction of lipids with regulatory binding sites on the transmembrane domain of the EGF receptor. **G. Hedger**, H. Koldsø, M.S. Sansom

**BIOL 46.** RNA-aminoglycoside interactions probed through platination kinetics. **S. Thalalla Gamage**, G. Dedduwa-Mudalige, C.S. Chow

**BIOL 47.** Probing the interaction of spider venom neurotoxins with the lipid bilayer using solid-state NMR, TEM and DSC. **G. Polido**, X. Shi, D. Xu, T. Doan, G.P. Holland

**BIOL 48.** Conjugation of BSA onto PEG<sub>8</sub> via strain-promoted azide-alkyne cycloaddition (SPAAC) as a drug delivery system. **J. Hill**, M. Rhodes, K.W. Olsen

**BIOL 49.** Benzotriazine di-N-oxides as fluorogenic substrates for hypoxia and one-electron reductases involved in the activation of bioreductive anticancer prodrugs. **X. Shen**, K.M. Johnson, R. Hillebrand, U. Sarkar, G.A. Baker, C. Laber, K.S. Gates

**BIOL 50.** Comparison of activating agents for conjugation of bovine serum albumin onto eight-arm polyethylene glycol (PEG) via strain promoted azide alkyne cycloaddition (SPAAC) as a pharmaceutical carrier. **M. Rhodes**, J. Hill, K.W. Olsen

**BIOL 51.** Natural and non-canonical mutagenesis studies of receptor gating in 5-HT<sub>3A</sub> receptors. **R. Mosesso**, S.C. Lummis, D.A. Dougherty

- BIOL 52.** Self-therapeutic HDL mimicking nanoparticles for detection of atherosclerotic plaques. **B. Banik, S. Dhar**
- BIOL 53.** Withdrawn.
- BIOL 54.** Mitochondria-targeted nanoparticle for understanding  $\alpha$ -Tocopheryl succinate action on cancer cells. **R. Wen, S. Dhar**
- BIOL 55.** Expression and characterization of straight  $\alpha$ -helix concatemers for nanosheet formation. **R.A. Bartlett**
- BIOL 56.** Development of alkyne-containing pyrazolopyrimidines to overcome drug resistance of BCR-ABL kinase. **X. Liu, C. Zhang, A. Kung**
- BIOL 57.** Experimental and computational studies to explore the impact of macromolecular crowding on the structure and function of *Escherichia coli* of prolyl-tRNA synthetase. **R. Andrews, L.M. Adams, A.N. Hodac, H. Schmit, S. Bhattacharyay, S. Hati**
- BIOL 58.** Binding studies of mutated C2 domain in coagulation factor VIII. **S. Thompson**
- BIOL 59.** Pathogenesis of type III secretion system effector IpaD in *Shigella*. **K. Smith, O. Arizmendy, W.D. Picking, W.L. Picking**
- BIOL 60.** Role of F365 in inhibitor binding by *Escherichia coli* beta-glucuronidase. **L. Lesure, C. Folsom, K.T. Lane**
- BIOL 61.** Novel mechanism-based inhibitors of flavin-dependent oxidation domains. **I. McCulloch, J.J. La Clair, M.J. Jaremko, M.D. Burkart**
- BIOL 62.** Hsp90 inhibitors as lead molecules for histidine kinase inhibition: Toward novel antibiotics. **J. Blair**
- BIOL 63.** Sequence-specific 2-cyanobenzothiazole ligation identified through phage-assisted interrogation of reactivity. **C. Ramil, Q. Lin**
- BIOL 64.** Potent natural soluble epoxide hydrolase inhibitors from Oubli plant *Pentadiplandra brazzeana* baillon. **S. Kitamura, C. Morisseau, S.G. Kamita, B. Inceoglu, G.R. De Nicola, M. Nyegue, B.D. Hammock**
- BIOL 65.** Investigation of the mechanism of CYP199A4 catalyzed dehydrogenation. **S. Wong, J. Stok, J. De Voss**
- BIOL 66.** Influence of conserved cysteines and pre-pheromone on Enterococcal plasmid pCF10 replication initiation protein activity. **A. Bruefach, B. Buttaro, E. Laughlin, N. Mourabet**
- BIOL 67.** Cancer gene therapy: Purification and characterization of lyase activity of methionine gamma lyase-deaminase (*MglA*) from *Porphyromonas gingivalis*. **N. Ledra, K. Venk**
- BIOL 68.** Stress-responsive signaling pathways as targets for modulating biofilm growth and composition. **S.J. Loewus, E.M. Curley, L.M. Ryno**
- BIOL 69.** Optimization of myxin production from *Lyso bacter antibioticus* OH13 to study the antibiotic's mechanism of action. **J. Monroy, Y. Zhao, L. Du**
- BIOL 70.** Membrane-bound selenoprotein T. **M. Willoughby, B. Hallahan, Z. Zhang, S. Rozovsky**
- BIOL 71.** Computational study of anticancer activities of ruthenium(II) complexes against selected cancer receptors. **P.A. Ajibade, A.A. Adeniyi**
- BIOL 72.** Kinetic study on enzymatic hydrolysis of model cellulose films using surface plasmon resonance. **M. Anuganti, R. Kamat, C.V. Kumar, Y. Lin**
- BIOL 73.** Conserved flexible tetraglycine loop in HDAC8 is vital for catalytic activity. **N.J. Porter, N.H. Christianson, C. Decroos, D.W. Christianson**
- BIOL 74.** Phenotypic screen for functional mutants of human adenosine deaminase acting on RNA 1. **Y. Wang, J. Havel, P.A. Beal**
- BIOL 75.** Design of a novel module n-methylbenzimidazole thiophene for specific recognition of G•C base pairs. **P. Guo, A. Paul, A. Kumar, A.A. Farahat, D.W. Boykin, W. Wilson**
- BIOL 76.** Elucidation of the aggregation pathways of helix-turn-helix peptides: Stabilization at the turn region is critical for fibril formation. **T. Do, A. Chamas, X. Zheng, A. Barnes, D. Chang, T. Veldstra, H. Takhar, N. Dressler, B. Trapp, K. Miller, A. McMahon, S.C. Meredith, J.E. Shea, K.L. Lazar Cantrell, M.T. Bowers**
- BIOL 77.** Oxidative stress mediates drug binding by calmodulin. **H.T. Niedermaier, R.J. Bieber Urbauer, J.L. Urbauer**
- BIOL 78.** Development of E2F-responsive luciferase reporters for the investigation of p27<sup>kip1</sup> mediated cell cycle regulation. **M. McCabe, M.J. Sever**
- BIOL 79.** Impact of excess metals on microRNA dysregulation and CD47 protein expression in U87 cells. **D.Y. Xia, M.J. Sever**
- BIOL 80.** Understanding oncostatin M mediated regulation of miR-21 in cancer cell lines. **S.T. Ahmed, M.J. Sever**
- BIOL 81.** Toxic doses and effects of the manufactured nanomaterial buckminsterfullerene or C<sub>60</sub> to mouse liver cells in culture. **U. Maharjan, Z. Miller, K. Albahrani, C. Thomas**
- BIOL 82.** Dose-dependent inhibition of succinoxidase by buckminsterfullerene (C<sub>60</sub>). **J.C. Flores, Z. Miller, U. Maharjan, C. Thomas**
- BIOL 83.** Identification of putative LuxS inhibitors by computational screening. **M.E. Bolitho, P. Gernon, C. Morgan, K. Wang**
- BIOL 84.** Regulation of cytidine triphosphate synthetase activity in *Burkholderia cepacia*. **T.P. West**
- BIOL 85.** Enzymatic hydrolysis of 2,2-diphenylethyl glucosinolate. **C.A. Klingaman, M.J. Wagner, J.R. Mays**
- BIOL 86.** Molecular view of HIV-1 restriction factors. **M.E. Akana, A. Bhattacharya, Z. Wang, D. Ivanov**
- BIOL 87.** Withdrawn.
- BIOL 88.** Development of selective, irreversible inhibitors for a receptor tyrosine kinase EphB3. **A. Kung, Y. Chen, F. Ni, C. Zhang**
- BIOL 89.** Copper inhibits AlkB family DNA repair enzymes and the relationship with Wilson's disease. **K. Bian, F. Chen, Q. Tang, D. Li**
- BIOL 90.** *In vivo* reduction of arsenic from inhaled mine waste. **K. Cablay, M. Bisoffi, C. Kim**
- BIOL 91.** Determination of 4-hydroxy-2-nonenal covalent binding sites on electron transfer flavoprotein using liquid chromatography-mass spectrometry. **M. Breen-Lyles, C.M. Byron**
- BIOL 92.** Pattern recognition for the classification of long non-coding RNA. **C.S. Eubanks**
- BIOL 93.** Detection of fear conditioning induced changes in a transcription factor in the prefrontal cortex by western blotting assay. **A.H. Saheb**
- BIOL 94.** Development of the quadricyclane ligation into a multimodal bioorthogonal reaction: Click, unclick, re-click. **F.M. Tomlin, C.G. Gordon, C. Bertozzi**
- BIOL 95.** Construction of an acetate kinase gene deleted plasmid for validation of its essentiality in methicillin resistant *Staphylococcus aureus* as a novel drug target. **J. Tice, C. Wu**
- BIOL 96.** Urine metabolic biomarkers for mouse ischemic acute kidney injury. **T. Chihanga**
- BIOL 97.** Understanding electrostatic effects on binding kinetics and affinities of ETS transcription factor proteins and DNA interaction. **T.D. Vo, S. Wang, G.M. Poon, W. Wilson**
- BIOL 98.** Determining the ligand coordination sphere and functionality of the Zn<sup>2+</sup> linchpin motif of the DNA repair glycosylase MUTYH. **N. Nuñez, S.S. David**
- BIOL 99.** Withdrawn.
- BIOL 100.** Identification of histidine 303 as the catalytic base of lysyl oxidase via site-directed mutagenesis. **R.N. Oldfield, K.M. Lopez**
- BIOL 101.** Enhanced oligonucleotide binding by RNA tethering in deaminase acting on RNA 2 (ADAR2). **C. Palumbo, K.T. Tran**
- BIOL 102.** Development of drug-like inhibitory agents of Nek2 kinase. **A. Finkelstein, R. Giri, Y. Sosa, D. Gloster, S. Kumar**
- BIOL 103.** Identification of S-glutathionylation by metabolic synthesis of alkene-glutathione. **D.N. Kekulandara, Y. Ahn**
- BIOL 104.** Adenosine deaminase acting on double strand RNA (ADAR) protein substrate preference, interactions indicated by the new RNA bound ADAR2 crystal structure. **Y. Zheng, P.A. Beal**
- BIOL 105.** Characterization of enzyme product profiles in specialized metabolism through heterologous expression. **M. Moore, J. Jin, S.P. Matsuda**
- BIOL 106.** Structural characterization of the ACCH domain of angiomin family members. **P. Vitanen, H. Petrache, A. Kimble-Hill**
- BIOL 107.** Fine-tuning triazabutadiene stability for controlled diazonium release. **L. Guzman, F. Kimani, J.C. Jewett**
- BIOL 108.** Effects of substrate sequestration on the fatty acid biosynthesis carrier protein. **D. Lee, H.N. Vuong, J.J. Hale, M.D. Burkart**
- BIOL 109.** Defining and exploiting APOBEC3A's cytidine deaminase activity on the extended epigenome. **E.K. Schutsky, J.E. DeNizio, C.S. Nabel, R.M. Kohli**
- BIOL 110.** Novel KinExA-based immunosensor for real-time measurement of the breast cancer biomarker carcinoembryonic antigen in serum. **I. Darwish, T. Wani, S. Zargar**
- BIOL 111.** Structure of the C-terminal domain of EcoR1241 restriction enzyme. **N. Luedtke, P. Grinkevich, B. McIntosh, T. Baikova, M. Lapkouski, J. Carey, R. Ettrich**
- BIOL 112.** Glutathione levels in human lung cancer (A549 cells) and 3T3-L1 preadipocytes following exposure to the calpain inhibitor (KR-185). **S.P. Falekun, E.L. Myles, I. Donkor, W. Boadi**
- BIOL 113.** H-transfer mechanisms in human vs *E. coli* thymidylate synthase. **Z. Islam, I. Gurevic, T. Iqbal, A. Ghosh, A. Kohen**
- BIOL 114.** Cyclopropanones are stable bio-orthogonal chemical reporters. **R. Row, H. Shih, J.A. Prescher**
- BIOL 115.** Site specific protein labeling of genetically encoded strained alkene/alkyne functionalities *in vivo* via rapid catalyst-free click chemistry. **K.A. Odoi, Y. Kurra, Y. Lee, W. Li**
- BIOL 116.** Trifunctional cyclooctyne for modifying azide-labeled biomolecules with photocrosslinking and affinity tags. **B. Piligian, J.A. Stewart, S. Rundell, B.M. Swarts**
- BIOL 117.** Engineering *E. coli* nitroreductase for targeted small molecule release. **T.D. Gruber, M.R. Tadross, J. Grimm, L.D. Lavis**
- BIOL 118.** Elucidation of lipoxigenase membrane association via hydrogen deuterium exchange. **K. Droege, M.E. Keithly, E.B. Prage, C.R. Sanders, R.N. Armstrong**
- BIOL 119.** Withdrawn.
- BIOL 120.** Development of "inside-out" PEGylated crosslinked hemoglobin polymers: A novel hemoglobin-based oxygen carrier (HBOC). **K.D. Webster, D. Dahhan, C. Frost, J.B. Chaires, K.W. Olsen**
- BIOL 121.** Novel Na<sup>+</sup>-independent Ca<sup>2+</sup>/dopamine/ MPP<sup>+</sup> uptake system is present in dopaminergic cells. **V.Q. Le, K. Wimalasena**
- BIOL 122.** Engineering virus like particles towards directing immunologic responses. **D. Patterson, B. Western, M. Terra, P. Krugler, M. Hicks, A. Rynda-Applé, A. Harnsen, T. Douglas**
- BIOL 123.** Zinc sensors reveal that proteomic zinc buffering is dependent on sulfhydryl groups. **M. Karim**
- BIOL 124.** Potentially bioactive ferrocene-based ureas: Synthesis, characterization, *in vitro* bioactivities, interaction with SS-DNA and DFT study. **F. Asghar, A. Badshah, B. Lal, I.S. Butler**
- BIOL 125.** New strategy to end-tether extracellular matrix proteins to polymer hydrogel surfaces. **J.P. Lee, M.B. Francis, S. Kumar**
- BIOL 126.** Catalytic activities of tumor-specific human cytochrome P450 CYP2W1 towards endogenous substrates. **Y. Zhao, P.R. Ortiz De Montellano**
- BIOL 127.** Clickable, photoactive NAADP analogs for identification of the NAADP binding protein. **T.Y. Asfaha, J.T. Slama, T. Walseth**
- BIOL 128.** Effects of rotational and translational position on T-T CPD formation in a T<sub>11</sub>-tract in a nucleosome. **K. Wang, S. Pondugula, V. Cannistraro, J.S. Taylor**
- BIOL 129.** Short hairpin-like peptide induces non-leaky membrane fusion. **H. Kan**
- BIOL 130.** Withdrawn.
- BIOL 131.** Investigations of an RNA thermometer using SHAPE assays. **K. Ulanowicz, C. Cempre, P. Dunn, Y. Nguyen, R.M. Mitton-Fry**
- BIOL 132.** Photochemical evidence for the presence of a reverse hoogsteen hairpin conformation in human telomeric DNA sequences. **C. Lu, J. Smith, J.S. Taylor**

### My Comments to the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

### My Experience with & Advice for Improving Diversity in Chemistry

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### My Experiences in & Advice for Organic Chemistry Courses

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## MONDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Marina Salon D

#### Frontiers in Biomolecular Recognition: From Materials to Cells

A. K. Mapp, *Organizer*

J. L. Meier, *Presiding*

9:00 Introductory Remarks.

9:05 BIOL 133. Synthesis at the interface of chemistry and biology: From stem cells to the genetic code. P.G. Schultz

9:30 BIOL 134. Mechanistic studies on a new menaquinone biosynthetic pathway. T.P. Begley

9:55 BIOL 135. Discovery of *in vivo* targets of transcriptional activators via covalent chemical capture. A.K. Mapp

10:20 Intermission.

10:40 BIOL 136. Riboswitches in diverse biological processes. S.A. Strobel

11:05 BIOL 137. Breaking the central dogma: Selectivity in adenosine to inosine RNA editing. P.A. Beal, A.J. Fisher, J. Thomas, M. Matthews, Y. Zheng, K.T. Tran, K. Phelps, A. Erickson, J. Havel

11:30 BIOL 138. Small-molecule strategies for mapping RNA structure and sequence. E.T. Kool

11:55 Concluding Remarks.

### Multiscales Chemistry

#### Bio

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#### Is There a Crisis in Organic Chemistry Education?

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

#### Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory

#### Active Sites

Sponsored by PHYS, Cosponsored by BIOL

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## MONDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Marina Salon D

#### Young Investigators in Biological Chemistry

V. Bandarian, *Organizer*

W. C. Pomerantz, *Presiding*

1:00 BIOL 139. Biochemical characterization of two evolutionary distant ten-eleven translocation enzymes and their utility in 5-methylcytosine sequencing in the genomes at single-base resolution. L. Saleh, E. Tamanaha, J. Pais, R. Vaisvila, N. Dai, S. Guan, I. Correa, Y. Zheng

1:20 BIOL 140. Ghrelin acylation by human ghrelin O-acyltransferase: Substrate selectivity, mechanism, and inhibitor development. J. Hougland, J. Darling, K. McGovern, E. Cleverdon

1:40 BIOL 141. Microbial synthesis of modified alkaloids for the generation of known and novel therapeutics. P. Peralta Yahya

2:00 BIOL 142. Metallation of misfolding tau peptides/protein: Aggregation, phosphorylation and catalytic activity. S. Martic

2:20 BIOL 143. Modified macrophages for cancer study and treatment. M.A. Mingroni, J.J. Elliott, J. Hardie, A. Basabrain, M.E. Farkas

2:40 BIOL 144. Investigating zinc finger recognition of epigenetically modified DNA. B.A. Buck-Koehntop

3:00 Intermission.

3:15 BIOL 145. Investigating mechanisms of human c-MYC oncogene-induced mutagenesis in cancer. I. del Mundo, M. Zewail-Foote, S. Kerwin, K. Vasquez

3:30 BIOL 146. Targeting virulence as an approach to bacterial pathogenesis: Efforts towards the development of chemical biology tools and anti-chlamydial therapeutics. K. Alser, K.R. Maksimchuk, J. Schreiner, C. Brackeen, D.G. McCafferty

3:45 BIOL 147. Enhanced detection of bacteria in environmental waters: An RNA-based approach. V. Kapoor, J. SantoDomingo

4:00 BIOL 148. Insights into the mechanism of a cobalt-type nitrile hydratase. M.T. Nelp, V. Bandarian

4:15 BIOL 149. Novel regulation of tumor suppressor P27<sup>kip1</sup> by transglutaminase. L. Zhang, R. Sheaff

4:30 BIOL 150. Bioorthogonal chemistry for the investigation of viral infection. S.M. Jensen, J.C. Jewett

4:45 BIOL 151. Non-canonical proline analogs reveal mechanistic trends among GLIC and other ligand-gated ion channels. M. Rienzo, A.R. Rocchi, S.D. Threatt, D.A. Dougherty, S.C. Lummiss

### Multiscales Chemistry

#### Mini-Platform

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#### Diversity-Quantification-Success?

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#### LGBT Chemists' Symposium on Chemical Biology

Sponsored by PROF, Cosponsored by BIOL, BIOT, MEDI, ORGN, PRES and WCC

#### Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory

#### Beyond the Active Site

Sponsored by PHYS, Cosponsored by BIOL

#### Undergraduate Research Posters

#### Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

V. Bandarian, *Organizer*

8:00 - 10:00

65, 74, 88, 98, 108, 113, 115, 117-118. See previous listings.

178, 186, 190, 194-195, 198, 214, 223, 235, 237, 259. See subsequent listings.

## TUESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Marina Salon D

#### Chemistry in Service of Biology: Tools for Probing Cellular Processes

J. A. Prescher, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 BIOL 152. Chemical probes for the functional analysis of O-GlcNAc modifications. M. Pratt

9:35 BIOL 153. Building new materials from chemically modified proteins. M.B. Francis

10:05 BIOL 154. Chemically arming viruses with triazabutadienes. J.C. Jewett

10:35 Intermission.

10:45 BIOL 155. Spatial and temporal control of cellular processes using chemical tools. D.M. Chenoweth

11:15 BIOL 156. Breaking down bacterial cell walls to understand Crohn's disease. C.L. Grimes, J.E. Melnyk, A.K. Schaefer

11:45 BIOL 157. Development of approaches for long-term time lapse imaging of host-pathogen interactions. A.E. Palmer

### Multiscales Chemistry

#### Soft Matter

Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS

#### ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in honor of Carol A. Fierke

Sponsored by WCC, Cosponsored by BIOL

#### Computer-Aided Drug Design

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

#### Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory

#### Photons, Protons, Electrons

Sponsored by PHYS, Cosponsored by BIOL

## TUESDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Marina Salon D

#### ACS Chemical Biology Award Symposium

Financially supported by ACS Chemical Biology

L. L. Kiessling, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 BIOL 158. Application of chemical biology strategies to probe and manipulate proteostasis. M. Shoulders

2:35 BIOL 159. Development of small molecule inhibitors of the menin-MLL protein-protein interaction for cancer therapy". J. Grembecka, D. Borkin, H. Miao, K. Kempinska, J. Pollock, T. Purohit, S. Klossowski, D. Sun, T. Cierpicki

3:05 BIOL 160. Discovery and engineering of plant chemistry for plant and human health. E. Sattely

3:35 BIOL 161. Chemical biology approaches to innate immunity and vaccine design: Probing a code without a key. A. Esser-Kahn

4:05 BIOL 162. Chemist's foray into translational research: From stem cells to orphan disease. P.G. Schultz

### Multiscales Chemistry

#### Liquids

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#### Computer-Aided Drug Design

#### Computational Biophysics

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## TUESDAY EVENING

### Section A

San Diego Convention Center  
Hall E

#### Current Topics in Biochemistry

V. Bandarian, *Organizer*

7:00 - 9:00

BIOL 163. Using proteomics and biochemical approaches to evaluate the function of SAKS1 in p97-associated process. S. Li, D. Wang, T. Chou

BIOL 164. Towards an understanding of nonenzymatic glycation #1: The role of inorganic phosphate in the non-covalent initial binding. B. Cundick, A. Awadh, G. Titus, B. Park, P. Ropski, M. Finkbeiner, K. Rodnick, R.W. Holman

BIOL 165. Towards an understanding of nonenzymatic glycation #2: The role of 2, 3-bisphosphoglycerate in nonenzymatic glycation of human hemoglobin and formation of HbA1c. G. Titus, K. Pickett, M. Finkbeiner, K. Rodnick, R.W. Holman

BIOL 166. Towards an understanding of nonenzymatic glycation #3: The formation of phosphate-catalyzed glucose degradation products. P. Ropski, B. Park, M. Finkbeiner, K. Rodnick, R.W. Holman

BIOL 167. Towards an understanding of nonenzymatic glycation #4: The role of phosphate-catalyzed glucose degradation products in non-covalent protein binding. B. Park, P. Ropski, T. Hintze, M. Finkbeiner, B. Cundick, G. Titus, K. Rodnick, R.W. Holman



- BIOL 168.** Towards an understanding of non-enzymatic glycation #5: Potential mechanistic roles of taurine. **M. Finkbeiner**, A. Jensen, K. Rodnick, R.W. Holman, T. Hintze
- BIOL 169.** Towards an understanding of nonenzymatic glycation #6: The role of inorganic phosphate in the transition from the non-covalent to covalent stage of glycation. **A. Awadh, B. Cundick**, K. Rodnick, R.W. Holman
- BIOL 170.** Enzyme responsive pro-gel cyclic peptides. **A.S. Carlini**, B. Han, N.C. Gianneschi
- BIOL 171.** Role of enzymatic processing on seawater and sea spray aerosol properties. **J. Michaud**, J. Sauer, K. Moore, O.S. Ryder, C. Lee, K. Mayer, K.A. Prather, M.D. Burkart
- BIOL 172.** Role of matrix metalloproteinases in the outcome of bone marrow transplant for junctional epidermolysis bullosa. **P. Caballero**, J. Tolar
- BIOL 173.** Molecular modeling of the Z-77 inhibitor binding to the bacterial loop of *E. coli* beta-glucuronidase. **H. Gullickson**, K.T. Lane
- BIOL 174.** Evaluation of off-target effects due to RNA interference in *C. elegans*. **R. Drazenovic**, C. Carter, T. Dwyer
- BIOL 175.** Chemoenzymatic protein labeling and isolation from eukaryotic cell lysates using prenyltransferases with reengineered substrate selectivity. **M.J. Blandin**, B. Hampton, J. Hougland
- BIOL 176.** Effects of polyphenolic acids on amyloid formation. **T. Nghiem**, R. Vitale, S. Posson, S. Nalluri, J. Gao, **D.F. Moriarty**
- BIOL 177.** Synthesis and evaluation of allyloxy containing substrates for protein farnesyltransferase capable of tetrazine ligation. **J. Wollack**
- BIOL 178.** Cation- $\pi$  interactions: Computational analyses of the aromatic box motif and the fluorination strategy for experimental evaluation of cyst-loop receptors and related structures. **M.R. Davis**, D.A. Dougherty
- BIOL 179.** Nearest neighbor parameters for 7-deaza-adenosine•uridine pairs in RNA duplexes. **K.E. Richardson**, B. Znosko
- BIOL 180.** Investigating the active site of LpxC in gram-negative bacteria through interactions with synthesized natural substrate analogues. **G. Lamanilao**, K. Wilson, S. Malkowski, M.L. Cafiero, L. Peterson
- BIOL 181.** Effect of fatty acid binding protein 2 Ala54Thr gene polymorphism on obesity and metabolic syndrome in Korean middle-aged women. **Y. Kim**, S. Woo, T. Han
- BIOL 182.** Photo-reactivity of the triazabutadiene. **J. He**, F. Kimani, J.C. Jewett
- BIOL 183.** Adenovirus mediated delivery of engineered DNA sequence for pancreatic cancer treatment. **F. Hassan**, T. Arnett, S. Ni, M. Kennedy
- BIOL 184.** Covalent capture of oxidized protein tyrosine phosphatase 1B (PTP1B) by carbon nucleophiles: Toward selective inactivation of PTP1B. **K. Ruddaraju**, K.S. Gates
- BIOL 185.** Imino proton NMR in the reprogramming of AT specific minor groove binders for mixed-sequence recognition. **N. Harika**, M.W. Germann, A. Paul, Y. Chai, E. Stroeve, D.W. Boykin, W. Wilson
- BIOL 186.** Defining the metabolic regulation of epigenetics using chemical proteomics. **D.C. Montgomery**, J.L. Meier, A. Sorum
- BIOL 187.** Mutagenesis study to disrupt electrostatic interactions on the two-fold symmetry interface of bacterioferritin. **Y. Zhang**
- BIOL 188.** Characterizing novel peptides as anti-thrombosis agents. **K. Gentile**, S. Martin, D. Guarracino
- BIOL 189.** Development of stabilized cyclic peptides with potential anti-thrombosis activity. **D.H. Nguyen**, S. Knox, D. Guarracino
- BIOL 190.** Organelle transport controlled by a photocleavable chemical inducer of dimerization. **C. Aonbangkhen**, E. Ballister, M. Lampson, D.M. Chenoweth
- BIOL 191.** Borylbenzodiazonium reagent for library fluorophore synthesis and biological application. **B. Mehari**, J.C. Jewett
- BIOL 192.** Effects of Fe<sup>3+</sup> and ascorbic acid on AlkB family DNA repair enzymes. **Z. Humulock**, K. Bian, D. Li
- BIOL 193.** Calorimetric study of the conformational change of calmodulin and troponin C chimera proteins. **N. Kaufman**, K. Schafer, D. Jensen, C. Wei
- BIOL 194.** Determination of immune signal transduction activation thresholds. **B. Moser**, T.J. Albin, R. Mancini, A. Esser-Kahn
- BIOL 195.** Chemical modulation of cystathionine gamma lyase/hydrogen sulphide system in mammalian cells. **F. Ndombura**
- BIOL 196.** Isolation of a chromate reductase from *Pseudomonas veronii*. **A. Staidle**
- BIOL 197.** Characterization of thermal, pH, and UV-induced aggregates of human  $\gamma$ S-crystallin and its aggregation prone variants. **D.M. Montelongo**, C.D. Anorma, D.N. Bandak, R.W. Martin
- BIOL 198.** Biophysical characterization of Nur from *Streptomyces coelicolor*. **O.M. Manley**, N.E. Grosseohme
- BIOL 199.** Understanding packing defects and loop interactions in the four-helix bundle protein, Rop. **A. Kumar**, J. Lohmeyer, T.J. Magliery
- BIOL 200.** Consensus, correlation and combinatorics based approaches in engineering triosephosphate isomerase stability. **S. Mohan**, N.W. Callahan, K.R. Stephany, B.J. Sullivan, T.J. Magliery
- BIOL 201.** Purification of lambda phage protein phosphatase. **J. Schmoeyer**, Y. Koo
- BIOL 202.** Kinetic characterization and chemotherapeutic relevant inhibition of human malate dehydrogenase 1 and 2. **C. Carter**, R. Drazenovic, H. Drake, T. Dwyer
- BIOL 203.** Oxidative damage in triplex-forming DNA sequences increases the mutation frequency in mammalian cells. **O. Drummond**, S. Coe, I. del Mundo, **M. Zewail-Foote**, K. Vasquez
- BIOL 204.** Exploring the sequence landscape of the model protein Rop. **N. Panneerselvam**, K.R. Stephany, T.J. Magliery
- BIOL 205.** Modifying the stability of tumor suppressor p53 through S7-S8 loop mutagenesis as suggested by comparison of human and worm structures. **D.R. Bowles**
- BIOL 206.** Exploring the role of xCT in neuroregeneration through laser ablation of zebrafish neurons. **N.A. Ladd**, B.P. Krueger, L.A. Chase, A.P. Putzke
- BIOL 207.** Linking pH, temperature and conformation for the DNA I-motif. **R.D. Sheardy**, T. Sutorius, T. Nguyen, J. Dominguez
- BIOL 208.** Withdrawn.
- BIOL 209.** Mutagenicity and toxicity of DNA adducts repaired by the AlkB family repair enzymes. **F. Chen**, K. Bian, Q. Tang, D. Li
- BIOL 210.** Development of protein-based, folate directed photodynamic therapy agents. **R.N. Jones**, K. Kiernan, K.W. Olsen, S. Kanzok, R. Dale
- BIOL 211.** Investigating the binding interactions between ubiquitin c-terminal hydrolases and inhibitors. **J. An**, D. Xiao
- BIOL 212.** Biochemical characterization of neutral cholesterol ester hydrolase 1 (NCEH1), a membrane bound serine hydrolase. **A. Jemas**, M.M. Klems, B.J. Bahnson
- BIOL 213.** Synthesis and proteomic evaluation of novel peptidic inhibitors for the thrombin-induced activation of platelet aggregation. **C.C. Clement**, E.L. Ewul, A. Babinska, J. Gonzalez, M. Dzieciatkowska, E. Timpo, M.O. Salifu, M. Philipp
- BIOL 214.** Discovery of a new class of  $\beta$ -lactamase inhibitors. **J. Gonzalez**, J. Barquero, **C.C. Clement**, M. Philipp
- BIOL 215.** Riboflavin lyase: An intriguing flavoenzyme in the riboflavin catabolic pathway. **Y. Chakrabarty**, H. Xu, B. Phimus
- BIOL 216.** Withdrawn.
- BIOL 217.** Identification of critical binding interactions in Nod2, an innate immune receptor. **M. Lauro**, K. DeMeester, C. Hou, B.J. Bahnson, C.L. Grimes
- BIOL 218.** Biophysical characterization and solution NMR structure of J2-crystallin: A novel eye lens protein. **D. Khago**, R.W. Martin
- BIOL 219.** Protein-protein interactions in biological nitrogen fixation. **C. Owens**
- BIOL 220.** Direct encapsulation of functional proteins from mammalian plasma membranes into nanodisc libraries. **J. Roy**, H. Pondenis, T. Fan, A. Das
- BIOL 221.** Split spinach aptamer for fluorescent analysis of specific nucleic acids. **N. Kikuchi**, D. Kolpashchikov
- BIOL 222.** Role of the P27 tumor suppressor protein in cancer cell metabolism. **A. Alarbi**
- BIOL 223.** Functionalization of the bacterial cell wall utilizing peptidoglycan O-acetyltransferase B (PatB). **Y. Wang**, K. DeMeester, C. Hou, C.L. Grimes
- BIOL 224.** Lipoprotein structure dependency on its lipid cargo and exchange dynamics: Implications for atherosclerosis development. **S. Maric**, T. Lind, M. Cardenas
- BIOL 225.** Alternative HDAC3 and HDAC6 deacetylase activities and the structural activity relationship of a selective HDAC3 inhibitor. **C. Zhang**, E. Inks, J. McClure, **C. Chou**
- BIOL 226.** Linking gene expression with phospholipid vesicle formation in a recombinant system. **A. Bhattacharya**, N.K. Devaraj
- BIOL 227.** Testing the dimerization hypothesis of BACE1-GFP fusion protein in cultured cells using integrated fluorescence spectroscopy. **A.A. Heikal**, S. Gardeen, J.L. Johnson
- BIOL 228.** Activation of carbonic anhydrase and its role in enhancing memory and learning. **M.A. Ilies**
- BIOL 229.** FOX-4 cephamycinase: An analysis of structure and function. **S.T. Lefurgy**, V. Malashkevich, B. Biju, M.A. Noel, A. Rafalowski, A. Brodovskaya, E.C. Mundorff, J. Aguilan, E. Nieves, E. Caselli, F. Prati, R. Toro, S.C. Almo, K. Papp-Wallace, J. Frere, G. Bou, R.A. Bonomo
- BIOL 230.** Withdrawn.
- BIOL 231.** Withdrawn.
- BIOL 232.** Revving and listening to proteins with vortex fluids and carbon nanocircuits. **G.A. Weiss**, P.G. Collins, C.L. Raston, J. Britton, M.V. Akhterov, K. Peck, M. Iftikhar, L. Meneghini, T.Z. Yuan, C.F. Ormonde
- BIOL 233.** Controlling miRNA-like Off-target effects of an siRNA with nucleobase modifications. **R. Valenzuela**, A. Ball-Jones, S. Suter, J. Ibarra-Soza, P. Beal
- BIOL 234.** Antibacterial activity of the novel c5-curcumin-2-hexadecyloic acid conjugate. **D.J. Sanabria-Rios**, Y. Rivera-Torres, J. Rosario, R. Gutiérrez, Y. Torres-García, N. Montano, G. Ortiz-Soto, E. Rios-Olivares, J.W. Rodríguez, N.M. Carballeira
- BIOL 235.** Design and synthesis of pyridone luciferins for bioluminescence imaging. **B.S. Zhang**, D.C. McCutcheon, J.A. Prescher
- BIOL 236.** "Inside-out" site directed PEGylation of cross-linked hemoglobin. **C. Frosti**, D. Dahhan, K.D. Webster, W.L. Dean, J.B. Chaires, K.W. Olsen
- BIOL 237.** Toolkit to interrogate polyketide acyltransferase domains. **T.D. Davis**, J. Michaud, M.D. Burkart
- BIOL 238.** Does loss of glutathione with cell washing lead to increased cell death in the presence of oxidative compounds? **A.M. Khobeir**, J. White, J. Shultz, J.J. Cali, J. Kelts
- BIOL 239.** ROS-activatable agent elicits homologous recombination DNA repair and synergizes with pathway compounds. **F.S. Thowfeik**, S. Abdul Salam, E.J. Merino
- BIOL 240.** Evolution of phospholipases A<sub>2</sub> in catalysis and allosteric regulation by membranes. **V.D. Mouchlis**, J. McCammon, E.A. Dennis
- BIOL 241.** Mechanisms behind benzaldehyde suppression of the enzyme tyrosinase. **A. Murray**, I. Kubo
- BIOL 242.** Structure guided design of potent and selective inhibitors for RIPK1 linked to necroptotic cell death. **S. Ray**, A. Degterev, G.D. Cuny

## WEDNESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Marina Salon D

### RNA Structure & Function: Perspectives from Inside the Cell & Out

J. Wedekind, *Organizer, Presiding*

#### 9:00 Introductory Remarks.

**9:05** **BIOL 243.** Structural analysis of the dynamic *Schizosaccharomyces pombe* spliceosome using single particle cryo-electron microscopy. **E. Binshtein**, S. Collier, Y. Takizawa, **M. Ohi**

**9:40** **BIOL 244.** Revealing RNA structure-function relationships *in vivo* and genome-wide. **P.C. Bevilacqua**, Z. Su, L.E. Ritchey, Y. Tang, S.M. Assmann

**10:15** **BIOL 245.** RNA pathways dissected at the single molecule level: The power of integrating experimental and computational approaches. **N.G. Walter**

**10:50** **BIOL 246.** Combining chemistry and transcriptomics for a holistic view of RNA structure inside living cells. **R. Spitale**

**11:25** **BIOL 247.** How diverse RNA folds recognize a common metabolite to control protein translation in bacteria. **J. Wedekind**

## Section B

Marriott Marquis San Diego Marina  
Marina Salon E

**Young Investigators in Biological Chemistry**

V. Bandarian, *Organizer*

J. C. Jewett, *Presiding*

**9:00 BIOL 248.** Experimental and computational studies of the effects of highly concentrated solutes on proteins: Insights into the causes and consequences of quinary protein structure and cytoplasmic organization. L. Abriata, E. Spiga, M. Dal Peraro

**9:20 BIOL 249.** Small molecule and nucleic acid modulators of NF- $\kappa$ B p65. D.A. Harki, J.C. Widen, N.B. Struntz, K.T. Passow, A.M. Kempema

**9:40 BIOL 250.** Enzymatic incorporation and utilization of an emissive fluorescent 6-aza uridine. P.A. Hopkins, L.C. McCoy, Y. Tor

**9:55 BIOL 251.** Polymerization of peptides into high density brush polymers: A general strategy for conferring tunable protection from proteolysis and cellular uptake. A.P. Blum, J.K. Kammeyer, N.C. Gianneschi

**10:10 BIOL 252.** Using mechanistic cross-linkers to study the substrate selectivity and protein-protein interactions of the *E. coli* fatty acid dehydratase, FabA. K. Finzel, C. Nguyen, D.R. Jackson, A. Gupta, S. Tsai, M.D. Burkart

**10:25 BIOL 253.** General method for analysis of nucleic acid structures by deoxyribozyme sensors. R.J. Karadeema

10:40 Intermission.

**10:50 BIOL 254.** Solution-state NMR structure and biophysical characterization of the *Ciona intestinalis*  $\beta$ -crystallin, an ancestral eye lens protein. N. Koziyuk, R.W. Martin

**11:05 BIOL 255.** Inhibitory effects of H69-targeting peptides on protein translation in bacteria. N. Muthunayake, C.S. Chow

**11:20 BIOL 256.** Chemical biology approaches to combat Parkinson's disease. F. Nwogbo, K. Alser, B.D. Bradaric, L. Olivere, D.G. McCafferty

**11:35 BIOL 257.** Integrative computational modeling reveals the intricacies of the two-metal-aided mechanism. G. Palermo, L. Casalino, A. Magistrato, U. Roethlisberger

**11:50 BIOL 258.** Chemical proteomic approaches to discover and characterize lysine acetyltransferase biology. D.C. Montgomery, J.L. Meier, A. Sorum

**12:05 BIOL 259.** Ligand-responsive viral RNA switches: Simple conformational switching modules in noncoding RNA. M.A. Boerneke, T. Hermann

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## Computer-Aided Drug Design

## Real World Dynamics

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

**Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory**

## The World of Vibrations

*Sponsored by PHYS, Cosponsored by BIOL*

## WEDNESDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
Marina Salon D

**Goodman Award: Symposium in honor of Joan Steitz**

*Financially supported by Biopolymers*

J. Steitz, *Organizer, Presiding*

2:00 Introductory Remarks.

**2:05 BIOL 260.** CRISPR-Cas9 genome engineering revolution. J.A. Doudna

**2:50 BIOL 261.** Overarching U1 snRNP-controlled gene expression mechanism. G. Dreyfuss

**3:35 BIOL 262.** PRC2, long noncoding RNAs and epigenetic silencing. C. Davidovich, X. Wang, K. Goodrich, A. Gooding, K. Luger, T.R. Cech

**4:20 BIOL 263.** RNA triple helices in cellular and viral biology. J. Steitz

## Multiscales Chemistry

## Sustainable

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

## Computer-Aided Drug Design

## New Modalities RNA

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

## THURSDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Marina Salon D

**Young Investigators in Biological Chemistry**

V. Bandarian, *Organizer*

L. Saleh, *Presiding*

**9:00 BIOL 264.** Elucidating the Role of Deamidation in human  $\gamma$  s-crystallin. K. Roskamp, J. Ceballos, R.W. Martin

**9:15 BIOL 265.** Targeting protein-protein interactions for disruption of KDM1A (LSD1) complexes. J. Link, S. Hwang, J. Burg, S. Wardell, D.G. McCafferty

**9:30 BIOL 266.** Trapping of the enoyl-acyl carrier protein reductase and acyl carrier protein interaction. L. Tallorin, K. Finzel, Q. Nguyen, J. Beld, J.J. La Clair, M.D. Burkart

**9:45 BIOL 267.** RNA-TAG as a platform for the identification of RNA-protein interactions. K.N. Busby, S.C. Alexander, N.K. Devaraj

**10:00 BIOL 268.** Probing binding interactions of agonists at a nicotinic acetylcholine receptor subtype important to addiction and Parkinson's disease. M.R. Post, H. Lester, D.A. Dougherty

**10:15 BIOL 269.** Structure and function of fusicoccadiene synthase, a bifunctional diterpene synthase with an alpha-alpha fold. M. Chen, D.W. Christianson

**10:30 BIOL 270.** Magnetic isolation of respiration active mitochondria using Mito-magneto. B. Banik, S. Dhar

10:45 Intermission.

**11:00 BIOL 271.** Unusual Lys-to-Trp cross-link catalyzed by a radical SAM enzyme. K. Schramma, M. Seyedsayamdoost

**11:15 BIOL 272.** Design and synthesis of triazabutadiene-based fluorogenic probe for tyrosine-specific labeling of proteins. M. Shadmehr, J.C. Jewett

**11:30 BIOL 273.** BluRph: A genetically targetable, far-red ratiometric pH sensor to study lysosomal trafficking. M. Naganbabu, L.A. Perkins, M.P. Bruchez

**11:45 BIOL 274.** Determination of cold adaptation in Antarctic toothfish lens proteins by structural comparison. J. Bierma, C. Kingsley, R.W. Martin

**12:00 BIOL 275.** Development of novel luciferin-luciferase pairs for multicomponent imaging. W.B. Porterfield, C.M. Rathbun, D. McCutcheon, K. Jones, J.A. Prescher

**12:15 BIOL 276.** Enzymatic characters of apoptosis signaling-kinase 1. J.M. Pleinis, D. Qiu, C. Cantrell, X. Zhan

## Big Data Science

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

## Computer-Aided Drug Design

## New Modality Therapeutics

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

## BMGT

**Division of Business Development and Management**

D. Daly, *Program Chairs*

## OTHER SYMPOSIA OF INTEREST:

**Computers in Chemistry** (see MPPG, Sun)

**Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications** (see COMP, Sun, Mon)

**Computers in Chemistry: Bridging the Gap between Clients & Software** (see SCHB, Mon)

## SOCIAL EVENTS:

**Symposium, 2:00 PM: Sun**

## SUNDAY AFTERNOON

## Section A

The Westin San Diego Gaslamp Quarter  
Balboa

**Current Topics in Chemical Business Development & Management**

*Cosponsored by MPPG‡*

J. L. Bryant, *Organizer*

D. T. Daly, *Organizer, Presiding*

**1:30 BMGT 1.** Business of sharing crystal structures. S. Ward, I. Bruno, C. Groom

**2:00 BMGT 2.** Capturing student interest with digital course materials. A. Campbell

**2:30 BMGT 3.** Development of a chemical drawing program that provides scientifically correct and engaging first impression for students. A.D. Costache

3:00 Intermission.

**3:15 BMGT 4.** Software to guide decision-making in compound optimization. M.D. Segall

**3:45 BMGT 5.** ADF modeling suite for Software for Chemistry & Materials aka Scientific Computing & Modelling. F. Goumans

**Discussions with the President's Task Force on Employment**

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

**Industrial Research at the Interface of Inorganic Chemistry & Polymer Science**

*Sponsored by POLY, Cosponsored by BMGT and INOR‡*

## SUNDAY EVENING

**My Comments to the President's Task Force on Employment**

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

## MONDAY MORNING

**Women in Innovation: Science & Technology**

*Sponsored by PROF, Cosponsored by BMGT‡ and WCC‡*

## MONDAY AFTERNOON

**Industrial Innovation in Polymer Chemistry: Sustainable Polymerization Feedstocks & Process Technology**

*Sponsored by POLY, Cosponsored by BMGT*

## TUESDAY AFTERNOON

## Chemical Angel Network

*Sponsored by PROF, Cosponsored by BMGT and SCHB*

## TUESDAY EVENING

**Industrial Research at the Interface of Inorganic Chemistry & Polymer Science**

*Sponsored by POLY, Cosponsored by BMGT and INOR‡*

## Division of Carbohydrate Chemistry

N. Snyder, Program Chair

### OTHER SYMPOSIA OF INTEREST:

**Biomedical & Drug Delivery Applications of Polysaccharide-Based Materials** (see CELL, Wed, Thu)

**Functional Lignocellulosics & Nanotechnology** (see CELL, Sun, Mon, Tue, Wed)

**Chemistry in Service of Biology: Tools for Probing Cellular Processes** (see BIOL, Tue)

**Frontiers in Biomolecular Recognition: From Materials to Cells** (see BIOL, Mon)

### SOCIAL EVENTS:

Dinner, 6:30 PM: Mon

### BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Sun

## SUNDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Marina Salon F

#### Wolfrom Award

Cosponsored by AGRO

N. L. Snyder, Organizer

X. Huang, Organizer, Presiding

**9:00 CARB 1.** Us versus them: A lectin as a microbial cell surface detector. L.L. Kiessling

**9:40 CARB 2.** Chemoenzymatic glycoengineering of antibodies: Enzyme substrate specificity is the name of the game. L. Wang

**10:20 CARB 3.** Nanoparticles with siglec ligands for modulating immune responses. J.C. Paulson, S. Duan, M.S. Macauley, R. McBride, C. Nycholot, L. Pang, W. Peng

### Functional Lignocellulosics & Nanotechnology

#### Lignocellulosics & Nanotechnology

Sponsored by CELL, Cosponsored by CARB

## SUNDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Marina Salon F

#### Isbell Award

X. Huang, Organizer

N. L. Snyder, Organizer, Presiding

**1:30 CARB 4.** Molecular recognition of *Brucella* A and M antigens dissected by synthetic oligosaccharide glycoconjugates. D.R. Bundle, N. Ganesh, S. Mandal, S. Sarkar, J. Sadowska, J. McGiven

**2:00 CARB 5.** Fluorescence-quenched substrates for live cell imaging of endogenous human glucocerebrosidase activity. D.J. Vocadlo

**2:30 CARB 6.** Production and inhibition of the polysaccharide intercellular adhesin. B. Difrancesco, A. Forman, R. Ariyakumaran, M. Nitz

### Section A

Marriott Marquis San Diego Marina  
Marina Salon F

#### Gin New Investigator Award

X. Huang, Organizer

N. L. Snyder, Organizer, Presiding

**3:15 CARB 7.** Total synthesis of periploside A, a steroid hexasaccharide containing a unique formyl acetal bridged orthoester linkage. B. Yu

**3:45 CARB 8.** Sweet interplay between *Helicobacter pylori* and gastric epithelial cell. C.H. Lin

**4:15 CARB 9.** Chemical tools for probing glycosylation dynamics *in vivo*. X. Chen

### Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

### Functional Lignocellulosics & Nanotechnology

#### Surface Interactions on Lignocellulosic Materials

Sponsored by CELL, Cosponsored by CARB

## SUNDAY EVENING

### My Comments to the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## MONDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Miramar Room

#### Glycosylases: Inhibition & Therapeutic Applications

Cosponsored by CELL  
Financially supported by Shimadzu Scientific Instruments, Inc; P212121, LLC

D. Ronning, S. Strigler, S. J. Sucheck, Organizers

S. Strigler, Presiding

#### 8:30 Introductory Remarks.

**8:35 CARB 10.** General mass-spectrometry-based assays for full characterization of glycosidase substrate specificity. N.L. Pohl

**9:05 CARB 11.** Assessing GlgE structures to inform inhibitor design and tuberculosis drug development. D. Ronning

**9:35 CARB 12.** Generation of brain active O-GlcNAcase inhibitors for use in preclinical animal models. D.J. Vocadlo

**10:05 CARB 13.** Explore series of Gluco-configured tetrahydroimidazopyridines as new pharmacological chaperones for Gaucher disease. P.G. Wang, J. Li, W. Zhao

**10:35** Intermission.

**10:50 CARB 14.** Utilizing an iminosugar-based glycosidase inhibitor as a pharmacological chaperone to treat the lysosomal storage disorder, Fabry disease. K. Valenzano

**11:20 CARB 15.** Chemical tools to probe the role of human neuraminidase enzymes in cell adhesion. C.W. Cairo

**11:50 CARB 16.** Will imino sugars always be the broad acting antiviral drugs of the future? T. Block

### Functional Lignocellulosics & Nanotechnology

#### Lignocellulosic Nanomaterials & Their Applications

Sponsored by CELL, Cosponsored by CARB

## MONDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Miramar Room

#### Glycosylases: Inhibition & Therapeutic Applications

Cosponsored by CELL  
Financially supported by Shimadzu Scientific Instruments, Inc; P212121, LLC

D. Ronning, S. Strigler, Organizers

S. J. Sucheck, Organizer, Presiding

**1:30 CARB 17.** 1-Deoxynojirimycin (DNJ) and pyrrolizidine derivatives as glycosidase inhibitors. L. Cipolla, F. Cardona, B. La Ferla, P. Fusi

**2:00 CARB 18.** Galactonoamides as inhibitors of glycosylases. S. Strigler, Q. Fan, J.B. Pickens

**2:30 CARB 19.** Thio-linked glycoside ketones and heterocycles as new generation of glucosidase inhibitors. Z.J. Witzczak

#### 3:00 Intermission.

**3:10 CARB 20.** Synthesis of pyrrolidine *N*-alkyl-phosphonates: Transition state inhibitors of *S. coelicolor* GlgE-V279S. S.K. Valetti, J.J. Lindenberger, D. Ronning, S.J. Sucheck

**3:35 CARB 21.** Synthesis of steryl glycoside analogs to study glycolipid biology. J. Gervay-Hague

**4:05 CARB 22.** NAD glycohydrolase (CD38): A cell regulatory NAD(P) transglycosidase useful for the chemoenzymatic synthesis of pyridine dinucleotide analogs. J.T. Slama, R. Ali, T. Astfaha, D. Andy, D.R. Giovannucci, K.A. Wall, T. Walseth

**4:35 CARB 23.** Proton transfer and hydrogen bonding in glycosylation reactions. D.M. Whitfield

### Functional Lignocellulosics & Nanotechnology

#### Lignocellulosic Nanomaterials & Their Applications

Sponsored by CELL, Cosponsored by CARB

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

N. L. Snyder, Organizer

8:00 - 10:00

37, 39-41, 45-46, 48-50, 52, 55, 57-58, 60, 62, 66, 71, 76-77, 79. See subsequent listings.

## TUESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Marina Salon F

#### Carbohydrate Research at Predominantly Undergraduate Institutions

Cosponsored by CELL

N. L. Snyder, Organizer, Presiding

#### 8:30 Introductory Remarks.

**8:35 CARB 24.** Drug discovery at primarily undergraduate institutions: From choosing an appropriate target to encouraging student-led research design. R.L. Woodward, M. Simpson, A. Dragan, A. Greenwell, E. Loosli, C. Holmes

**9:05 CARB 25.** Breaking down the wall: Small molecule inhibitors of bacterial N-acetylglucosaminidases as chemical probes and antimicrobials. C. Reid

**9:35 CARB 26.** Functional amphiphilic polymeric materials from starch synthons. A. Sengupta, A.R. Linehan, L.M. Ryno, J. Nettleton, P.M. Iovine

#### 10:05 Intermission.

**10:15 CARB 27.** Glycans in pathogenic bacteria – potential for selective targeting. D.H. Dube

**10:45 CARB 28.** Chemoenzymatic synthesis of trehalose analogs for targeting mycobacteria. P. Woodruff

**11:15 CARB 29.** Adventures in carbohydrate chemistry. N.L. Snyder

#### 11:45 Concluding Remarks.

### Functional Lignocellulosics & Nanotechnology

#### Dispersions, Gels, Foams, Colloids, Films

Sponsored by CELL, Cosponsored by CARB

## TUESDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Marina Salon F

#### Carbohydrate Research at Predominantly Undergraduate Institutions

Cosponsored by CELL

N. L. Snyder, Organizer, Presiding

#### 1:30 Introductory Remarks.

**1:35 CARB 30.** Examples of metabolic labeling of cancer cell and virus glycosylation with azido sugars. L. Cai, Q. Wang

**2:05 CARB 31.** Trehalose analogues: New synthetic methods and applications in mycobacteria research. B. Swarts, P. Woodruff

**2:35 CARB 32.** Synthetic studies of luteo-side B. J.L. Koviach-Cote, A. Jones

#### 3:05 Intermission.

**3:15 CARB 33.** Design of and synthetic progress toward a novel C-linked GalNAc- $\alpha$ -serine. E.G. Nolen

**3:45 CARB 34.** Towards a better understanding of the O-4 effect in sialylation reactions. C. De Meo

- 4:15 CARB 35.** 2,3-Oxazolidinone derivatives of 2-allylamine, 2-gulosamine, 2-mannosamine, and 2-talosamine via intramolecular metallanitrene additions of all four D-glycal 3-carbamate diastereomers. **C.M. Rojas**
- 4:45 CARB 36.** Incorporating carbohydrates into the undergraduate laboratory. **J.S. Rhoad, K. Cooper, M. Edlin, N. Chapman**
- 5:15 Concluding Remarks.**

## TUESDAY EVENING

### Section A

San Diego Convention Center  
Hall D

#### General Posters

N. L. Snyder, *Organizer*

**7:00 - 9:00**

- CARB 37.** Synthesis of carbohydrate phthalocyanine conjugates. **S.A. Cooper, G. Cambroner, R.Q. Wiggins, N.L. Snyder**
- CARB 38.** Progress towards the synthesis of alpha-1,4-linked fungal galactosylaminoglycans. **E.W. Watkins, N.L. Snyder**
- CARB 39.** Modular synthesis of the repeating tetrasaccharide subunit of *Streptococcus pneumoniae* serotype 8. **A. Mason, N.L. Snyder**
- CARB 40.** Comparison of covalent delivery methods for immune-mediated targeting of *Helicobacter pylori*. **J.E. Feldman, D.H. Dube**
- CARB 41.** Glycan-based strategy for selectively targeting *Helicobacter pylori*. **K.L. Krupp, E. Clark, I. Kline, D.H. Dube**
- CARB 42.** Analysis of glycoproteins in *Helicobacter pylori* overexpressed in the presence of host cells. **J. Muscato, D.H. Dube**
- CARB 43.** Addition of basic sites to the glycans of *Helicobacter pylori* to increase MS/MS peak abundance. **H.S. Miller, D.H. Dube, E.A. Stemmler**
- CARB 44.** Reduction of sugar lactones to lactols with lithium triethylborohydride. **C. Gonzalez, S. Kavooosi, A. Sanchez, S.F. Wnuk**
- CARB 45.** Genetically-encoded fragment-based discovery of glycopeptide ligands for carbohydrate-binding proteins. **R. Derda**
- CARB 46.** Dynamic kinetic transformations of lactols for *de novo* synthesis of carbohydrate. **H. Wang, W. Tang**
- CARB 47.** One-step chemoenzymatic synthesis of trehalose analogues. **L.M. Meints, A.W. Poston, Z. Wagar, B. Urbanek, I. Lopez-Casillas, B.M. Swarts**
- CARB 48.** Withdrawn.
- CARB 49.** Sulfation pattern dictates the conformation of heparan sulfate. **P. Hsieh, D.F. Thieker, M. Guernini, J. Liu**
- CARB 50.** New old favorite: Glycosylations using septanosyl bromides as donors. **A. Pote, R. Vannam, M. Peczu**
- CARB 51.** Reaction mechanism of the rhodium-catalyzed arylation of fullerene with organoboron compounds in water. **A. Poater, J. Martinez**
- CARB 52.** Quality control of cell based on the binding pattern of sugar chain-immobilized fluorescent nanoparticles (SNFPs). **H. Shinchi, T. Nakamura, M. Wakao, Y. Suda**
- CARB 53.** Withdrawn.
- CARB 54.** Synthesis and conformational analysis of fluorine-modified trehalose analogues. **S. Rundell, Z. Wagar, L.M. Meints, A.W. Poston, B. Piligian, C. Olson, B.M. Swarts**
- CARB 55.** Expanding the scope of a chemoenzymatic method for the synthesis of trehalose analogue. **C. Olson, L.M. Meints, A.W. Poston, B. Piligian, B. Swarts**
- CARB 56.** Cellular microarray strategy for the investigation of glycosaminoglycan-protein interactions as they relate to stem cell differentiation. **G.W. Triege, K. Krug, A. Michalak, M. Huang, K. Godula**
- CARB 57.** Novel 1→6- & 6→6-linked ester disaccharide analogs – synthesis and structural evaluation. **S. Hackbusch, A. Franz**
- CARB 58.** Development of Karplus equations for 1,6-linked disaccharides. **A. Watson, A. Franz**
- CARB 59.** Identification of a versatile fucosidase for glycoprotein remodeling and glycan sequencing. **T. Tsai, C. Wong**
- CARB 60.** Synthesis of carbohydrate modified analogues of  $\alpha$ -galactosylceramide for NKT cell activation. **D. Chennamadhavuni, S.K. Richardson, A. Saavedra, L. Carreno, W. Yuan, S.A. Porcelli, A.R. Howell**
- CARB 61.** Investigating the substrate specificity of the trehalose-recycling transporter SugABC-LpQY. **M. O'Neill, Z. Wagar, L. Meints, B. Urbanek, B. Swarts**
- CARB 62.** Targeting cancer cell metabolism using N-glycoconjugate based small-molecule modulators of reactive oxygen species. **F. Ndombera**
- CARB 63.** Modular synthesis of N-glycans for homogeneous and mixed-glycan arrays to study hetero-ligand binding of HIV-1 broadly neutralizing antibodies. **C.Y. Wu, S.S. Shivatare, C. Wong**
- CARB 64.** Synthesis of chondroitin sulfate partial structure and interaction analysis with GAG-binding proteins by SPR imaging. **M. Wakao, K. Miyachi, Y. Ichiki, Y. Suda**
- CARB 65.** Synthesis of sulfatide ligands for type II NKT cell activation. **K. Luvaga, K. Camara, S.K. Richardson, E.C. Kanyo, M. Terabe, J. Berzofsky, A.R. Howell**
- CARB 66.** Carbon-linked cyanogenic glycosides as potential non-lethal pesticides. **G. Gutierrez, K.V. Waynant**
- CARB 67.** Chemical synthesis of azido inositols via Ferrier rearrangement. **M. Hogue, S. Rundell, C.J. Wilson, B.M. Swarts**
- CARB 68.** Development of a liposome based assay for Lipid II and analog translocation by flippase MurJ. **H. Wang, K. Chen, W. Cheng, P. Liang**
- CARB 69.** Synthesis of GPI-0100 based saponin derivatives as potent vaccine adjuvants. **Y. Lai, P. Liang**
- CARB 70.** Is there a structural role for 3-O-sulfation in heparan sulfate? **A. Green, C.K. Larive**
- CARB 71.** Synthesis and evaluation of dinutrophenyl-modified trehalose analogues for the delivery of antibody-recruiting small molecules (ARMs) to mycobacteria. **A. Rylski, B. Swarts**
- CARB 72.** Catalytically promoted glycosylation for the synthesis of O- and S- linked glycolipids. **D. Hanrahan, R. Palos Pacheco, L. Szabo, L.L. Kegel, J.E. Pemberton, R.L. Pelt**
- CARB 73.** Inulin is immunogenic as shown by development of an immunoassay for inulin. **E.V. Groman**
- CARB 74.** Bioorthogonal chemical reporters for selective *In Situ* probing of mycomembrane components in mycobacteria. **H. Foley, J.A. Stewart, H.W. Kavunja, S. Rundell, B.M. Swarts**
- CARB 75.** Development of carbon-linked glycosides of threonine and serine: A synthetic approach to study the *in vivo* effects of glycosylation on alpha-synuclein. **C. Deleon, M. Pratt**
- CARB 76.** Effect of monochloroacetyl in sialylation reactions. **C. De Meo, S. Aalaei, C. Yu**
- CARB 77.** Applying hydrogen-bond-mediated aglycone delivery (HAD) in sialylations: Scope and limitations. **C. De Meo, S. Geringer, F. Najafi Khosroshahi**
- CARB 78.** Withdrawn.
- CARB 79.** Stereoselective synthesis of  $\beta$ -mannopyranosides via anomeric O-alkylation. **H.P. Nguyen, J. Zhu**
- CARB 80.** Chemical and structural characterization of xylans from sugarcane bagasse and sugarcane straw. **D.M. Carvalho, A. Martinez Abad, J. Colodette, M.E. Lindström, F. Vilaplana, O. Sevastyanova**
- CARB 81.** Glycocalyx based strategies to modulate embryonic stem cell fates. **M. Huang, K. Godula, R. Smith, M. Christy, C.J. Fisher, A. Michalak**
- CARB 82.** Withdrawn.
- CARB 83.** Glycolipids as ancient weapons for mycobacteria against humans and potential weapons for humans against mycobacteria. **T. Houston, T. Mosaib, D. Farr, S. Boiteux, I.D. Grice, M.J. Kiefel**
- CARB 84.** Design and synthesis of a new class of oligomannose immunogens for recapitulation of the 2G12 HIV epitope. **C. Toonstra**
- CARB 85.** Superabsorbent cellulose-clay nanocomposite hydrogels for hygienic application. **C. Chang, N. Peng, L. Zhang**
- CARB 86.** Withdrawn.
- CARB 87.** Withdrawn.
- CARB 88.** Green avenue for dehydration of biomass using alternative technologies. **C. Len, S. Le Guenic, C. Ceballos, F. Delbecq**
- CARB 89.** Subtle structural changes effect the metabolic fate of four different chemical reporters of glycosylation. **A. Batt, M. Pratt**
- CARB 90.** Optimization of O-GlcNAc chemical reporter allows identification of proteins implicated in cell death. **K.N. Chuh, A. Batt, C. Brennan, M. Pratt**

**10:00** Intermission.

**10:15 CARB 94.** Chemical-genetics strategy to identify covalent cysteine-reactive small molecules. **E. Weerapana**

**10:45 CARB 95.** Metal free click reactions for glycoconjugate modification. **G. Boons**

### Section B

Marriott Marquis San Diego Marina  
San Diego Ballroom B

#### From mAb to ADCs: Tailored Antibodies & Dedicated Chemistry Technologies for Site Specific ADCs

*Cosponsored by MEDI*

O. J. Marcq, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:40 CARB 96.** Preparation of well-defined antibody-drug conjugates through glycan remodeling and strain promoted azide-alkyne cycloadditions. **G. Boons**

**9:05** Discussion.

**9:10 CARB 97.** Developing site-specifically modified ADCs using a chemoenzymatic approach. **D. Rabuka**

**9:35** Discussion.

**9:40 CARB 98.** Antibodies conjugated through glycans to small molecule drugs: Stability and specific killing of cancer cells. **D. Dimitrov, Y. Feng, R. Sussman, J. Maris, S. Smith, S. Degrado, N. Jain, Z. Zhu**

**10:05** Discussion.

**10:10** Intermission.

**10:25 CARB 99.** Glycan-conjugation of payloads to MAbs enables ADCs with improved therapeutic index. **R. van Geel, M. Wijdeven, J. Verkade, B. Janssen, S. van Berkel, A. DeBoer, F. van Delft**

**10:50** Discussion.

**10:55 CARB 100.** Site-specific conjugation of monomethyl auristatin E to anti-CD30 antibodies improves their pharmacokinetics and therapeutic index in rodent models. **F. Lhospice, B. Delphine, B. Christian, P. Drenner, E. Fischer, L. Gauthier, H. Rispaud, S. Savard, A. Represa, C. Bonnafous, R. Schibli, F. Romagne**

**11:20** Discussion.

**11:25 CARB 101.** Activation of innate immune cells with antibody conjugates of a fungal derived pathogen associated molecular pattern molecule, Imprime PGG. **M.E. Danielson, K.S. Michel, P.M. Will, R.B. Fulton, S.M. Leonardo, X. Qiu, A. Bykowski Jonas, B.C. Harrison, K.B. Gordon, N. Bose, A.S. Magee, J.R. Graff**

**11:50** Discussion.

**11:55** Panel Discussion.

## WEDNESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Marina Salon F

#### Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Symposium in honor of Professor Sharpless's 75th Birthday

*Cosponsored by CELL*

P. Wu, *Organizer, Presiding*

**8:30 CARB 91.** Click chemistry: History and new directions. **P. Wu**

**9:00 CARB 92.** Click chemistry for diagnostic and therapeutic glycoconjugates: *In Vivo* pattern recognition using "strong" and "weak" interactions. **K. Tanaka**

**9:30 CARB 93.** Thio-click tools and coupling strategies for synthesis of carbohydrate glycomimetics. **Z.J. Witzcak**

## WEDNESDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
Marina Salon F

**Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Symposium in honor of Professor Sharpless's 75th Birthday**

*Cosponsored by CELL*

P. Wu, *Organizer*

J. Dong, *Presiding*

**1:30 CARB 102.** Sulfur(VI) fluoride exchange (SuFEx): Another good reaction for click chemistry. Q. Zheng, J. Dong, P. Wu, K.B. Sharpless

**1:45 CARB 103.** Beyond orthogonality: Sulfur(VI) Fluoride Exchange (SuFEx), another good reaction for click chemistry. J. Dong

**2:15 CARB 104.** Chemical editing of cell-surface glycan structures to control cellular responses. K. Godula

**2:45 CARB 105.** Leveraging click reactions for the efficient synthesis of polymers with absolute control over mass, sequence, and stereochemistry. J.C. Barnes, D.J. Ehrlich, Y. Jiang, F.A. Leibfarth, T.F. Jamison, J.A. Johnson

**3:15** Intermission.

**3:35 CARB 106.** Post-polymerization modification of polymer brushes. J.J. Locklin

**4:05 CARB 107.** Bioorthogonal chemistry. C. Bertozzi

**Biomedical & Drug Delivery Applications of Polysaccharide-Based Materials**

**Wound Care, Antimicrobial Surfaces, Point-of-Care Diagnostics**

*Sponsored by CELL, Cosponsored by CARB*

**Functional Lignocellulosics & Nanotechnology**

**Paper: Fundamentals & Applications**

*Sponsored by CELL, Cosponsored by CARB*

## THURSDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Marina Salon F

**Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Symposium in honor of Professor Sharpless's 75th Birthday**

*Cosponsored by CELL*

P. Wu, *Organizer*

H. Wang, *Presiding*

**8:30 CARB 108.** Precise redox responses imprinted by on-demand redox targeting. Y. Aye

**9:00 CARB 109.** Self-reproducing catalysts capable of driving repeated phospholipid membrane synthesis and growth. N.K. Devaraj

**9:30 CARB 110.** Proteome reactivity of arylfluorosulfates. J.W. Kelly

**10:00** Intermission.

**10:15 CARB 111.** What click chemistry has taught us about cellular protein synthesis. D.A. Tirrell, B.M. Babin, S. Stone, K.P. Yuet

**10:45 CARB 112.** Chemistry and biology of glycosylation: Epitope identification and cancer vaccine development. C. Wong

**Biomedical & Drug Delivery Applications of Polysaccharide-Based Materials**

**Hydrogels, Regenerative Medicine, Tissue Engineering**

*Sponsored by CELL, Cosponsored by CARB*

## CATL

**Division of Catalysis Science and Technology**

E. Nikolla and K. Ramasamy, *Program Chairs*

**OTHER SYMPOSIA OF INTEREST:**

**Structure, dynamics and reactivity at complex interfaces with relevance in renewable energy and environmental applications** (see COMP, Sun, Mon)

**ENFL Distinguished Researcher Award: Symposium in honor of Stu Soled** (see ENFL, Mon, Tue)

**CO<sub>2</sub> Conversion & Utilization** (see ENFL, Mon, Tue, Wed)

**Application of Computational Chemistry for Energy & Fuel Production** (see ENFL, Tue, Wed, Thu)

**George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in honor of Mieczysław M. Boduszynski** (see ENFL, Wed)

**In Situ & Operando Characterization & Modeling of Reaction Kinetics** (see ENFL, Wed, Thu)

**BUSINESS MEETINGS:**

**Business Meeting, 5:30 PM:** Mon

## SUNDAY MORNING

## Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom B

**Amorphous Catalytic Materials**

B. Peters, S. L. Scott, *Organizers, Presiding*

**8:00 CATL 1.** Atomic scale understanding of Bronsted acidity and cracking activity of amorphous silica alumina using density functional theory. P. Raybaud, C. Chizallet

**8:35 CATL 2.** Long timescale simulations of diffusion and reactions in and on the surface of disordered solids. H. Jonsson

**9:10 CATL 3.** Systematic framework for modeling isolated catalyst sites on amorphous supports. B.R. Goldsmith, S. Seritan, E. Sanderson, S.L. Scott, B. Peters

**9:30 CATL 4.** Mechanistic approach to the characterization of surface sites on transitional aluminas. M. Kang, J. DeWilde, A. Bhan

**9:50** Intermission.

**10:10 CATL 5.** Characterization of amorphous silica based catalysts and materials using DFT computational methods. F. Tielens

**10:45 CATL 6.** Fundamentals of amorphous silica catalyst supports. K. Johnson, C. Ewing, A. Bagusetty, E. Patriarca, D. Lambrecht, G. Vesser, J.J. McCarthy

**11:20 CATL 7.** DMMP reactivity on zirconium hydroxide under in operando conditions. P. Pehrsson, W. Gordon, R. Balow, D. Barlow, V.M. Bermudez, I. Iordanov, C. Knox, J. Lundin, J.H. Wynne, C.J. Karwacki, G.W. Peterson

**11:40 CATL 8.** Activation of the Phillips polymerization catalyst by ethylene oxidative addition followed by homolysis: A computational assessment. A. Fong, S.L. Scott, B. Peters

## Section B

Manchester Grand Hyatt San Diego  
Coronado A

**Catalytic Materials for Methane Conversion**

*Cosponsored by ENFL*

B. A. Kilos, S. Linic, E. Nikolla, *Organizers, Presiding*

**9:00** Introductory Remarks.

**9:05 CATL 9.** Mechanistic insights into the catalytic conversion of methane over supported catalysts. M. Neurock

**9:50 CATL 10.** Metal-lattice oxygen site pairs in four-centered C-H bond activation of methane. J. Varghese, Q. Trinh, S. Mushrif

**10:15 CATL 11.** Enhancing light olefin selectivity in methanol-to-hydrocarbons conversion by co-feeding oxygenates. R. Khare, S.S. Arora, A. Bhan

**10:40** Intermission.

**11:00 CATL 12.** Structure-property relationships of palladium-catalyzed methane complete combustion using uniform nanoparticles. J. Willis, E. Goodman, M. Carnello

**11:25 CATL 13.** CO<sub>2</sub> conversion through methane reforming under visible light: Surface plasmon mediated nonpolar molecule activation. H. Liu

**11:50** Concluding Remarks.

## Section C

Manchester Grand Hyatt San Diego  
Harbor Ballroom C

**Computational Chemistry Across Catalysis**

**Modeling Complex Reaction Networks in Catalysis**

*Cosponsored by COMP, ENFL and WCC*  
*Financially supported by SCF*

A. W. Goetz, C. Michel, *Organizers*

P. Sautet, D. G. Vlachos, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 CATL 14.** Mechanistic study of zeolite catalyzed dehydration of bio-alcohols: Density functional theory and microkinetic analysis. G.B. Marin

**8:45 CATL 15.** Joint kinetics: New relationships between thermodynamic and kinetic characteristics with catalytic applications. G.S. Yablonsky, D. Constales, D. Branco-Pinto, G.B. Marin

**9:05 CATL 16.** Steady state kinetics of any catalytic network: Graph theory, the energy span model, the analogy between catalysis and electrical circuits, and the meaning of "mechanism". S. Kozuch

**9:25 CATL 17.** Alcohol dehydration kinetics over various zeolites using experimental and theoretical methods for catalytic fast pyrolysis. S. Kim, L. Kunz, R. Cywar, R. McDonough, L. Bu, M.R. Nimlos, R.S. Paton, D. Robichaud

**9:45** Intermission.

**9:55 CATL 18.** Unravelling the complexity of catalytic kinetics: Computational method development, applications, and perspective. M. Stamatakis

**10:35 CATL 19.** Withdrawn.

**10:55 CATL 20.** Dynamic steady-state detection with throttling in lattice kinetic Monte Carlo to increase computational efficiency of spatial chemical kinetics simulations. A. Savara, T. Danielson, C. Hin

**11:15 CATL 21.** Investigation of industrial NH<sub>3</sub> oxidation by computational fluid dynamics simulations including detailed surface kinetics. A. Wisler, M. Klingenberger, A. Drochner, H. Vogel, M. Votsmeier

**11:35 CATL 22.** Theoretical study of the reaction mechanism and structure sensitivity of the hydrodeoxygenation of propanoic acid over Pd catalysts in vapor and liquid phase environments. E. Walker, R. Solomon, S. Behtash, A. Heyden

**11:55** Concluding Remarks.

## Section D

Manchester Grand Hyatt San Diego  
Coronado B

**Fundamental Surface Chemistry of Non-oxide Transition Metal Ceramic Catalysts: Carbides, Nitrides, Sulfides, Phosphides, Selenides**

*Cosponsored by ENFL*

S. Laursen, N. M. Schweitzer, *Organizers, Presiding*

**8:00 CATL 23.** Lattice nitrogen reactivity in Co<sub>2</sub>Mo<sub>2</sub>N catalysts: Understanding the role of surface structure and composition through application of depth resolved XPS and computational modelling. J.S. Hargreaves, A. McFarlane, C.A. Catlow, C.D. Zeinalipour-Yazdi, W.R. Flavell, M. Leontiadou, H. Radtke

**8:40 CATL 24.** Vapor-phase upgrading over oxophilic molybdenum carbide catalysts: From model compounds to biomass pyrolysis vapors. J.A. Schaidle, C. Nash, C. Mukarakate, M. Griffin, C. Farberow, J. Blackburn, K. Steirer, D. Robichaud, D. Ruddy

**9:00 CATL 25.** Surface characterization of iron-nickel phosphides to understand their role in prebiotic phosphorylation. H.L. Abbott-Lyon, D. Qasim

**9:20 CATL 26.** Photocatalyst sheets based on non-oxide particulate semiconductors. K. Dömen

**10:00 CATL 27.** Understanding the role of surface chemical reactivity in CO<sub>2</sub> photoreduction. S. Poudyal, S. Laursen

**10:20 CATL 28.** Aromatic amine catalyzed photoelectrochemical reduction of CO<sub>2</sub>: What is the surface doing? A.B. Bocarsly, R.J. Cava, J. Frick, Y. Hu, J.W. Krizan

**10:40 CATL 29.** Metal carbides for catalysis and electrocatalysis. J.G. Chen

**11:20 CATL 30.** Engineering heterometallic transition metal carbide nanoparticles for electrocatalysis. S.T. Hunt, M. Milina, Y. Roman-Leshkov

**11:40 CATL 31.** Electrocatalytic overall water splitting on nickel selenide (Ni<sup>3</sup>Se<sub>2</sub>). A. Swesi, J. Masud, M. Nath

## Section E

Manchester Grand Hyatt San Diego  
Coronado D

## Catalysis at the Sub-Nanometer Scale

## Subnanometer (Selective) Oxidation Catalysts

*Cosponsored by WCC*

P. Christopher, J. R. Morris, *Organizers*

A. M. Karim, *Organizer, Presiding*

**8:00 CATL 32.** Cu-oxide clusters in nanoporous materials: Structural and chemical factors determining oxidation properties. **J.A. Lercher**, S. Grundner, A. Vjunov, M. Sanchez

**8:45 CATL 33.** Structure and catalytic behavior of  $\text{Cu}_2\text{O}$  supported Pt atom. **A. Therrien**

**9:05 CATL 34.** Developing new sub-nm catalysts for water splitting and CO oxidation. **A. Orlov**, Q. Wu, Y. Li, S. Xiong, D. Su, S. Zhao

**9:35 CATL 35.** Supported Ir single atoms, subnanometer clusters and nanoparticles for CO oxidation. **Y. Lu**, X. Ma, H. Xin, A.M. Karim

**9:55** Intermission.

**10:10 CATL 36.** Are single atom species really catalysts? **K. Ding**, A. Gulec, N.M. Schweitzer, L. Marks, **P.C. Stair**

**10:40 CATL 37.** High-load Pt, single-atom catalysts for CO oxidation. **S. Duan**, R. Wang, **J. Liu**

**11:00 CATL 38.** Site specific analysis of isolated Pt atoms on oxide supports for oxidation catalysis. **L. DeRita**, J. Matsubu, P. Christopher

**11:20 CATL 39.** Electrocatalysis on nickel complexes at the atomic scale. **D. Tafen**, D. Alfonso, D. Kauffman, C. Matranga

**11:40** Discussion.

## Alpha Olefin Catalysis: Production &amp; Transformations

## Catalytic Production

*Sponsored by I&EC, Cosponsored by CATL and INOR‡*

## Fuel Cells

*Sponsored by ENFL, Cosponsored by CATL*

## Structure, Dynamics &amp; Reactivity at Complex Interfaces with Relevance in Renewable Energy &amp; Environmental Applications

*Sponsored by COMP, Cosponsored by CATL and PHYS*

## SUNDAY AFTERNOON

## Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom B

## Amorphous Catalytic Materials

B. Peters, S. L. Scott, *Organizers, Presiding*

**1:00 CATL 40.** Characterization of amorphous catalytic materials by DNP-enhanced solid-state NMR methods. **T. Kobayashi**, F.A. Perras, **M. Pruski**

**1:35 CATL 41.** Novel amorphous silica-alumina with unique structure and strong acidity for catalytic reactions. **J. Huang**

**2:10 CATL 42.** Well-defined group VI oxo derivatives supported on silica by SOMC: Model of industrial olefin metathesis catalyst. **N. Merle**, Y. Bouhoute, K. Szeto, A. De Mallmann, I. Del Rosal, L. Maron, C.P. Nicholas, R. Gauvin, L. Delevoye, M. Taoufik

**2:30 CATL 43.** Synthesis-structure-function relations of silica-supported niobium(V) catalysts for alkene epoxidation with  $\text{H}_2\text{O}_2$ . **N.E. Thornburg**, J.M. Notestein

**2:50** Intermission.

**3:10 CATL 44.** Spectroscopy of single site metal oxide catalyst on silica. **N. Peek**, D. Jeffcoat, Y. Wang, L.J. Van De Burgt, S.L. Scott, **A.E. Stigman**

**3:45 CATL 45.** Molecular design of cooperative interactions for heterogeneous catalytic materials to tune catalytic rates and selectivities. **N.A. Brunelli**, N. Deshpande, L. Pattanaik, K. Sherman, C.W. Jones

**4:20 CATL 46.** Reactions of molecular metal complexes with amorphous silica surfaces. **S.L. Scott**

**4:40 CATL 47.** Mineral phase stability, constant internal oxidation enthalpy, and low surface energy contribute to catalytic ability of nanosheet CaMn-oxides. **N.R. Birkner**, A. Navrotsky

## Section B

Manchester Grand Hyatt San Diego  
Coronado A

## Catalytic Materials for Methane Conversion

## Oxidation &amp; Oxidative Coupling of Methane

*Cosponsored by ENFL*

B. A. Kilos, S. Lincic, E. Nikolla, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:05 CATL 48.** Oxidative coupling of methane: Active sites and mechanisms. **J. Sauer**

**1:50 CATL 49.** Mechanism for direct partial oxidation of methane to methanol in 8MR zeolites. **A.R. Kulkarni**, Z. Zhao, J.K. Norskov, F. Studt

**2:15 CATL 50.** Partial oxidation of methane to methanol over ZSM-5 from first-principles. **A. Arvidsson**, P. Carlsson, H. Gronbeck, A. Hellman

**2:40 CATL 51.** First-principles microscopic modeling of methane oxidation over PdO(101). **M.C. Van den Bossche**, H. Gronbeck

**3:05** Intermission.

**3:25 CATL 52.** Oxidative coupling of methane (OCM) with supported tungstate catalysts. **M. Zhu**, Z. Fink, W. Taifan, M. Ford, F. Tielens, **J. Baltrusaitis**, I.E. Wachs

**3:50 CATL 53.** Iron-oxo catalysts for CH bond cleavage: Insights from modeling. **C. Michel**, P. Andrikopoulos, P. Sautet

**4:15 CATL 54.** Effect of dopant ionic radius on methane activation at the alkaline earth metal doped (111) surface of ceria. **J.J. Carey**, **M. Nolan**

**4:40** Concluding Remarks.

## Section C

Manchester Grand Hyatt San Diego  
Harbor Ballroom C

## Computational Chemistry Across Catalysis

## QMMM &amp; Reaction Pathway Sampling

*Cosponsored by COMP, ENFL and WCC*

P. Sautet, D. G. Vlachos, *Organizers*

A. W. Goetz, C. Michel, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:05 CATL 55.** Metalloenzyme design. **A. Alexandrova**, C. Valdez, M.R. Nechay

**1:45 CATL 56.** Development and application of advanced methods for QM/MM simulations of enzyme catalysis. **E.G. Kratz**, R.E. Duke, D. Fang, **G.A. Cisneros**

**2:05 CATL 57.** Computational modeling of artificial metalloenzymes. **A. Lledos**, L. Alonso-Cotichico, J. Marechal

**2:25 CATL 58.** Understanding the formation of hydrogen peroxyde in superoxide reductase: A metadynamic QM/MM study. **R. David**, Y. Moreau, H. Jamet, A. Milet

**2:45 CATL 59.** Catalytic and biocatalytic iron porphyrin carbene formation: Effects of binding mode, carbene substituent, porphyrin substituent, and protein axial ligand. **R. Khade**, **Y. Zhang**

**3:05** Intermission.

**3:15 CATL 60.** Using metadynamics for quantitative estimates of chemical reaction kinetics. **J. Pfaendtner**, K. Fleming, P. Tiwary

**3:35 CATL 61.** Reaction pathway sampling from molecules to solids using stochastic surface walking method. **Z. Liu**

**3:55 CATL 62.** Advanced molecular simulations of elementary steps in zeolite catalysis under reaction conditions. **K. De Wispelaere**, S. Bailleul, V. Van Speybroeck

**4:15 CATL 63.** Cu coordination and dynamics under reaction conditions for  $\text{NO}_x$  selective catalytic reduction. **C. Paolucci**, H. Li, W.F. Schneider

**4:35 CATL 64.** Skeletal isomerization of 1-butene catalyzed by HFER, HMTT, and HMRE zeolites: A theoretical study. **M. He**, **Y. Li**

**4:55** Concluding Remarks.

## Section D

Manchester Grand Hyatt San Diego  
Coronado B

## Fundamental Surface Chemistry of Non-oxide Transition Metal Ceramic Catalysts: Carbides, Nitrides, Sulfides, Phosphides, Selenides

*Cosponsored by ENFL*

S. Laursen, N. M. Schweitzer, *Organizers, Presiding*

**1:00 CATL 65.** Tuning surface properties of sulfide Mo-based nanoslabs to control catalytic properties. **F. Mauge**, A. Travert, J. Chen, L. Olivierio

**1:40 CATL 66.** Nanoparticulate catalysts for acceptorless dehydrogenative coupling reactions. **L.R. McCullough**, R. Watson, D. Childers, B.A. Kilos, D.G. Barton, E. Weitz, H. Kung, J.M. Notestein

**2:00 CATL 67.** Nanoscale nickel phosphide catalysts for hydrodenitrogenation and hydrodesulfurization: Possible replacements for metal sulfides? **M.E. Bussell**, A. d'Aquino, S.J. Danforth, T.R. Clinkingbeard, C.E. Miles

**2:40 CATL 68.** Selecting and tuning non-noble metals to promote C-O bond cleavage and carbon-carbon coupling reactions. **Y. He**, S. Laursen

**3:00 CATL 69.** Novel metal carbide catalysts for desulfurization and the low temperature water-gas shift reaction. **J. Rodriguez**, P. Liu, F. Vines, F. Illas

**3:40 CATL 70.** Hydrodeoxygenation of lignin-derived phenolic compounds on transition metal carbides. **C. Chen**, W. Lee, A. Bhan

**4:00 CATL 71.** Design and synthesis of carbide supported metal catalysts. **L.T. Thompson**

**4:40 CATL 72.** Factors that control selectivity during hydrodeoxygenation on  $\text{Ni}_3\text{P}_y$  cluster. **M.E. Witzke**, D. Flaherty

## Section E

Manchester Grand Hyatt San Diego  
Coronado D

## Catalysis at the Sub-Nanometer Scale

## Challenges in Catalyst Synthesis, Stability &amp; Characterization

*Cosponsored by WCC*

A. M. Karim, J. R. Morris, *Organizers*

P. Christopher, *Organizer, Presiding*

**1:00 CATL 73.** Molecular metal catalysis on supports: Synthesis, characterization, and progress toward design. **B.C. Gates**

**1:45 CATL 74.** Tailoring the catalytic activity and stability of Pt clusters via encapsulation within CNTs. **F. Zhang**, X. Pan, J. Xiao, X. Bao

**2:05 CATL 75.** Challenges in characterizing the nature of supported single atoms and clusters. **J. Liu**

**2:35** Intermission.

**2:50 CATL 76.** Subnanometer metal clusters from a computational perspective. **D. Jiang**

**3:20 CATL 77.** Design of single atom heterogeneous catalysts having exceptional thermal stability. **A.K. Datye**, J. Jones, E. Peterson, A. DeLaRiva

**3:50 CATL 78.** Battling deactivation of sub-nano surface-deposited Pt cluster catalysts. **E. Jimenez-Izal**, M. Ha, **A. Alexandrova**

**4:20** Discussion.

## Alpha Olefin Catalysis: Production &amp; Transformations

## Alpha Olefin Transformations

*Sponsored by I&EC, Cosponsored by CATL and INOR‡*

## Fuel Cells

*Sponsored by ENFL, Cosponsored by CATL*

## Structure, Dynamics &amp; Reactivity at Complex Interfaces with Relevance in Renewable Energy &amp; Environmental Applications

*Sponsored by COMP, Cosponsored by CATL and PHYS*

## MONDAY MORNING

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom B

#### Amorphous Catalytic Materials

B. Peters, S. L. Scott, *Organizers, Presiding*

**8:00** *CATL* **79.** Amorphous surface oxide phases: Nature of catalytic active sites and their reactivity. I.E. Wachs

**8:35** *CATL* **80.** Fundamental understanding of ZnO doped ZrO<sub>2</sub> surface for C-C bond formation and deoxygenation of biomass derived-oxygenates. J. Sun, R. Baylon, D. Mei, Y. Wang

**9:10** *CATL* **81.** Bifunctional polymer architectures for cooperative catalysis: Tunable acid-base polymers for the aldol condensation. C.B. Hoyt, C.W. Jones

**9:30** *CATL* **82.** Nitrogen cleavage on porous organic polymers vs silica supported Ta-hydride catalysts: Comparative reaction energetics. J.M. Lopez-Encarnacion, K. Ortiz-Camacho, A. Alvelo-Aviles, A. Pagan-Luque, M. Alvarez-Cardona, V. Pantojas, J. Jellinek

**9:50** Intermission.

**10:10** *CATL* **83.** Propene metathesis and oxidation over silica-supported tungsten oxide catalysts. A.T. Bell

**10:45** *CATL* **84.** Comparing silica-supported tin(IV) with SnBeta for MPV reactions. S. Conrad, R. Verel, P. Wolf, I. Hermans

**11:20** *CATL* **85.** Catalytic dehydration of carbohydrates with solid acid catalysts in biphasic media. B. Saha, D. Gupta, A. Bhaumik

**11:40** *CATL* **86.** Tunable gelating networks to entrap, detect, and catalytically destroy toxic agents. K. Sullivan, C.L. Hill, Q. Yin, W.A. Neiwert, H. Zeng, A. Mehta, T. Liu, P. Yin, E.R. Weeks, S. Vivek

### Section B

Manchester Grand Hyatt San Diego  
Pier

#### Catalytic Materials for Methane Conversion

##### Methane Reforming

*Cosponsored by ENFL*

B. A. Kilos, S. Lincic, E. Nikolla, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05** *CATL* **87.** Synergetic effect of Ni and Co in Ni-Co/SBA-15-CD catalysts and their catalytic performance in carbon dioxide reforming of methane. H. Wu, H. Liu, W. Yang, D. He

**8:30** *CATL* **88.** Syngas production from methane dry reforming over Ni/SBA-15 catalyst: Effect of operating parameters. O. Omoregbe, J. Tan, H. Danh, H. Setiabudi, S. Abidin, D. Vo

**8:55** *CATL* **89.** Synthesis of novel carbon-resistant perovskite catalyst (CeCo<sub>3</sub>Ni<sub>1-x</sub>O<sub>3+δ</sub>) for methane dry reforming. R.L. Al-Otaibi

**9:20** Intermission.

**9:40** *CATL* **90.** Withdrawn.

**10:05** *CATL* **91.** Formation of highly active surface species induced by CO<sub>2</sub> on Ni/ZrO<sub>2</sub> in methane dry reforming. A. Jentys

**10:30** *CATL* **92.** Syngas production over Ba<sub>0.75</sub>Ni<sub>1</sub>Al<sub>12-y</sub>O<sub>19-3</sub> hydrocarbon reforming catalysts. T.H. Gardner, E.L. Kugler

**10:55** *CATL* **93.** Characterization and evaluation of Ni-based pyrochlore for the steam reforming of methane. D. Haynes, D. Shekhawat, D. Berry, M.W. Smith, J.P. Baltrus, J.J. Spivey

**11:20** *CATL* **94.** Syngas production through the steam-biogas reforming process. P.S. Roy, K. Kim, C.S. Park, A. Raju

**11:45** Concluding Remarks.

### Section C

Manchester Grand Hyatt San Diego  
Harbor Ballroom C

#### Computational Chemistry Across Catalysis

##### Towards Chemical Accuracy

*Cosponsored by COMP, ENFL and WCC*

C. Michel, D. G. Vlachos, *Organizers*

A. W. Goetz, P. Sautet, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05** *CATL* **95.** Embedded correlated wave-function methods for plasmon-induced photocatalysis. C.M. Krauter, E.A. Carter

**8:45** *CATL* **96.** Extending density-functional embedding theory to tackling heterogeneous catalysis that involves spin-polarized materials. C. Huang

**9:05** *CATL* **97.** Predictive framework for the understanding of lignin breakdown and conversion. P. Ramakrishnan, B.A. Simmons, S. Singh

**9:25** *CATL* **98.** Towards the accurate and efficient theoretical modelling of catalysis. X. Xu

**9:45** *CATL* **99.** Adsorption and reactivity of cellulosic aldoses on transition metals. Q. Trinh, S.H. Mushrif

**10:05** Intermission.

**10:15** *CATL* **100.** Role of anharmonicity in the confinement effect in zeolites: Structure, spectroscopy, and adsorption free energy of ethanol in H-ZSM-5. M. Lee, K. Alexopoulos, M. Reyniers, G.B. Marin, V. Glezakou, R. Rousseau, J.A. Lercher

**10:35** *CATL* **101.** Thermodynamic approach for exploring catalytic pathways using high accuracy computational methods. C. South, N. Kumar, S. Raugai, M. Dupuis, T.R. Cundari, A.K. Wilson

**10:55** *CATL* **102.** Evolution of quantum chemical methods for the simulation of reactions of organic molecules in zeolites. A.T. Bell

**11:15** *CATL* **103.** Accurate ab initio free energies of surface reactions from anharmonic vibrations. G. Piccini, J. Sauer

**11:35** *CATL* **104.** Theoretical analysis of proton-coupled electron transfer in benzimidazole-phenol complexes. M.T. Huynh, J.D. Gust, M.E. Tejada-Ferrari, A. Teillout, A.L. Moore, T.A. Moore, S. Hammes-Schiffer

**11:55** Concluding Remarks.

### Section D

Manchester Grand Hyatt San Diego  
Coronado B

#### Catalysis at the Sub-Nanometer Scale Selectivity

*Cosponsored by WCC*

P. Christopher, A. M. Karim, *Organizers*

J. R. Morris, *Organizer, Presiding*

**8:00** *CATL* **105.** Catalysis by subnanometer clusters. S. Vajda

**8:45** *CATL* **106.** Pt/Cu single atom alloys for highly selective formic acid decomposition. M. Marcinkowski, C.J. Murphy, M.L. Liriano, N.A. Wasio, F.R. Lucci, E.H. Sykes

**9:05** *CATL* **107.** Isolated Rh atoms on oxide supports as CO<sub>2</sub> reduction catalysts. J. Matsubu, P. Christopher

**9:25** *CATL* **108.** Selective hydrogenation of acetylene in ethylene over Cu-Pd catalysts. X. Cao, A. Mirjalili, W. Xie, W. Jang

**9:45** Intermission.

**10:00** *CATL* **109.** Single atomic Pt catalyst for electrocatalytic reactions with unique selectivity. H. Lee, S. Yang, J. Kim

**10:20** *CATL* **110.** Investigation of room-temperature N<sub>2</sub> bond-activation on size-selected W<sub>2-9</sub> clusters supported on highly ordered pyrolytic graphite (HOPG) by scanning tunneling microscopy (STM) and density functional theory (DFT). J.C. Robins

**10:40** *CATL* **111.** Catalytic properties controlled by the sub-nanometer windows in metal-organic frameworks. W. Huang, X. Li, T. Goh, C. Xiao

**11:00** *CATL* **112.** Control of Pd catalyst selectivity with mixed thiolate monolayer. C. Lien, J.W. Medlin

**11:20** *CATL* **113.** Withdrawn.

**11:40** Discussion.

### Section E

Manchester Grand Hyatt San Diego  
Coronado A

#### Ipatieff Prize: Symposium in honor of Aditya Bhan

*Financially supported by Ipatieff Trust Fund*

M. Neurock, M. Tsapatsis, *Organizers, Presiding*

**8:30** *CATL* **114.** Strategies for the synthesis of zeolites and for encapsulating clusters within their voids. S. Goel, S.I. Zones, E. Iglesia

**8:55** *CATL* **115.** Water activation by the supports for Pt catalysts during the water-gas shift reaction. V.J. Cybulskis, Y. Cui, M. Shekhar, J. Lovón Quintana, N. Delgass, F. Ribeiro

**9:20** *CATL* **116.** Metal oxide-like MOF nodes as catalyst supports. D. Yang, S.O. Odoh, J.D. Borycz, T.C. Wang, O.K. Farha, J.T. Hupp, C.J. Cramer, L. Gagliardi, B.C. Gates

**9:45** *CATL* **117.** Impact of water on dehydration of alcohols on molecular sieves. Y. Zhi, H. Shi, D. Mei, J.A. Lercher

**10:10** *CATL* **118.** Controlling zeolite growth at the single unit cell level: Implications for membranes and catalysis. M. Tsapatsis

**10:35** *CATL* **119.** Production of aromatic molecules from biomass-derived furans. R.F. Lobo

#### WCC 2016 Rising Stars Awards Symposium

*Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE*

#### CO<sub>2</sub> Conversion & Utilization

##### Conversion

*Sponsored by ENFL, Cosponsored by CATL*

#### Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications

*Sponsored by COMP, Cosponsored by CATL and PHYS*

## MONDAY AFTERNOON

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom B

#### Amorphous Catalytic Materials

B. Peters, S. L. Scott, *Organizers, Presiding*

**1:00** *CATL* **120.** *In situ* characterization of Ru nanocluster catalysts on K-Al<sub>2</sub>O<sub>3</sub> and their selective nitrile hydrogenation to primary amines. M. Tada, S. Muratsugu

**1:35** *CATL* **121.** Single-site iridium catalysts on MgO powder: Evidence of bonding at various support surface sites. A. Hoffman, L. Debeve, S. Zhang, D.A. Dixon, B.C. Gates

**2:10** *CATL* **122.** Highly dispersed, supported TaOx catalysts via a "nanocavity" route. Z. Bo, N.E. Thornburg, S. Nauerl, L. Pen, C.M. George, K. Schwartzberg, L. Marks, P.C. Stair, R.P. Van Duyne, J.M. Notestein

**2:30** Intermission.

**2:50** *CATL* **123.** Tuning catalytic performance via active site design. D.G. Vlachos

**3:25** *CATL* **124.** Phase-programmed nanofabrication: Effect of organophosphite precursor reactivity on the evolution of nickel and nickel phosphide nanocrystals. J. Vela-Becerra, H. Andaraarachchi, M. Thompson, M.A. White, H. Fan

**4:00** *CATL* **125.** Novel platform for studying catalyst precursors and synthesis on amorphous supports. M. Martynowicz, B. Hu, K. Andreev, D. Gidalevitz, A. Hock

**4:35** *CATL* **126.** Withdrawn.

### Section B

Manchester Grand Hyatt San Diego  
Coronado A

#### Computational Chemistry Across Catalysis

##### Oxide Catalysts & Key Industrial Reactions

*Cosponsored by COMP, ENFL and WCC*

A. W. Goetz, D. G. Vlachos, *Organizers*

C. Michel, P. Sautet, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:05** *CATL* **127.** Heterogeneous catalysis of metals and metal oxides: An accuracy status. A. Vojvodic

**1:45** *CATL* **128.** Is oxide hydrogenation equivalent to reduction? Fundamental differences between TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> from DFT. C. Spreatico, W. Karim, A. van Bokhoven, J. VandeVondele

**2:05** *CATL* **129.** Oxidative dehydrogenation of ethane on Co<sub>3</sub>O<sub>4</sub>: Effects of surface structure and doping. V. Fung, F. Tao, D. Jiang

**2:25** *CATL* **130.** Theoretical study on the unique electronic and structural effects in vanadia/ceria catalyzed reactions. X. Wu, X. Gong

**2:50** *CATL* **131.** DFT studies on a well-defined rhenium oxo complex grafted on Al-modified silica active in olefin metathesis. E. Lam, A. Comas-Vives, C. Coperet

**3:15** *CATL* **132.** New generations of olefin metathesis catalysts. A. Poater, R. Chauvin

**3:35** *CATL* **133.** Activation of C<sub>2</sub>H<sub>2</sub> over AuCl<sub>3</sub> and AuI: Their catalytic activity in hydrochlorination of acetylene. G. Hong, X. Tian, B. Jiang, J. Wang, Y. Yang, J. Zheng

- 3:55 CATL 134.** Lewis acid Al sites play in concert to promote carbon-carbon bond formation upon dimethylether activation on alumina. **A. Comas-Vives, M. Valla, M. Schwarzwalder, C. Coperet, P. Sautet**
- 4:15 CATL 135.** Direct amination of alcohols catalyzed by aluminum triflate: A DFT and experimental study. **R. Wischert, W. Guo, Q. Gu, Q. Wang, M. Corbet, C. Michel, P. Sautet**
- 4:35** Concluding Remarks.

### Section C

Manchester Grand Hyatt San Diego  
Harbor Ballroom C

#### Ipatieff Prize: Symposium in honor of Aditya Bhan

Financially supported by Ipatieff Trust Fund

M. Neurock, M. Tsapatsis, *Organizers, Presiding*

- 1:00 CATL 136.** Engineering active sites and their environments under working catalytic conditions. **M. Neurock**
- 1:25 CATL 137.** Oxidation of N-(phosphonomethyl)glycine to glyphosate in a trickle bed reactor. **D. Hickman, J.W. Ringer**
- 1:50 CATL 138.** Amine-modified silicates as acid/base bifunctional catalysts and catalyst supports. **C.W. Jones**
- 2:15 CATL 139.** High selectivity production of propylene via olefin metathesis over surface organometallic chemistry derived catalysts. **C.P. Nicholas**
- 2:40 CATL 140.** First-principles models of heterogeneity in catalysis. **W.F. Schneider**
- 3:05 CATL 141.** Ethylene carbonylation revisited: New paradigms. **B.A. Kilos, C. Yang, E. Weitz, J.M. Notestein, D.G. Barton**

### Section D

Manchester Grand Hyatt San Diego  
Coronado B

#### Surface Chemistry & Catalysis of Metal Oxides

A. Selloni, *Organizer*

A. Vojvodic, *Organizer, Presiding*

A. Sellinger, *Presiding*

- 1:00 CATL 142.** Oxide surface chemistry: From single crystals to supported particles. **H. Freund**
- 1:30 CATL 143.** First principles analysis of oxide and oxide-metal interfacial catalysis. **J.P. Greeley, T. Choksi, Z. Zhao, P. Majumdar**
- 2:00 CATL 144.** Surface and interface properties of transition metal oxide catalysts for solar fuels. **B.E. Koel**

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- 2:30 CATL 145.** Advances in theoretical studies of surface structures and adsorption of probe molecules at metal oxides. **Y. Yu, Z. Wen, X. Gong**
- 2:45 CATL 146.** Importance of attractive pair interactions in reactions on metal oxide surfaces. **M.C. Van den Bossche, B. Abrahamsson, H. Gronbeck**
- 3:00** Intermission.
- 3:15 CATL 147.** Approaches to tuning oxide reactivity through composition and structure. **J.R. Kitchin, Z. Xu**
- 3:45 CATL 148.** Understanding the roles of strong oxide-metal interactions in CO oxidation reaction. **L. Yu, H. Kim, J. Rodriguez, F. Yang, P. Liu**
- 4:15 CATL 149.** Plasma-enhanced atomic layer deposition of transition metal oxides for photoelectrochemical energy conversion. **I. Sharp, J. Yang, A. Schwartzberg, F.M. Toma, C. Kisielowski, J.K. Cooper, E. Crumlin, M. Favaro**
- 4:45 CATL 150.** Synthesis and simulation of amorphous TiO<sub>2</sub> for photoelectrochemical applications. **N.A. Deskins, P. Rao, D. Wang**

### Section E

Manchester Grand Hyatt San Diego  
Pier

#### Elucidation of Mechanisms & Kinetics on Surfaces

Cosponsored by COLL, ENVR and PHYS

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:10 CATL 151.** Correlating experimental data with computational models for active site model identification: A case study for the water-gas shift reaction. **A. Heyden, E. Walker, G.A. Terejanu, S.C. Ammal**
- 1:50 CATL 152.** Elucidation of mechanisms and kinetics using error estimation functionals. **T. Bligaard**
- 2:30 CATL 153.** Structure-energy-activity relations in heterogeneous catalysis. **P. Sautet, F. Calle-Vallejo, D. Loffreda**
- 3:10** Intermission.
- 3:30 CATL 154.** Simulation of temperature programmed reactions: TPR mechanism following adsorption of methanol on CeO<sub>2</sub>(111). **A. Savara**
- 4:10 CATL 155.** Microkinetics modeling using the MKMCXX software suite. **I. Filot, B. Zijstra, R. Broos, E. Hensen**

#### WCC 2016 Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE

#### CO<sub>2</sub> Conversion & Utilization

##### Capture & Utilization

Sponsored by ENFL, Cosponsored by CATL

##### Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications

Sponsored by COMP, Cosponsored by CATL and PHYS

#### Nanomaterials for Energy Conversion & Storage

##### Energy Conversion

Sponsored by ENFL, Cosponsored by CATL

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

E. Nikolla, *Organizer*

#### 8:00 - 10:00

- 2, 10-12, 21-22, 25, 30, 50, 61-63, 70, 72, 79, 81, 88, 92, 122, 128-130, 135, 146, 150. See previous listings.
- 159-161, 195, 197-198, 312-313, 317, 322, 328-329, 331, 335, 352, 365, 367, 400, 447. See subsequent listings.

## TUESDAY MORNING

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom B

#### Computational Chemistry Across Catalysis

##### Electrocatalysis & Photocatalysis

Cosponsored by COMP, ENFL and WCC

A. W. Goetz, D. G. Vlachos, *Organizers*

C. Michel, P. Sautet, *Organizers, Presiding*

#### 8:00

- Introductory Remarks.
- 8:05 CATL 156.** Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells. **S. Linic**
- 8:45 CATL 157.** Continuum embedding for photo-electrochemical surface processes. **M. Sinstein, H. Oberhofer, D. Berger, V. Blum, K.U. Reuter**
- 9:05 CATL 158.** Phenomenological models for carbon monoxide adsorption on platinum-based alloy catalysts for direct methanol fuel cells. **N. Dimakis, F. Flor, A. Salgado, K. Adjibi, E.S. Smotkin**
- 9:25 CATL 159.** Towards first-principles modeling of electrolytic solvent effects in photo-catalytic water splitting. **S. Ringe, H. Oberhofer, S. Matera, K.U. Reuter**
- 9:45 CATL 160.** Highly selective Cu-In catalyst for electrochemical reduction of CO<sub>2</sub> to CO. **A. Jedidi, S. Rasul, K. Takanebe, L. Cavallo**
- 10:05** Intermission.
- 10:15 CATL 161.** Computational studies on charge recombination in TiO<sub>2</sub> nanoparticles. **M. Muuronen, F.U. Furcher**
- 10:35 CATL 162.** Organic photocatalysts for atom transfer radical polymerization driven by visible light. **C. Lim, J. Theriot, H. Yang, G. Miyake, C. Musgrave**
- 10:55 CATL 163.** Tuning the photocatalytic activity of polymers for water splitting by changing their molecular weight; insights from computational modelling and experiment. **P. Guiglion, M. Zwijnenburg**
- 11:15 CATL 164.** Calculating photocatalytic conversion in bimetallic donor-acceptor systems. **L.A. Fredin**
- 11:35 CATL 165.** Interplay between trapped electronic states and protons at the TiO<sub>2</sub> water interface. **J. Cheng, M. Sprick**

- 11:55** Concluding Remarks.

### Section B

Manchester Grand Hyatt San Diego  
Coronado A

#### Ipatieff Prize: Symposium in honor of Aditya Bhan

Financially supported by Ipatieff Trust Fund

M. Neurock, M. Tsapatsis, *Organizers, Presiding*

- 8:30 CATL 166.** New insights into vapor phase ethanol carbonylation. **J.M. Notestein, S. Yacob, D. Childers, S. Park, L. McCullough, B.A. Kilos, D.G. Barton**
- 8:55 CATL 167.** Reactivity and stability investigation of supported molybdenum oxide catalysts for the hydrodeoxygenation (HDO) bio-oil components. **Y. Roman-Leshkov**
- 9:20 CATL 168.** Advanced synthesis methods and structure-performance relationships in zeolite catalysis. **J.D. Rimer**
- 9:45 CATL 169.** Hydrogen activation and hydrodeoxygenation over ceria-zirconia catalysts. **S. Schimming, G. Foo, O. Lamont, A. Rogers, M. Yung, A.D. D'Amico, C. Sievers**
- 10:10 CATL 170.** Solid-supported sulfonic acid catalysts: Influence of functional group conversion on cooperativity and kinetic influence of water during biomass conversion. **Y. Noda, K. Li, W.A. Elliott, J. Sutyak, R.M. Rioux**
- 10:35 CATL 171.** Kinetics of MFI zeolite surfaces. **P.J. Dauenhauer**

### Section C

Manchester Grand Hyatt San Diego  
Harbor Ballroom D

#### Condensed Phase Catalysis

Cosponsored by ENFL

R. Getman, R. M. Rioux, *Organizers*

J. Bond, *Organizer, Presiding*

- 8:30 CATL 172.** Heterogeneous catalysis in biphasic systems. **S. Crossley**
- 9:10 CATL 173.** Towards understanding acid-catalyzed alcohol dehydration in aqueous phase: Kinetics, mechanism and energetic landscapes. **H. Shi, A. Vjunov, Y. Liu, S. Eckstein, D. Mei, D.M. Camaioni, J.A. Lercher**
- 9:30 CATL 174.** Molecular-level insights into the role of water on Pt(111)-catalyzed glycerol and methanol reforming using a combined DFT/MD approach. **C.J. Bodenschatz, T. Xie, S. Sarupria, R. Getman**
- 9:50** Intermission.
- 10:10 CATL 175.** Mapping the energetically efficient catalysis of renewables with Pourbaix diagrams. **K. Saravanan, M. Groenenboom, J.A. Keith**
- 10:50 CATL 176.** Hydrothermal stability of zeolites under relevant biomass conversion reaction conditions. **D.W. Gardner, J. Huo, T.C. Hoff, R.L. Johnson, B.H. Shanks, J. Tessonnier**
- 11:10 CATL 177.** Selective oxidation of n-butane to 1-butanol over transition metal catalysts encapsulated by metal-organic frameworks. **S. Dix, D.A. Gomez-Gualdron, J. Zhu, J.K. Scott, C.T. Campbell, R. Getman**



## Section D

Manchester Grand Hyatt San Diego  
Coronado B

## Surface Chemistry &amp; Catalysis of Metal Oxides

A. Selloni, A. Vojvodic, *Organizers, Presiding*

**8:00 CATL 178.** Atomic layer deposited transition metal oxides as active electrocatalysts for the oxygen evolution reaction. K. Nardi, J.G. Baker, A.J. Mackus, S.F. Bent

**8:30 CATL 179.** Activity trends and design principles for multi-transition-metal (oxy) hydroxide oxygen evolution catalysts. S.W. Boettcher

**9:00 CATL 180.** Engineering complex, layered metal oxides: High performance nickelate oxide nanostructures for oxygen exchange/reduction. E. Nikolla

**9:30 CATL 181.** Perovskite electrocatalysts for energy storage and conversion. K.J. Stevenson, J.T. Mefford, R. Forslund

**10:00** Intermission.

**10:15 CATL 182.** Hydroxylation, wetting, and catalysis on perovskite oxide surfaces. K.A. Stoerzinger, W.T. Hong, Y. Lee, L. Giordano, Y. Shao-Horn

**10:45 CATL 183.** First-principles prediction of OER reaction mechanism, overpotential, and stability of perovskite oxide electrocatalysts. A. Kolpak

**11:15 CATL 184.** Electrochemical redox of late transition metal perovskite oxides. W. Chueh

**11:45 CATL 185.** Tailoring transition metal oxides for energy conversion devices: First-principles study of A-doped  $\text{Sr}_2\text{Fe}_{1-x}\text{Mo}_x\text{O}_{6-\delta}$ . A.B. Muñoz-García, M. Pavone

## Section E

Manchester Grand Hyatt San Diego  
Pier

## Elucidation of Mechanisms &amp; Kinetics on Surfaces

*Cosponsored by COLL, ENVR and PHYS*

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

**8:00 CATL 186.** Experimental measurements of the energies of adsorbed catalytic intermediates and the rate constants for their elementary reaction steps. C.T. Campbell

**8:40 CATL 187.** Activation, coupling, and selective oxidation of methane. C. Okolie, E. Stavitski, C. Sievers

**9:20 CATL 188.** Unraveling the kinetics of aqueous-phase carbonyl hydrogenation over supported Ru. J. Bond, O.A. Abdelrahman

**9:40** Intermission.

**10:00 CATL 189.** Alcohol amination catalyzed by metal supported catalysts: The role of co-adsorbed species revealed by DFT studies. C. Michel, A.S. Dumon, R. Wischert, M. Pera-Titus, P. Sautet

**10:40 CATL 190.** Interaction-aware saturation number as a reactivity descriptor for metal nanocatalysts. X. Ma, S. Wang, H. Xin

**11:00 CATL 191.** Is there something new under the sun? Myths and facts in the analysis of catalytic cycles. S. Kozuch

## Application of Computational Chemistry for Energy &amp; Fuel Production

## Computational Catalysis in Research

*Sponsored by ENFL, Cosponsored by CATL*

CO<sub>2</sub> Conversion & Utilization

## Electroreduction

*Sponsored by ENFL, Cosponsored by CATL*

## Nanomaterials for Energy Conversion &amp; Storage

## Energy Conversion: Characterization/Application

*Sponsored by ENFL, Cosponsored by CATL*

## TUESDAY AFTERNOON

## Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom B

## Computational Chemistry Across Catalysis

## From Metallic Nanoparticles to Isolated Metal Active Site

*Cosponsored by COMP, ENFL and WCC*

A. W. Goetz, C. Michel, *Organizers*

P. Sautet, D. G. Vlachos, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:05 CATL 192.** From large metallic particles to nanoclusters supported on alumina in reaction conditions: A theoretical viewpoint. P. Raybaud

**1:45 CATL 193.** Detailed reaction mechanisms for heterogeneous catalysis. W.A. Goddard, Q. An, M. Cheng, J. Qian

**2:05 CATL 194.** Correlating structure and function for nanoparticle catalysts. G.A. Henkelman

**2:25 CATL 195.** Site preference of chemisorption. R.A. Van Santen, I. Tranca

**2:45** Intermission.

**2:55 CATL 196.** Exchange interactions in transition-metal reactivity: The catalase activity of Mn-salen complexes. M. Swart, A. Romero-Rivera

**3:15 CATL 197.** Metal phlorin intermediates toward hydrogen evolution: New functionality resulting from ligand noninnocence. B.H. Solis, A.G. Maher, D.K. Dogutan, D.G. Nocera, S. Hammes-Schiffer

**3:35 CATL 198.** Electrochemical CO<sub>2</sub> reduction catalyzed by Mn catalysts: DFT investigations point to strategies for overpotential reduction and activity improvement. Y. Lam, R.J. Nielsen, W.A. Goddard, H.B. Gray

**3:55 CATL 199.** Methane activation at binuclear Iron sites in Fe-ZSM-5 is studied by using density functional theory (DFT) calculations. M. He, J. Zhang, X. Sun

**4:15 CATL 200.** C-H vs. C-C bond formation in a faujasite. Modeling a subtle balance for anchored Rh centers. S. Dinda, Y. Wu, A. Govindasamy, A. Genest, N. Roesch

**4:35** Concluding Remarks.

## Section B

Manchester Grand Hyatt San Diego  
Coronado A

## Ipatieff Prize: Symposium in honor of Aditya Bhan

*Financially supported by Ipatieff Trust Fund*

M. Neurock, M. Tsapatsis, *Organizers, Presiding*

**1:00 CATL 201.** Synthetic methods to control framework aluminum distribution in chabazite zeolites and consequences for NOx selective catalytic reduction with ammonia. J.R. Di Iorio, R. Gounder

**1:25 CATL 202.** Synthesis and catalytic characterization of hybrid lamellar-bulk zeolite catalysts. D. Liu

**1:50 CATL 203.** Mechanism of aromatic dealkylation in methanol-to-hydrocarbons conversion on H-ZSM-5: What are the aromatic precursors to light olefins? S. Ilias, A. Bhan

**2:15 CATL 204. Award Address** (Ipatieff Prize sponsored by the Ipatieff Trust Fund). Be practical: Mechanistic studies of industrially relevant catalytic systems. A. Bhan

## Section C

Manchester Grand Hyatt San Diego  
Harbor Ballroom C

## Surface Chemistry &amp; Catalysis of Metal Oxides

A. Selloni, A. Vojvodic, *Organizers, Presiding*

**1:00 CATL 205.** Surface chemistry of oxygen and water on anatase TiO<sub>2</sub> (101). M. Setvin, J. Hulva, B. Daniel, T. Simschitz, M. Schmid, U. Schauer, A. Selloni, U. Diebold

**1:30 CATL 206.** Non-band-gap photoexcitation of hydroxylated TiO<sub>2</sub>. Y. Zhang, D. Payne, C. Pang, H. Fielding, G. Thornton

**2:00 CATL 207.** Tailoring charge recombination in photoelectrodes using oxide nanostructures. A. Hellman

**2:30 CATL 208.** Nature of rutile nuclei in anatase-to-rutile phase transition. Z. Liu

**3:00** Intermission.

**3:15 CATL 209.** Imaging water reactions with reduced, stoichiometric, and oxidized RuO<sub>2</sub>(110) surfaces. Z. Dohnalek

**3:45 CATL 210.** Energetics and solvation effects at the photoanode/catalyst interface: Ohmic contacts versus Schottky barriers. G.A. Galli

**4:15 CATL 211.** Graphene/ (101) anatase TiO<sub>2</sub> interface: A DFT study. C. Di Valentin, L. Ferrighi

## Section D

Manchester Grand Hyatt San Diego  
Pier

## Elucidation of Mechanisms &amp; Kinetics on Surfaces

*Cosponsored by COLL, ENVR and PHYS*

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

**1:00 CATL 212.** Mechanism and kinetics of C-C bond forming reactions with carboxylic acids over Brønsted acid sites. S. Crossley

**1:40 CATL 213.** Theoretical investigation of the reactivity of carbonyl compounds on CeO<sub>2</sub>(111). C. Zhao, Y. Xu

**2:00 CATL 214.** Using modulation excitation spectroscopy to obtain insights in complex heterogeneous liquid-phase reactions. I. Hermans

**2:40 CATL 215.** Microkinetic analysis of  $\gamma$ -valerolactone ring opening and decarboxylation over solid acids. J. Bond, C. Jungong

**3:00** Intermission.

**3:20 CATL 216.** Ethanol condensation reaction networks that selectively form long chain alcohols or aromatics. D. Flaherty

**3:40 CATL 217.** Kinetic consequences of hydrophobic voids in Lewis acid zeolites for glucose isomerization catalysis in liquid water. M.J. Cordon, J.W. Harris, J.C. Vega-Vila, F. Ribeiro, R. Gounder

**4:20 CATL 218.** Anisole decomposition in UHV conditions: When DFT and experiments play ping-pong on a Pt(111) surface. R.J. Réocreux, C. Ould Hamou, C. Michel, J. Giorgi, P. Sautet

## Section E

Manchester Grand Hyatt San Diego  
Coronado B

## Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Cosponsored by ENFL*

E. Hensen, *Organizer*

M. Saeys, *Organizer, Presiding*

**1:00 CATL 219.** Overview of mechanism for Fischer-Tropsch synthesis. B.H. Davis

**1:30 CATL 220.** Optimally performing Fischer-Tropsch catalysis. I. Filot, R.A. Van Santen, E. Hensen

**2:00 CATL 221.** Surface science investigations of the Fischer-Tropsch reaction on cobalt. K. Weststrate, H. Niemantsverdriet

**2:30** Intermission.

**3:00 CATL 222.** Insights into CO activation and hydrocarbon chain growth in Fischer-Tropsch synthesis. D. Hibbitts, E. Dybeck, T. Lawlor, M. Neurock, E. Iglesia

**3:30 CATL 223.** Structural sensitivity of metal catalysts for Syngas conversion from first-principles theory. W. Li

**4:00 CATL 224.** Incorporating lateral interactions in the micro-kinetics of methanation over Fe(100). R.K. Abrahams, E. van Steen

**4:30 CATL 225.** Fe-based catalysts for Fischer-Tropsch process: Progress on theoretical study. X. Wen, Y. Li, Y. Yang, H. Jiao

## Application of Computational Chemistry for Energy &amp; Fuel Production

## Computational Catalysis in Research

*Sponsored by ENFL, Cosponsored by CATL*

CO<sub>2</sub> Conversion & Utilization

## Electroreduction

*Sponsored by ENFL, Cosponsored by CATL*

## Nanomaterials for Energy Conversion &amp; Storage

## Energy Storage: Synthesis/Characterization

*Sponsored by ENFL, Cosponsored by CATL*

## TUESDAY EVENING

## Section A

San Diego Convention Center  
Hall D

## Poster Session

E. Nikolla, *Organizer*

**8:00 - 10:00**

**CATL 226.** Withdrawn.

**CATL 227.** NO<sub>2</sub> assisted soot combustion over mesoporous manganese oxides. N.D. Wasalathanthri, T. SantaMaria, D. Kriz, S. Biswas, C. Kuo, S.L. Suib

**CATL 228.** Patterned Pd nanoparticles for investigating ligand-free Suzuki-Miyaura cross coupling. A.A. Gosavi, C.A. Mirkin, J.M. Notestein, N. Chernyakov

**CATL 229.** Combined Fe-Cu bimetallic nanoparticles-ozone process for degradation of indigo carmine dye in aqueous media. T. Torres Blancas

- CATL 230.** Improvement of platinum nano-catalysts via boron doping. E. Jimenez-Izal, M. Ha, J. Dadras, A. Alexandrova
- CATL 231.** Preparation of core-shell catalysts for epoxidation reaction of ethane. N. Kaewpornmongkol, S. Chavadej
- CATL 232.** Partial oxidation of methane on a nickel catalyst: Monte Carlo simulation study. S. Pruksawan, B. Kitiyanan, R.M. Ziff
- CATL 233.** Tuning the optical and catalytic properties of copper oxide nanosheets. Z. Fishman, Y. He, B. Liu, G.L. Haller, L. Pfefferle
- CATL 234.** B-site substitution effects in La-Co based perovskites. J. Simboeck, K. Simeonov, R. Palkovits
- CATL 235.** NiO-based trimetallic mixed metal oxide catalysts for oxidative dehydrogenation of ethane to ethylene. P. Unruean, B. Kitiyanan
- CATL 236.** High pressure - high temperature *in situ* scanning tunneling microscopy study of the dissociation of CO on Co(0001). B. Boeller, M. Ehrensperger, J. Wintterlin
- CATL 237.** Determination of the active site of the water-gas shift reaction over Pt/TiO<sub>2</sub> catalyst. E. Walker, G.A. Terejanu, S.C. Ammal, A. Heyden
- CATL 238.** Hydrogen generation from formic acid decomposition using a Ir-Pd nanoparticles supported on different supports. M.H. Alotaibi, O.F. Aldosari, R.L. Al-Otaibi
- CATL 239.** Direct conversion of methane to methanol by a controlled oxidation process at low temperature. C. Zhang
- CATL 240.** Visible light mediated upgrading of lignin components to biofuel. S. Verma, N.R. Baig, M. Nadagouda, R.S. Varma
- CATL 241.** Selective hydrogenation of biomass-derived 5-hydroxymethyl-furfural using Ru based catalyst. J. Hwang
- CATL 242.** Withdrawn.
- CATL 243.** CO<sub>2</sub> reforming of CH<sub>4</sub> to syngas over Ni/Nd/SBA-15 catalysts: Effects of Nd modification on catalytic performance. H. Liu, D. He
- CATL 244.** First-principles investigation of alloying effects in selective hydrogen production from formic acid on the Pd-M alloy catalysts. J. Cho, S. Lee, J. Han, S. Yoon, S. Nam, K. Lee, H. Ham
- CATL 245.** Withdrawn.
- CATL 246.** Experimental and theoretical investigation on possible catalytic hydrogen production from water using anionic small Mo-oxide clusters in the gas phase. M. Ray, A. Saha, K. Raghavachari, C. Jarrold
- CATL 247.** Oxygen reduction reaction mechanisms study for transition-metal phthalocyanine supported on graphitized carbon black. F. Wang, Z. Zhang, M. Dou, J. Ji, J. Liu, Z. Li
- CATL 248.** Unsupported palladium nanoparticle catalysts with near-surface ligand steric control: Influence on terminal alkene isomerization. P. Tieu, Y. Shon
- CATL 249.** Catalytic depolymerization of lignin by Cu-PMO: Preserving aromatic products through O-methylation. J. Barrett, Y. Gao, C.M. Bernt, M. Foston, P.C. Ford
- CATL 250.** How carboxylate bind to gold nanoparticle? Unraveling the exceptional charge effect. A. Jedidi, Z. Cao, L. Cavallo
- CATL 251.** Mesoporous sulfated zirconia (UCT-47): An efficient catalyst for biodiesel production. M.S. Seraji, A. Poyraz, C. Kuo, A.R. Howell, S.L. Suib
- CATL 252.** Dual gold catalysis to functionalize alkynes. A. Poater
- CATL 253.** Oxidative dehydrogenation of ethane to ethylene over alumina-supported V<sub>0.2</sub>Mo<sub>0.1</sub>Ni<sub>0.1</sub>Nb<sub>0.1</sub> catalyst. S. Narasa, B. Kitiyanan
- CATL 254.** Preparation of N-doped carbon supported Co<sub>3</sub>O<sub>4</sub> nanoparticles as electrocatalysts for oxygen reduction reaction. J. Liu, M. Liu, F. Wang
- CATL 255.** Carbon nanotube supported ultrafine Pt-Co-P nanoparticles for methanol electro-oxidation. J. Sun, F. Wang, H. Liu, M. Dou, J. Liu, J. Ji, Z. Li
- CATL 256.** Enhancing the reactivity of CuPMOs with Lewis and Bronstead acids towards desired products from lignin model compounds and biomass. M. Chui, G. Metzger, T. Azumi, C.M. Bernt, A. Tran, M. boscolo, P.C. Ford
- CATL 257.** Zeolite-supported manganese oxides for photochemical water oxidation. S. Shrestha, P. Dutta
- CATL 258.** Bimetallic nitrogen-doped graphene-like carbon derived from iron and cobalt phthalocyanine-based conjugated polymer networks as superior electrocatalyst for oxygen reduction. F. Wang, Z. Zhang, J. Liu, M. Dou, J. Ji, Z. Li
- CATL 259.** Size dependent oxygen affinity and CO oxidation activity of small Au nanoclusters. H. An, H. Ha, M. Yoo, H. Kim
- CATL 260.** Effect of additives on the etherification of glycerol using heterogeneous catalysts. T. Han, J. Lee, J. Lee
- CATL 261.** Dynamic structural evolution of Au-Pd nanoparticles under CO oxidation condition. H. An, H. Ha, M. Yoo, H. Kim
- CATL 262.** Exploring the activation parameters for lignin model compounds over Cu-doped porous metal oxide catalysts. C.M. Bernt, H. Maneesuwann, F. Brunner, G. Metzger, M.A. Chui, A. Tran, K. Barta, P.C. Ford
- CATL 263.** Methanol production from syngas on the (0001) surface of doped Cr<sub>2</sub>O<sub>3</sub>: The role of H<sub>2</sub>O formation. J.J. Carey, M. Nolan
- CATL 264.** Silica-based hybrid catalysts and their application in alkane oxidation. M. Yadav, A.J. Karkamkar
- CATL 265.** Silver nanoparticle enhanced formate production by semiconductor photocatalyst. A. Do, M.D. Heagy
- CATL 266.** Electrochemical study of the effect of adsorbates and precursors in the synthesis of well-defined bimetallic platinum-rhodium nanoparticles using water-in-oil microemulsion. R.A. Martinez-Rodriguez, F.J. Vidal-Iglesias, J. Solla-Gullón, C.R. Cabrera, J.M. Feliu
- CATL 267.** Oxidative aromatization of propane with CO<sub>2</sub> over bi-functional MFI zeolite catalyst. Y. Mo, Y. Choi, S. Park
- CATL 268.** Dry reforming of methane over NiO-MO<sub>x</sub>/MgO catalysts. H. Dang, M. Czaun, A. Goepfert, S.G. Prakash, G.A. Olah
- CATL 269.** Mechanistic insights into non-directed, platinum-catalyzed C(sp<sup>3</sup>)-H functionalization. M. Lee, M.S. Sanford
- CATL 270.** Ruthenium catalyzed amide hydrogenation en route methanol generation. D.C. Samblanet, M.S. Sanford
- CATL 271.** Real biogas reforming with carbon dioxide over Ni-based bimodal pore catalyst. Z. Bao, Y. Lu, Y. Li, F. To, F. Yu
- CATL 272.** Theoretical study on the mechanism of the alkylation reaction between isobutene and isobutane catalyzed by chloroaluminate ionic liquid. X. Liu, S. Li, D. Wang, Y. Ma
- CATL 273.** Synthesis, structure, and catalytic use of chiral pinene-containing N-heterocyclic carbenes. M. Jackson, S. Nadakal, L. Freeman, C.M. Garner
- CATL 274.** Strategies to reduce leaching of soluble polymer-supported catalysts in thermomorphic systems. J. Bianga, M.L. Harrell, T. Banks, D.E. Bergbreiter
- CATL 275.** Catalytic membrane process for effective treatment of endocrine disrupting compounds in water. H. Kim, T. Corbett, J. Lee, K. Yeung
- CATL 276.** Metal doped catalyst development for lignin liquefaction and optimization of the process variables using design of experiments. S. Pourjafar, W. Seames, A. Kubatova, E.I. Kozliak
- CATL 277.** Effect of the alkyl substituents and a catalyst choice on the decomposition of beta-diketones to ketones and carboxylates via retro Claisen condensation reaction. J.R. LaPenna, A.V. Ignatchenko
- CATL 278.** Synthesis of nickel nanoparticles from N,N'-dialkylimidazolium chloronickel(II) ionic liquid and their application as catalysts. A.M. Alsalmeh, M.H. Siddiqui
- CATL 279.** Fabrication and characterization of LDH and graphitic carbon nitride hybrid material for photoelectrochemical oxidation of organics. L. Mohapatra, S. ZaidiZaidi, M. Al-Maadeed
- CATL 280.** DNA directed immobilization approach for heterogenizing a biological catalyst. T. Hurlburt, K. Palla, M.B. Francis, G.A. Somorjai
- CATL 281.** Towards a continuous bioprocessing synthesis of levomilnacipran. C. Ayoub, M. Nguyen, A.C. Evans
- CATL 282.** Use of methyl and monomethyl viologens as catalysts in the production of hydrogen from glucose for the use in hydrogen fuel cells and as electron carriers in glucose fuel cells. J. Nguyen, G. Watt, J. Harb, R.S. Lewis
- CATL 283.** Preparation of catalytically active octanethiolate-capped platinum nanoparticles using sodium S-octylthiosulfate ligand precursor for hydrogenation of alkenes and alkynes. K. San, Y. Shon
- CATL 284.** Oxidation of reduced Keggin heteropolytungstates by dioxygen in water catalyzed by Cu(II). M. Kim, I.A. Weinstock, Y.V. Geletii, C.L. Hill
- CATL 285.** Photodegradation of hydroquinone on TiO<sub>2</sub> in presence of additives used for inks manufacture. A. Barbosa Lopez, M. Lozano
- CATL 286.** CdS-MoS<sub>2</sub> hybrid for hydrogen evolution reaction: p-n junction photoelectrode with enhanced photoelectrocatalysis. J. Ji
- CATL 287.** Aromatic chemicals production through various heterogeneous catalytic lignin depolymerization processes. S. Zhang, J. Kruger, R. Katahira, G. Beckham
- CATL 288.** Sterical index to predict the reactivity of alkynes. A. Poater, M. Michalak
- CATL 289.** Withdrawn.
- CATL 290.** Reaction sampling and reactivity prediction using stochastic surface walking method. X. Zhang, Z. Liu
- CATL 291.** Conformationally rigid chiral bipyridine N,N'-dioxide as organocatalyst: Asymmetric ring opening of meso-epoxides. G. Elumalai, S. Nagamalla, S. Jayakumar, R.R. Chinnasamy
- CATL 292.** Generating isopeptide bonds using sortase A homologs. L. Nguyen, J.M. Antos
- CATL 293.** Catalytic asymmetric hydroboration (CAHB) of phosphonate functionalized vinyl arenes. R.O. Carr, S. Chakrabarty, J.M. Takacs
- CATL 294.** Effect of additives on the etherification of glycerol using homogeneous catalysts. T. Han, J. Lee, J. Lee
- CATL 295.** Metal removal from discovery to commercialisation-scaling up your scavenger. S. Purser, A. Blanco, P. Murray
- CATL 296.** Removal of adsorbed carbonates/bicarbonates from Zr(OH)<sup>4</sup> and its effect on the reactions of VX, GD, and HD. G.W. Wagner, G.W. Peterson
- CATL 297.** Photodynamic medical device tips and their resistance to fouling for *in vivo* sensitizer release. A.A. Ghogare, J.M. Miller, B. Mondal, A.M. Lyons, K. Cengel, T. Busch, A. Greer
- CATL 298.** Catalytic modification of natural proteins with Rh(II) metalloproteids. S. Knudsen, F. Vohidov, Z.T. Ball
- CATL 299.** Synthesis of two novel ligand scaffolds for bimetallic catalytic hydroformylation reactions. P.J. Roy, R.J. Rosso
- CATL 300.** Development of an anchoring bis-dirhodium catalyst for selective proximity-driven protein modification. A.E. Mangubat, Z.T. Ball
- CATL 301.** Fischer-Tropsch synthesis: Effect of Cu, Mn, and Zn addition on the activity and product selectivity of cobalt ferrite catalyst. M. Gnanamani, H.H. Hamdeh, G. Jacobs, W.D. Shafer, B.H. Davis
- CATL 302.** Fischer-Tropsch synthesis: Effect of ammonia on supported cobalt catalysts. V.R. Pendyala, G. Jacobs, B.H. Davis
- CATL 303.** Development of MOF supported catalysts for commercially relevant processes. V. Pascanu, M.J. Johansson, X. Zou, B. Martin-Matute
- CATL 304.** Dielectric barrier discharge plasma-based dry reforming: Determining the discharge characteristics and the optimum condition. M.K. Nikoo, N. Saidina Amin, K.D. Murray
- CATL 305.** Role of CO<sub>2</sub> on the reactivity of Zr(OH)<sub>4</sub> nanopowders in real-world conditions: Towards *in operando* chemical warfare agent decomposition. R. Balow, D. Barlow, J. Lundin, J.H. Wynne, G.W. Wagner, W. Gordon, G.W. Peterson, V. Bermudez, C.J. Karwacki, I. Iordanov, C. Knox, P. Pehrssson
- CATL 306.** Efficient methanol to olefin (MTO) catalyst based on hierarchical SAPO-34 Efficient methanol to olefin (MTO) catalyst based on hierarchical SAPO-34. Z. Liu
- CATL 307.** Solvothermal synthesis of WS<sub>2</sub> quantum dots for photocatalytic oxidative coupling of amines. M. Kim, D. Yim, J. Park, F. Raza, S. Jeon, H. Kim, T. Kang, H. Lee, J. Ju, J. Kim
- CATL 308.** WS<sub>2</sub> nanosheets bearing metal nanoparticles for photocatalyzed C-C coupling reactions. D. Yim, J. Park, F. Raza, H. Lee, H. Kim, M. Kim, S. Jeon, J. Kim
- CATL 309.** Synthesis and batch reactor evaluation of novel constrained geometry catalysts. S.G. Brown, R.M. Jenkins, L. Sun
- CATL 310.** Computation as a tool for designing molecular catalysts for the conversion of CO<sub>2</sub> into more useful products. R. Raju, E. Brothers
- CATL 311.** Withdrawn.

## WEDNESDAY MORNING

## Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom B

## Catalytic Processes at Interfaces: Fundamentals &amp; Applications

D. Hibbitts, *Organizer*

R. Gounder, B. Xu, *Organizers, Presiding*

**8:00** CATL **312**. Alloy catalysis across composition space. I. Sen, G. Gumuslu, A.J. Gellman

**8:20** CATL **313**. Revisiting the structure insensitivity of CO oxidation on supported Pt catalysts. M. Kale, P. Christopher

**8:40** CATL **314**. Contrasting metal-catalyzed C–C and C–O hydrogenolysis. D. Hibbitts, D. Flaherty, E. Gurbuz, E. Iglesias

**9:00** CATL **315**. Reaction pathways for phenolics hydrodeoxygenation governed by the oxophilicity of the metal catalysts. D.E. Resasco

**9:40** CATL **316**. Conversion of lactic acid to bio-acrylic acid on lanthanum phosphate catalysts. C. Wang, D. Theng, A. Borgna

**10:00** CATL **317**. 3D printed sensitizer surface for photooxidation chemistry: Aspects on water disinfection. N. Walalawela, Y. Liu, Y. Zhao, A.M. Lyons, A. Greer

**10:20** CATL **318**. Colloidal Pd nanoparticles design: *In situ* characterization combined with kinetic modeling. A.M. Karim, W. Li, C. Thompson, S. Mozaffari, S. Ivanov, S. Seifert

**11:00** CATL **319**. Energetics of adsorbed methyl on Ni(111) by microcalorimetry. W. Zhao, S. Carey, C.T. Campbell

**11:20** CATL **320**. Application of phosphate-based self-assembled monolayers for chemoselective hydrogenation. J. Zhang, L. Ellis, J.W. Medlin

**11:40** CATL **321**. Carbon support effects on liquid-phase hydrogenation reactions. R.G. Rao, J. Tessonnier

## Section B

Manchester Grand Hyatt San Diego  
Coronado B

## Computational Chemistry Across Catalysis

## From Heterogeneous to Homogeneous Catalysis

*Cosponsored by COMF, ENFL and WCC*

C. Michel, P. Sautet, *Organizers*

A. W. Goetz, D. G. Vlachos, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05** CATL **322**. Ab initio studies of plasma: Surface interactions in the plasma-catalytic dry reforming of methane. K. Stocker, W. Lin, G.C. Schatz

**8:25** CATL **323**. Modeling promoter effects in iron-based Fischer-Tropsch catalysis. M.J. Louwerse, J. Xie, K. De Jong

**8:45** CATL **324**. Theoretical insights into the “green” synthesis of aniline from benzene and ammonia using a Ni catalyst. Z. Alsunaidi, T.R. Cundari, A.K. Wilson

**9:05** CATL **325**. Theoretical study of carbon deposition through the disproportionation of carbon monoxide on the supported nickel catalyst. Y. Izumi, N. Mizukami, H. Kamata, H. Ushiyama

**9:25** CATL **326**. H<sub>2</sub>S decomposition on bare and doped (0001) surface of Cr<sub>2</sub>O<sub>3</sub>: Doping changes the thermodynamic selectivity towards H<sub>2</sub>O formation. J.J. Carey, M. Nolan

**9:45** Intermission.

**10:05** CATL **327**. Withdrawn.

**10:25** CATL **328**. Computational investigation of enhanced activity and stability in Mo-doped Pt–Ni octahedral nanoparticles using a cluster expansion. L. Cao, T. Mueller

**10:45** CATL **329**. Modelling the properties of AuAg bimetallic nanoparticles for H<sub>2</sub> production. A.L. Gould, A. Logsdail, C.A. Catlow

**11:05** CATL **330**. Elucidation of the mechanism of activation of dioxygen by iron (II)polypyridylamine complexes in water. D. Angelone, J. Chen, A. Darksharapu, W.R. Browne, M. Swart

**11:25** CATL **331**. Structure and stability of open zwitterionic versus closed spirocycle structures in organocatalysis promoted by n-heterocyclic carbenes. L. Falivene, L. Cavallo

**11:45** Concluding Remarks.

## Section C

Manchester Grand Hyatt San Diego  
Harbor Ballroom C

## Surface Chemistry &amp; Catalysis of Metal Oxides

A. Selloni, A. Vojvodic, *Organizers, Presiding*

**8:00** CATL **332**. Surface chemistry and catalysis on the magnetite Fe<sub>3</sub>O<sub>4</sub>(100) surface. G. Parkinson

**8:30** CATL **333**. Role of dopands and surface polarity in the water oxidation at transition metal oxide surfaces: Insights from DFT+U calculations. H. Hajiyani, R. Pentcheva

**9:00** CATL **334**. Withdrawn.

**9:15** CATL **335**. Activation, regeneration, and active site identification of oxide-based olefin metathesis catalysts. K. Ding, P.C. Stair

**9:30** CATL **336**. Carbon–carbon bond formation upon dimethylether activation on alumina. P. Sautet, A. Comas-Vives, M. Valla, C. Coperet

**9:45** Intermission.

**10:00** CATL **337**. Activation of the carbon-hydrogen bond by oxides and halides. H. Metiu

**10:30** CATL **338**. On the performance of aluminium substituted lanthanum based perovskite type oxides in methane partial oxidation by framework oxygen. F. Mudu, U. Olsbye, B. Arstad, S. Diplas, Y. Li, H. Fjellvåg

**11:00** CATL **339**. Adsorption of water and carbon oxides on monoclinic zirconia from first principles calculations. K. Honkala

**11:30** CATL **340**. Oxidation reactions on yttria-stabilized zirconia: Redox chemistry on an irreducible oxide. D. Chaopradith, D.O. Scanlon, C.A. Catlow

**11:45** CATL **341**. Identification and exclusion of reaction intermediates in photocatalytic CO<sub>2</sub> reduction to methane. J. Strunk, A.R. Pougin, M. Dilla

## Section D

Manchester Grand Hyatt San Diego  
Pier

## Elucidation of Mechanisms &amp; Kinetics on Surfaces

*Cosponsored by COLL, ENVR and PHYS*

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

**8:00** CATL **342**. Mechanistic bridge between homogeneous and heterogeneous catalysis for the liquid phase CO<sub>2</sub> hydrogenation to formates. G. Filonenko, W. Vrijburg, R. van Putten, E. Hensen, E. Pidko

**8:40** CATL **343**. Using “active site” kinetics models to understand the role of water in Au catalyzed oxidations. B.D. Chandler, J. Saavedra, S. Luikart, M. Santos, C.J. Pursell

**9:20** CATL **344**. *In situ* studies and the mechanism of the water-gas shift reaction on Cu-ceria catalysts. J. Rodriguez, D.J. Stacchiola, S.D. Senanayake, P. Liu, J. Hanson, A. Martinez-Arias, J. Evans, J. Graciani, J.F. Sanz

**9:40** Intermission.

**10:00** CATL **345**. Reaction mechanism and kinetics of olefin metathesis by supported ReO<sub>3</sub>/Al<sub>2</sub>O<sub>3</sub> catalysts. S. Lwin, I.E. Wachs

**10:40** CATL **346**. Manipulating the reactivity of Rh catalysts via anionic strong metal support interactions. J. Matsubu, P. Christopher

## Section E

Manchester Grand Hyatt San Diego  
Coronado A

## Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Cosponsored by ENFL*

M. Saeys, *Organizer*

E. Hensen, *Organizer, Presiding*

**8:00** CATL **347**. Catalyst structure and C–O activation during Fischer-Tropsch synthesis: New ideas from computational catalysis. K.K. Gunasooriya, M. Saeys

**8:30** CATL **348**. Size-selected subnanometer cobalt clusters in Fischer-Tropsch reaction. S. Lee, B. Lee, S. Seifert, R.E. Winans, S. Vajda

**9:00** CATL **349**. Tracking down the loss of cobalt active sites at birth and during aging of a Fischer-Tropsch catalyst. P. Raybaud, M. Corral Valero, K. Larmier, C. Chizzallet

**9:30** CATL **350**. CO on CoCu: Induced surface (anti)segregation and outcomes on CO dissociation. G. Collinge, N. Kruse, J. McEwen

**10:00** Intermission.

**10:30** CATL **351**. Fischer-Tropsch synthesis over Co(0001): An approach to the atomic scale by *in situ* STM. J. Winterlin

**11:00** CATL **352**. Self-assembly of Fischer-Tropsch products on Co(0001) observed by high pressure scanning tunneling microscopy. V. Navarro

**11:30** CATL **353**. Visualization of compression and spillover in a co-adsorbed system: Syngas on cobalt nanoparticles. E.H. Sykes

## Section F

Manchester Grand Hyatt San Diego  
Coronado D

## James Flack Norris Award in Physical Organic Chemistry: Symposium in honor of Juan C. Scaiano

G. Cosa, *Organizer, Presiding*

K. Stamplecoskie, *Presiding*

**8:00** Introductory Remarks.

**8:05** CATL **354**. Optimizing photocatalytic activity of metal clusters through precise synthesis. K. Stamplecoskie

**8:50** CATL **355**. Cleaning the stream:

Catalytic H<sub>2</sub> release from ammine metal borohydrides. M. Mostajeran, M.A. Reynen, R. Baker

**9:35** CATL **356**. Probing samarium oxide nanoparticle catalysis at the single molecule level with fluorescence microscopy. G.K. Hodgson, S. Impellizzeri, J. Scaiano

**9:55** CATL **357**. N-heterocyclic carbenes as novel, stable ligands for self-assembled monolayers on 2-dimensional metal surfaces, metal nanoparticles, and metal nanoclusters. C.M. Crudden

**10:40** CATL **358**. New opportunities for old heterogeneous catalysts: Noble metal nanoparticles driving isomerization and photo-redox C–C coupling reactions. A.E. Lanterna, J. Scaiano

**11:00** CATL **359**. Helping nature regain control of the global carbon cycle. T.A. Moore, A.L. Moore, J.D. Gust

## Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of Donna G. Blackmond

*Sponsored by ORGN, Cosponsored by CATL and WCC*

## In Situ &amp; Operando Characterization &amp; Modelling of Reaction Kinetics

## In Situ Studies, Oxidation &amp; Gold Catalysts

*Sponsored by ENFL, Cosponsored by CATL*

## Application of Computational Chemistry for Energy &amp; Fuel Production

## Computational Catalysis in Research

*Sponsored by ENFL, Cosponsored by CATL*

CO<sub>2</sub> Conversion & Utilization Conversion

*Sponsored by ENFL, Cosponsored by CATL*

## Nanomaterials for Energy Conversion &amp; Storage

## Energy Storage: Computational/ Application

*Sponsored by ENFL, Cosponsored by CATL*

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## WEDNESDAY AFTERNOON

## Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom B

## Catalytic Processes at Interfaces: Fundamentals &amp; Applications

B. Xu, *Organizer*

R. Gounder, D. Hibbitts, *Organizers, Presiding*

**1:00 CATL 360.** Role of the metal-oxide support for methane activation on supported metal clusters. J.J. Carey, M. Nolan

**1:20 CATL 361.** Heterogeneous catalysed production of green C6 diols and triols. B. Kühne, M. Kunz, H. Vogel

**1:40 CATL 362.** Propylene from bio-derived propionic acid: Acid hydrogenation and alcohol dehydration. T.R. Eaton, X. Wang, A. Settle, D. Vardon, E. Karp, G. Beckham

**2:00 CATL 363.** Shape-selective zeolite catalysis for polyester bioplastics production. M. Dusseier

**2:40 CATL 364.** Probing reactivity and selectivity of surface species during alkene chain growth on solid Brønsted acids. M. Sarazen, E. Iglesia

**3:00 CATL 365.** Science and technology of framework metal-containing molecular sieves catalysts. L. Nemeth, S.R. Bare

**3:20 CATL 366.** Plasma-assisted catalytic dry reforming of methane: Exploring the effects of dielectric barrier discharge plasma on catalyst performance. J.C. Hicks

**4:00 CATL 367.** Developing polymeric platforms for the enhancement of molecular catalysts via secondary sphere effects. S. Sahu, C.W. Machan, C.P. Kubiak, N.C. Gianneschi

**4:20 CATL 368.** Studies on crystal growing for morphology control of ZSM-5. J. Shi, J. Teng, Y. Wang, Z. Xie

**4:40 CATL 369.** Role of non-bulk interfacial structure in charge localisation in rutile-anatase TiO<sub>2</sub> composites. M. Nolan, N.A. Deskins, K. Schwartzberg, K.A. Gray

## Section B

Manchester Grand Hyatt San Diego  
Coronado B

## Surface Chemistry &amp; Catalysis of Metal Oxides

A. Selloni, A. Vojvodic, *Organizers, Presiding*

**1:00 CATL 370.** Structural and dynamic aspects of site isolation at the surface of selective oxidation catalysts. A. Trunschke

**1:30 CATL 371.** Mechanistic insights for propane ammoxidation over Mo-V-Te-Nb mixed metal oxide M1 phase from density functional theory. J. Yu, C. Zhao, Y. Xu, V.V. Gullants

**2:00 CATL 372.** Cation synergies and support effects in V-W oxide catalysts for NO<sub>x</sub> abatement. M.E. McBriarty, Z. Feng, G.P. Campbell, T.L. Drake, J. Elam, P.C. Stair, D.E. Ellis, M.J. Bedzyk

**2:15 CATL 373.** Adsorption and adhesion energetics of Au on MgO(100) studied by single crystal adsorption calorimetry: Comparison to Cu and Ag on MgO(100) and Au on CeO<sub>2-x</sub>(111). S.L. Hemmingson, G.M. Feeley, T. James, C.T. Campbell

**2:30** Intermission.

**2:45 CATL 374.** Surface chemistry and catalysis of cerium oxide-based systems: Theoretical and experimental model catalysts. M. Ganduglia-Pirovano

**3:15 CATL 375.** Multi-scale modelling and reactivity of cerium oxide. K. Hermansson, P. Broqvist, M. Wolf, J. Kullgren

**3:45 CATL 376.** Dynamic formation of catalytic active sites during CO oxidation on TiO<sub>2</sub> and CeO<sub>2</sub>-supported gold nanoparticles. Y. Wang, Y. Yoon, D.C. Cantu, M. Lee, V. Glezakou, R. Rousseau

**4:15 CATL 377.** Controlling the nature of mixed-metal oxide catalysts at the nanometer level: CeO<sub>2</sub>/TiO<sub>2</sub> and the importance of Ce<sup>3+</sup> as an active site. J. Rodriguez, D.J. Stacchiola, S.D. Senanayake, P. Liu, J. Evans, J. Graciani, J.F. Sanz

**4:45 CATL 378.** C-H bond activation at ceria-supported vanadia catalysts: DFT studies on the selective oxidation of methanol. T.E. Kropp, J.A. Paier, J. Sauer

## Section C

Manchester Grand Hyatt San Diego  
Pier

## Elucidation of Mechanisms &amp; Kinetics on Surfaces

*Cosponsored by COLL, ENVR and PHYS*

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

**1:00 CATL 379.** Impact of reaction conditions on active sites in zeolite catalysis. F. Goeltl, A. Love, P. Sautet, I. Hermans

**1:40 CATL 380.** *In situ* NMR measurements shed light on the kinetics and mechanism of glucose isomerization in NaX zeolite. S.L. Scott, L. Qi

**2:20 CATL 381.** Probing the surface kinetics of high temperature, millisecond reactions. P.J. Dauenhauer

**3:00** Intermission.

**3:20 CATL 382.** Understanding and tuning the surface chemistry of ceramic non-oxide metal catalysts. S. Laursen, Y. He, S. Poudyal, Y. Song

**4:00 CATL 383.** Low pressure CO<sub>2</sub> hydrogenation to methanol at oxide-metal interfaces. D.J. Stacchiola, J. Rodriguez, P. Liu, S.D. Senanayake

## Section D

Manchester Grand Hyatt San Diego  
Harbor Ballroom C

## Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Cosponsored by ENFL*

E. Hensen, M. Saeys, *Organizers*

J. Gascon, *Presiding*

**1:00 CATL 384.** Combined transient kinetic and computational study of Co-catalyzed Fischer-Tropsch synthesis. E. Hensen, W. Chen, B. Zijstra, I. Filot, R. Pestman

**1:30 CATL 385.** Coverage-dependent mechanisms of CO hydrogenation over Co-based catalysts. N. Kruse

**2:00 CATL 386.** Selectivity of C<sub>5</sub>+ in Co-based Fischer-Tropsch synthesis. A. Holmen, N. Tsakoumis, E. Rytter

**2:30 CATL 387.** Impact of readsorption of olefins at the product slate in FT. H. Oosterbeek, S. van Bavel

**3:00** Intermission.

**3:30 CATL 388.** Influence of metal oxide promoters on Fischer Tropsch synthesis over Co. A.T. Bell

**4:00 CATL 389.** Elucidating fundamental aspects of the cobalt-catalyzed Fischer-Tropsch synthesis by using model catalyst systems and *in situ* spectroscopic characterization. A. Martinez

**4:30 CATL 390.** Fischer-Tropsch synthesis catalysts: Strategies to enhance the sensitivity of *in situ* characterization techniques. M. Ronning

## Section E

Manchester Grand Hyatt San Diego  
Coronado A

## James Flack Norris Award in Physical Organic Chemistry: Symposium in honor of Juan C. Scaiano

G. Cosa, *Organizer, Presiding*

**1:00 CATL 391.** From chemoselective fluorescence imaging to autocatalytic singlet oxygen generation enabled by activatable probes. G. Cosa

**1:45 CATL 392.** Design and applications of single-molecule switches for the investigation of inorganic catalysts with fluorescence microscopy. S. Impellizzeri, J. Scaiano

**2:05 CATL 393.** Photochemistry within a water-soluble organic capsule. V. Ramamurthy

**2:50 CATL 394.** Solid state photochemistry and spectroscopy with nanocrystalline suspensions. M.A. Garcia-Garibay

**3:35** Introduction of Awardee.

**3:40 CATL 395. Award Address** (James Flack Norris Award in Physical Organic Chemistry sponsored by the ACS Northeastern Section). From the mole to the molecule: Nanocatalysis, one molecule at a time. J. Scaiano

## In Situ &amp; Operando Characterization &amp; Modelling of Reaction Kinetics

## Microkinetics &amp; Renewables

*Sponsored by ENFL, Cosponsored by CATL*

## Application of Computational Chemistry for Energy &amp; Fuel Production

## Computational Catalysis in Research

*Sponsored by ENFL, Cosponsored by CATL*

CO<sub>2</sub> Conversion & Utilization

## Photoconversion

*Sponsored by ENFL, Cosponsored by CATL*

## George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in honor of Mieczyslaw M. Boduszynski

*Sponsored by ENFL, Cosponsored by CATL*

## THURSDAY MORNING

## Section A

Manchester Grand Hyatt San Diego  
Coronado A

## Catalytic Processes at Interfaces: Fundamentals &amp; Applications

R. Gounder, *Organizer*

D. Hibbitts, B. Xu, *Organizers, Presiding*

**8:00 CATL 396.** Single cobalt molecular catalyst for splitting CO<sub>2</sub> and H<sub>2</sub>O into CO and O<sub>2</sub>. N. Morlanes, V. Rodionov, K. Takanabe

**8:20 CATL 397.** Efficient electrocatalysts prepared by pulse electrochemical deposition for PEM fuel cells. C.D. Cooper, J.J. Burk, S.K. Buratto

**8:40 CATL 398.** Electrodeposited MnO<sub>x</sub>/PEDOT thin films as catalysts for the oxygen reduction reaction. T.N. Lambert, J.A. Vigil, K. Eldred

**9:00 CATL 399.** First principles studies of heterogeneous catalysis: Complexity at interfaces. J.P. Greeley

**9:40 CATL 400.** Size-selected vanadium oxide clusters on TiO<sub>2</sub>(110) and iron oxide clusters on Pt(111): Discovering mechanisms of oxidative reactions at interfaces: Every atom counts. J.W. Buffon, H.L. Neilson, J.C. Robins, S.K. Buratto

**10:00 CATL 401.** Exploring thermocatalytic and electrocatalytic properties of organic and inorganic porous materials. B.G. Trewyn

**10:20 CATL 402.** Direct synthesis of H<sub>2</sub>O<sub>2</sub>: Competition between heterolytic and homolytic processes at the liquid-solid interface. D. Flaherty

**11:00 CATL 403.** DFT study of liquid environment effects on water and hydrogen peroxide formation on platinum. R. Ferreira de Moraes, F. Calle-Vallejo, A.A. Franco, P. Sautet, D. Loffreda

**11:20 CATL 404.** Energetics of Au and Cu adsorption and film growth on Pt(111) measured by single-crystal adsorption calorimetry. G.M. Feeley, S.L. Hemmingson, T. James, C.T. Campbell

**11:40 CATL 405.** Implications of acid strength, confinement, and site proximity for reactivity and selectivity in bifunctional metal-alc catalysis. G. Noh, E. Iglesia

## Section B

Manchester Grand Hyatt San Diego  
Coronado B

## General Papers

R. Ghose, E. Nikolla, *Organizers*

V. Schwartz, *Presiding*

**8:00 CATL 406.** Withdrawn.

**8:15 CATL 407.** Bimetallic iron and nickel nanoparticles for oxygen evolution and methanol oxidation under alkaline conditions for fuel cells. S. Candelaria, N. Bedford, T. Woehl, L. Greenlee

**8:30 CATL 408.** Transition metal chalcogenides as viable water oxidation/reduction catalysts. M. Nath, A. Swesi, J. Masud

**8:45 CATL 409.** Multimetallic alloy nanocatalysts for energy production, conversion, and storage. H. Cronk, S. Kim, Z. Skeete, Y. Zhao, S. Shan, J. Lou, C. Zhong

**9:00 CATL 410.** Plasmon induced heating of Au modified ZnO for CO<sub>2</sub> hydrogenation. S. Hammache, C. Wang, C. Matranga

**9:15 CATL 411.** C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> core-shell nanowire arrays for efficient visible-light photoelectrocatalytic bisphenol A degradation. Y. Wang, Q. Wu, W. Bai, G. Jiang, Z. Zhao, J. Chen

**9:30 CATL 412.** Pd@Pt core-shell concave decahedra: A class of catalysts for enhancing the oxygen reduction reaction. M. Vara, X. Wang, M. Luo, H. Huang, A. Ruditskiy, J. Park, S. Bao, J. Liu, J. Howe, M. Chi, Z. Xie, Y. Xia

**9:45** Intermission.

**10:00 CATL 413.** Multi-component hybrid material structures for electrocatalytic hydrogen generation. H. Wang

**10:15 CATL 414.** Glycerol oxidation on supported electroless CuNiMoP. O. Elendu

- 10:30 CATL 415.** Speciation and kinetic study of iron promoted sugar conversion to 5-hydroxymethylfurfural (HMF) and levulinic acid (LA). **Y. Jiang**, L. Yang, C.M. Bohn, G. Li, D. Han, N.S. Mosier, J.T. Miller, H.I. Kenttamaa, M.M. Abu-Omar
- 10:45 CATL 416.** Formation of 1,3-butadiene from ethanol in a two-step process using modified zeolite- $\beta$  catalysts. **A. Klein**, R. Palkovits
- 11:00 CATL 417.** Platinum-catalyzed, terminal selective C(sp<sup>3</sup>)-H oxidation of aliphatic amines. **M. Lee**, M.S. Sanford
- 11:15 CATL 418.** Rational design of ZSM-11 catalyst with tunable physicochemical properties. **Y. Shen**, J.D. Rimer
- 11:30 CATL 419.** Withdrawn.
- 11:45 CATL 420.** Preparation of a floating metal catalyst on solution surface. **M. Li**, C. Liu

## Section C

Manchester Grand Hyatt San Diego  
Pier

### General Papers

R. Ghose, E. Nikolla, *Organizers*  
V. Schwartz, *Presiding*

- 8:00 CATL 421.** TiO<sub>2</sub> supported Ru, Fe, and Co nano-catalysts coated in microchannel Si-microreactor for Fischer-Tropsch synthesis. **R. Abrokwah**, M. Rahman, V.G. Deshmehane, S. Woosley, S. Aravamudan, D. Kushla
- 8:15 CATL 422.** Uniform nanostructures for heterogeneous catalysis by fast annealing of monodisperse metal nanocrystals. **M. Cargnello**, C. Chen, R.J. Gorte, C.B. Murray
- 8:30 CATL 423.** Selective oxidative upgrading of ethane under mild reaction conditions over Fe- and Cu- ZSM-5 catalysts; a stirred batch and continuous flow study. **R.D. Armstrong**, M. Forde, S.J. Freakley, C. Hammond, Q. He, R.L. Jenkins, S.A. Kondrat, J. Lopez-Sanchez, S.H. Taylor, D.J. Wilcock, C.J. Kiely, G. Hutchings
- 8:45 CATL 424.** Removal of nitrogen species from bitumen-derived gas oil prior to hydrotreating: Efficient approach towards improving refinery feedstock. **P. Misra**, A.K. Dalai, J. Adjaye
- 9:00 CATL 425.** Mesoporous manganese oxide as an efficient heterogeneous catalyst for solvent free oxidative activation of C-H bond. **K. Mullick**, S. Biswas, A.M. Angeles Boza, S.L. Suib
- 9:15 CATL 426.** Particle size effects of Ag/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub> for ethylene epoxidation. **J. van den Reijen**, S. Kanungo, A. Nijhuis, K. de Jong, P. de Jongh
- 9:30 CATL 427.** Graphene-oxide-supported Cu-Al and Co-Al hydroxalicates as enhanced catalysts for carbon-carbon coupling via Ullmann reaction. **R. Menzel**, M.M. Mostafa, **S.M. Bawaked**, S.N. Basahel, S.A. Al-Thabaiti, M. Shaffer
- 9:45 Intermission.**
- 10:00 CATL 428.** Improving stability of zeolites in aqueous phase via selective structural defect removal. **S. Prodingner**, M. Derewinski, A. Vjunov, I. Arslan, S. Burton, J.A. Lercher
- 10:15 CATL 429.** Cu/SiO<sub>2</sub> catalysts: Influence of reduction on particle size and stability. **L. Pompe**, R. van den Berg, K. de Jong, P. de Jongh
- 10:30 CATL 430.** Recyclable gold nanoparticles as routine benchtop catalysts: efficient hydration, semihydrogenation of alkynes and reductive amination. **S. Liang**, B. Xu, G.B. Hammond

- 10:45 CATL 431.** Synthesis of mesoporous zeolite Y and its applications in catalytic reaction. **J. Zhao**, L. Qin, G. Wang, Y. Chen, B. Liu
- 11:00 CATL 432.** Mechanism for the direct synthesis of H<sub>2</sub>O<sub>2</sub> on Pd clusters: Heterolytic reaction pathways at the liquid-solid interface. **N.M. Wilson**, D. Flaherty
- 11:15 CATL 433.** Acceptorless alcohol dehydrogenation catalyzed by a bifunctional Ir-NHC catalyst. **E. Martinez-Castro**, G. González Miera, B. Martin-Matute
- 11:30 CATL 434.** Earth abundant metals in catalysis: The reduction of carbonyl compounds using iron catalysts. **F.S. Wekesa**, Z. Sumner, L. Kong, R. Arias-Ugarte, **M. Findlater**
- 11:45 CATL 435.** Performance evaluation of proton exchange membrane fuel cells using cobalt oxide based anodic electrocatalyst. **S. Bashir**, J.L. Liu

## Section D

Manchester Grand Hyatt San Diego  
Coronado E

### Elucidation of Mechanisms & Kinetics on Surfaces

*Cosponsored by COLL, ENVR and PHYS*

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

- 8:00 CATL 436.** Elementary steps in surface reactions: Mechanisms, kinetics, and thermodynamics. **S. Schauerermann**
- 8:40 CATL 437.** Vinyl acetate formation pathways and selectivity on model metal and alloy catalyst surfaces. **W.T. Tysoe**
- 9:20 CATL 438.** Mechanism of CO<sub>2</sub> hydrogenation on Pd/Al<sub>2</sub>O<sub>3</sub> catalysts: Kinetics and transient DRIFTS-MS studies. **X. Wang**, H. Shi, J. Kwak, **J. Szanyi**
- 10:00 Intermission.**
- 10:20 CATL 439.** Modeling bulk composition dependent properties of Cu<sub>x</sub>Pd<sub>1-x</sub> alloy surfaces. **J.R. Kitchin**, J. Boes, A.J. Gellman
- 11:00 CATL 440.** Use of effusive molecular beams to measure kinetics of catalytic reactions. **F. Zaera**
- 11:40 CATL 441.** Understanding site isolation of Pd and Ni in Zn- and Ga-based bulk intermetallics during the selective hydrogenation of alkynes. **A. Dasgupta**, C. Spanjers, M.J. Janik, **R.M. Rioux**

## Section E

Manchester Grand Hyatt San Diego  
Coronado D

### Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Cosponsored by ENFL*

E. Hensen, M. Saeys, *Organizers*

J. W. Thybaut, *Presiding*

- 8:00 CATL 442.** MOF-mediated synthesis of highly active and stable catalysts for syngas chemistry. **T. Wezendonk**, X. Sun, L. Oar-Arteta, M. Makkee, F. Kapteijin, **J. Gascon**
- 8:30 CATL 443.** Fischer-Tropsch synthesis: Improved C5+ selectivity with pore-modified alumina. **G. Jacobs**, C. Bertaux, V.R. Pendyala, W.D. Shafer, B.H. Davis
- 9:00 CATL 444.** Selectivity control in Fischer-Tropsch synthesis for the production of liquid fuels. **K. Cheng**, J. Kang, **Q. Zhang**, **Y. Wang**
- 9:30 Intermission.**

- 10:00 CATL 445.** Size and promoter effects in supported iron Fischer-Tropsch catalysts: Insights from experiment and theory. **K. de Jong**, J. Xie, J. Yang, A. Holmen, D. Chen, M. Louwerse
- 10:30 CATL 446.** Insight into iron-based Fischer-Tropsch synthesis reaction. **D. Ma**
- 11:00 CATL 447.** Combating the detrimental effects of water in Fe-based CO<sub>2</sub> hydrogenation catalysts. **M.J. Bradley**, R. Ananth, F. Dimascio, D. Hardy, B. Jeffrey, H. Willauer

### In Situ & Operando Characterization & Modelling of Reaction Kinetics

#### In Situ Techniques & Electrocatalysis

*Sponsored by ENFL, Cosponsored by CATL*

### Application of Computational Chemistry for Energy & Fuel Production

#### Computational Catalysis in Research

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## THURSDAY AFTERNOON

### Section A

Manchester Grand Hyatt San Diego  
Coronado A

### General Papers

R. Ghose, E. Nikolla, *Organizers*

V. Schwartz, *Presiding*

- 1:00 CATL 448.** Organometallic studies of catalytically relevant nickel complexes for aromatic fluoroalkylation. **J.R. Bour**, M.S. Sanford
- 1:15 CATL 449.** Withdrawn.
- 1:30 CATL 450.** Withdrawn.
- 1:45 CATL 451.** Withdrawn.
- 2:00 CATL 452.** Insights into a bifunctional iridium complex-promoted *N*-alkylation of amines with alcohol. **G. González Miera**, B. Agnieszka, R. Marcos, P. Norrby, B. Martin-Matute
- 2:15 CATL 453.** Smartest silica technology: Getting the most from your Pd-catalysed process. **S. Purser**, C. North, P. Murray
- 2:30 CATL 454.** Broad spectrum antimicrobial activity of photocatalytically active nanostructured graphitic carbon nitride (ns-g-C<sub>3</sub>N<sub>4</sub>) coatings under visible radiation. **J.H. Thurston**, N.M. Hunter, K. Cornell
- 2:45 Intermission.**
- 3:00 CATL 455.** Novel catalysts excellent for preparation of the lower Mooney HNBR specialty rubbers. **Z.J. Zhan**, L. Xin, W. Ren
- 3:15 CATL 456.** Azobenzene and micellar catalysis. **C. Len**, F. Mangin, E. Leonard
- 3:30 CATL 457.** Enhanced visible light photocatalytic activities of TiO<sub>2</sub> reduced graphene oxide nanoparticles and its application in rhodamine B degradation. **Y. Chen**, Y. Cao, X. Dong
- 3:45 CATL 458.** Influence of Cu and Pd substitution on catalysis of selective catalytic oxidation of NH<sub>3</sub> to N<sub>2</sub>. **P. Li**, R. Zhang, B. Chen
- 4:00 CATL 459.** Catalyst of benzene alkylation with dilute ethylene and its commercial applications. **Z. Shen**, B. Zhang, H. Sun, W. Yang
- 4:15 CATL 460.** Promotional effect of boron in catalytic tar reforming: First principles investigation using toluene as a model compound. **Q. Trinh**, S.H. Mushrif

- 4:30 CATL 461.** Biomass-derived gas-phase alkali as a tar reforming catalyst promoter in sulfur-laden biomass gasification gas. **P. Haghghi Moud**, K. Andersson, K. Engvall
- 4:45 CATL 462.** Insight into factors affecting the selectivity of light olefins in MTO process. **Y. Gao**, S. Chen, Y. Wang

## Section B

Manchester Grand Hyatt San Diego  
Promenade A

### General Papers

R. Ghose, E. Nikolla, *Organizers*

V. Schwartz, *Presiding*

- 1:00 CATL 463.** Effect of organic salt on the yields of trioxane in reaction solution and in distillate. **W. Haiyan**, H. Yufeng, Y. Liuyi
- 1:15 CATL 464.** Study on design, synthesis, and catalytic application of microporous triptycene-based polymers. **X. Zhang**, Y. Lv, X. Liu, G. Du, S. Yan, J. Liu, Z. Zhao
- 1:30 CATL 465.** Synthesis of polyoxymethylene dimethyl ethers catalyzed by the pyridolone-based ionic liquids. **Y. Zhenyu**, H. Yufeng, M. Weiting
- 1:45 CATL 466.** CuS/RGO hybrids by one-pot method for efficiently electrochemical sensing of hydrogen peroxide. **X. Zhang**, W. Liu
- 2:00 CATL 467.** Synthesis of glycol-based bolaamphiphile cobalt-Schiff base complexes for catalytic breakdown of lignin in whole biomass. **W.T. Hartwig**, J.J. Bozell
- 2:15 CATL 468.** Novel brønsted-acidic ionic liquids as catalysts for synthesizing trioxane. **J. Qi**, H. Yufeng, M. Weiting
- 2:30 CATL 469.** Combining mutagenesis and the use of a chemical auxilliary for the hydroxylation of non-activated CHs by P450 3A4. **P. Schiavini**, J. Pottel, N. Moitessier, K. Auclair
- 2:45 Intermission.**
- 3:00 CATL 470.** Analysis of fractionated bio-oils. **M.V. Olarte**, J. Ferrell, A. Padmameruma, E. Christensen, C. Drennan
- 3:15 CATL 471.** Recyclable multicatalytic colloids with scalable functionalities and high dispersion stability in organic and aqueous media via layer-by-layer assembly. **D. Kim**, Y. Ko, J. Cho
- 3:30 CATL 472.** Novel strategy for producing highly dispersed Pd particles on ZIF-8 through the occupation and unoccupation of carboxyl groups and its application in selective diene hydrogenation. **X. Jia**, Y. Fan
- 3:45 CATL 473.** Three-dimensional graphene-based bimetallic hybrids with flexibly switchable peroxidase-like catalytic activity. **F. Yuan**, H. Zhao, X. Quan
- 4:00 CATL 474.** Simple synthesis of three-dimensionally ordered macroporous ZrO<sub>2</sub>-supported Pt@CeO<sub>2-x</sub> core-shell nanoparticles with high catalytic activity and stability for soot oxidation. **Y. Li**, Z. Zhao, Y. Wei, B. Jin
- 4:15 CATL 475.** Different effect of Cu species on highly active Cu-SAPO-18 catalysts for selective catalytic reduction of NO with ammonia. **Y. Li**, J. Liu, Z. Zhao
- 4:30 CATL 476.** Role of PEG on the formation of polyphenols with laccase enzymes. **J. Su**, A. Cavaco-Paulo
- 4:45 CATL 477.** Silicon nanocrystals as catalysts for dehydrogenation of secondary alcohols into ketones: The case of room-temperature production of acetone and hydrogen from isopropanol. **J. El Demellawi**, C. Holt, E. Abou-Hamad, Z. Al-Talla, Y. Sait, S. Chaieb

## Section C

Manchester Grand Hyatt San Diego  
Pier

### Elucidation of Mechanisms & Kinetics on Surfaces

*Cosponsored by COLL, ENVR and PHYS*

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

**1:00 CATL 478.** Mechanistic study of methanol synthesis from CO<sub>2</sub> and H<sub>2</sub> on a modified model Mo sulfide-based catalysts. C. Liu, P. Liu

**1:40 CATL 479.** Surface dynamics of first row transition metal and alloy clusters and their catalytic consequences for C-H bond activation. Y. Chin, W. Tu

**2:20 CATL 480.** Electrochemical reduction of CO<sub>2</sub> on Au: An *in situ* spectroscopic study. M. Dunwell, Q. Lu, Y. Yan, F. Jiao, B. Xu

**2:40 CATL 481.** Withdrawn.

**3:00** Intermission.

**3:20 CATL 482.** Normal loading induced catalytic effect on tribopolymer formation on RuO<sub>2</sub>(110) surface. J. Yang, Y. Qi, H. Kim, A.M. Rappe

**3:40 CATL 483.** Acid and base properties of graphitic carbons evaluated by local electronic structures. D. Guo, R. Shibuya, T. Kondo, J. Nakamura

**4:00** Concluding Remarks.

## Section D

Manchester Grand Hyatt San Diego  
Coronado E

### Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Cosponsored by ENFL*

E. Hensen, M. Saeyes, *Organizers*

B. H. Davis, *Presiding*

**1:00 CATL 484.** Deactivation and regeneration of commercial type Fischer-Tropsch co-catalysts. E. Rytter, A. Holmen

**1:30 CATL 485.** Kinetic modeling of primary and secondary reactions in Fischer-Tropsch synthesis. B. Todic, D.B. Bukur

**2:00 CATL 486.** From microkinetic understanding to industrial reactor simulation for Fischer-Tropsch synthesis. J.W. Thybaut, J. Van Belleghem, G.B. Marin

**2:30 CATL 487.** Effect of water over iron-based catalysts for Fischer-Tropsch synthesis using biomass-derived syngas. Z. Wang, K. Mai, J.J. Spivey

**2:45 CATL 488.** Withdrawn.

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## CELL

## Division of Cellulose and Renewable Materials

C. Frazier, *Program Chair*

### OTHER SYMPOSIA OF INTEREST:

**Chemical Modification of Natural Bio-based Material: Design & Application for Value Added Products** (see AGFD, Tue)

**Chemical Imaging: Applications, Advances, & Challenges** (see ANYL, Wed, Thu)

**Biofuel & Biobased Chemical Production: Biomass Pretreatment and Hydrolysis** (see BIOT, Mon)

**Proteins & Polymers Under Confinement** (see COLL, Sun)

**Bioresponsive & Biomimetic Synthetic Polymers & Materials** (see PMSE, Sun, Mon)

**Sustainable Polymers, Processes & Applications** (see POLY, Sun, Mon, Tue)

### BUSINESS MEETINGS:

**CELL Business Meeting**, 5:30 PM: Mon

## SUNDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Cardiff

### Biomass & Polymer Extrusion, Composite & Reaction Technologies: New Insights, Future Potential & Principles to Practice

*Cosponsored by PMSE and POLY*

A. Ayoub, L. A. Lucia, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 CELL 1.** Reactive extrusion of zein with glyoxal and polyethylene maleic anhydride. G.W. Selling, K. Utt

**8:30 CELL 2.** Extraction of cellulose consisted of nanofibers from brown algae and its applications. Y. Du, H. Gao, B. Duan, L. Zhang

**8:55 CELL 3.** From compatibilizing polymer blends to enzymatic polymerizations using reactive extrusion. S. Spinella, C. Samuel, J. Raquez, M. Ganesh, P. Dubois, R.A. Gross

**9:20 CELL 4.** Spinnability and water sensitivity of filaments spun from cellulose nanofibril hydrogels. M. Lundahl, G. Cunha, E. Rojo, H. Orelma, T. Papageorgiou, J.C. Arboleda, O.J. Rojas

**9:45** Intermission.

**10:15 CELL 5.** Genetic engineering of functional large amyloid fibers. D. Roth, D. Ridgley, F.B. Gillam, J.R. Barone

**10:40 CELL 6.** Interest, progress and limitations of reactive extrusion applied to natural polymers. F. Becquart, M. Taha

**11:05 CELL 7.** Inducing silk fibroin nano-particles by chemical oxidation. K. Zheng, Y. Chen, Y. Fan, D.L. Kaplan

**11:30 CELL 8.** Extrusion fiber spinning of polyethylene reinforced with cellulose nanocrystals. N. Brandquist, R.A. Venditti, A. Ayoub

## Section B

Marriott Marquis San Diego Marina  
La Costa

### Lignin Refining, Functionalization & Utilization

#### Refining & Fractionation

C. Crestini, *Organizer*

D. Argyropoulos, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 CELL 9.** Homogeneous technical lignins as phenolic precursors to heat stable polymers & carbon fibers. D. Argyropoulos

**8:30 CELL 10.** Isolation and characterization of sulfur-free lignin produced by Gamma-Valerolactone/Water fractionation of Eucalyptus wood. H. Le, M. Ståhl, M. Borrega, H. Sixta

**8:55 CELL 11.** Chemical and thermal characterization of organosolv yellow poplar lignins fractionated by different time periods. J. Tao, O. Hosseinaei, P. Kim, D.P. Harper, J.J. Bozell, T.G. Rials, N. Labbe

**9:20 CELL 12.** Biomass lignin fractionation using amine-sulfonate functionalized ionic liquids. P. Yan, Z. Xu, C. Zhang, X. Liu, W. Xu, Z. Zhang

**9:45** Intermission.

**10:15 CELL 13.** On the crossflow membrane fractionation of lignoboost kraft lignin: Characterization of low molecular weight fractions. S. Aminzadeh, T. Mattsson, G. Henriksson, M.E. Lindström

**10:40 CELL 14.** Global protocol for the mild quantitative fractionation of lignin carbohydrate complexes (LCC). N. Giummarella, L. Zhang, G. Henriksson, M. Lawoko

**11:05 CELL 15.** Using the DOE bioenergy feedstock library as a tool for lignin structure/property relationship research. S. Fox, R. Emerson, A. Hoover, V. Walker, G. Gresham

**11:30 CELL 16.** Chemical valorisation of lignins toward fine chemicals and polymers: The ChemLiVal project. D. Da Silva Perez, B. Andrioletti, M. Beyerle, C. Cabral-Almada, C. Crestini, L. Djakovitch, V. Dufraud-Niccolai, P. Fongarland, E. Framery, L. Jean-Gerard, R. Kieffer, A. Nunes Coelho, S. Woldemichael, S. Tapin-Lingua

## Section C

Marriott Marquis San Diego Marina  
Point Loma

### New Horizons in Sustainable Materials Nanocellulose

*Cosponsored by DAC<sup>‡</sup> and POLY*

*Financially supported by EPNOE*

P. R. Navard, *Organizer*

K. J. Edgar, *Organizer, Presiding*

**8:25** Introductory Remarks.

**8:30 CELL 17.** Organized thin films of cellulose nanocrystals: From model to optically active films. Y. Habibi

**8:55 CELL 18.** Cross-linked cellulose nanocrystal aerogels as universal 3D substrates for functional nanoparticles. X. Yang, K. Shi, H. Zhu, S. Zhu, I. Zhitomirsky, E.D. Cranston

**9:20** CELL 19. Withdrawn.

**9:45** Intermission.

**10:15 CELL 20.** Amphiphilic and resilient cellulose nanofibril aerogel: Assembling, structural and properties analyses. F. Jiang, Y. Hsieh

**10:40 CELL 21.** Modifying cellulose nanocrystals for enhanced dispersion in polylactide. S. Spinella, C. Samuel, J. Raquez, G. Lo Re, P. Dubois, R.A. Gross

**11:05 CELL 22.** Structure-property relationships of cellulose nanofiber films. M. Zhao, M. Takeuchi, M. Shimizu, T. Saito, A. Isogai

## Section D

Marriott Marquis San Diego Marina  
Marina Salon G

### Structure of Native Celluloses & Variety of Nano-celluloses That Can Be Formed from Them: Anselme Payen Award Symposium in honor of Akira Isogai

*Financially supported by U.S. Forest Service*

U. P. Agarwal, R. H. Atalla, O. J. Rojas, J. Sugiyama, *Organizers*

R. Moon, A. Rudie, *Presiding*

**8:00** Introductory Remarks.

**8:05 CELL 23.** Beyond the crystal structure of cellulose microfibril. Y. Nishiyama, T. Kuribayashi, Y. Ogawa

**8:30 CELL 24.** Brand-new concept for surface modification of TEMPO-oxidized cellulose nanofibers. Y. Yoshida, Y. Kumamoto, K. Yamato, A. Isogai

**8:55 CELL 25.** Comments on chirality and cellulose nanocrystals. D.G. Gray

**9:20 CELL 26.** Periodate oxidation of cellulose – a straightforward reaction that gives a complex product. A. Potthast, T. Rosenau, M. Siller, H.M. Amer, S. Koprivica

**9:45** Intermission.

**10:15 CELL 27.** Mechanistic and kinetic aspects of TEMPO mediated oxidation of cellulose. T. Pääkkönen, C. Bertinetto, R. Pönni, G. Tummala, M. Nuopponen, T. Vuorinen

**10:40 CELL 28.** Developments of nano-cellulose paper for printed electronics. M. Nogi

**11:05 CELL 29.** Potential of cellulose nanofibrils in tissue engineering. K. Syverud, A. Rashad, K.B. Mustafa

**11:30 CELL 30.** Probing the hydrogen bonding network in native cellulose using computational modeling with IR, Raman and sum-frequency-generation (SFG) vibration spectroscopy. C. Lee, J.D. Kubicki, M. Jarvis, S.H. Kim

## Section E

Marriott Marquis San Diego Marina  
Solana

### Functional Lignocellulosics & Nanotechnology

#### Lignocellulosics & Nanotechnology

*Cosponsored by CARB*

*Financially supported by BioNavis; EPNOE*

T. Nypelö, S. Spirk, *Organizers*

I. Piipponen, M. S. Peresin, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 CELL 31.** Photoluminescence in highly ordered transparent cellulose aerogels imparted by surface-grafted carbon dots. S. Plappert, S. Ouraishi, T. Rosenau, F. Liebner

**8:30 CELL 32.** Tailoring the surface chemistry of cellulose nanocrystals in aqueous media: From small molecules to polymer brushes. J.O. Zoppe, L. Johansson, J. Seppälä, H.A. Klok

**8:55** CELL **33.** Processing and high-resolution solution-state NMR analysis of nanocellulose using ionic liquids. A. Holding, J. Helminen, L. Lemetti, S. Heikkinen, V. Mäkelä, S. Kedzior, E.D. Cranston, I. Filpponen, I. Kilpeläinen, A. King

**9:20** CELL **34.** Hybrid materials from hemicelluloses oligomers and fatty acids. D. Da Silva Perez, M. Chemin, Ham-Pichavant, G. Chollet, M. Petit-Conil, H. Cramail, S. Grelier

**9:45** Intermission.

**10:15** CELL **35.** Preparation and stabilization of metal nanoparticles using cellulose. R. Liu, H. Kang, M. Chen, W. Li, J. Tan, Y. Huang

**10:40** CELL **36.** *In-Situ* synthesis of semi-conducting metal sulfide nanoparticles in a polysaccharide matrix. D. Reishofer, H. Ehmann, S. Dunst, G. Trimmel, S. Spirk

**11:05** CELL **37.** Biocidal nanofiber system based on curdlan/polyethylene oxide. M. Elnaggar, A.M. Abdelgawad, C.L. Salas, O.J. Rojas

**11:30** CELL **38.** Cellulose acetate/lignin/copper ii-complex nanofiber composites for hygienic applications: Germicidal and deodorizing materials. A.M. Abdelgawad, M. Elnaggar, O.J. Rojas

## SUNDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Cardiff

#### Biomass & Polymer Extrusion, Composite & Reaction Technologies: New Insights, Future Potential & Principles to Practice

Cosponsored by PMSE and POLY

A. Ayoub, L. A. Lucia, *Organizers, Presiding*

**1:15** Introductory Remarks.

**1:20** CELL **39.** Sustainable thermosets from epoxidized sucrose soyate and carboxylic acids with the assistance of solvents. S. Ma, D.C. Webster

**1:45** CELL **40.** Processing of natural fiber polymer composites: Mechanisms of fiber breakage, composite microstructure and rheology. A. Abdennadher, A. Le Duc, B. Vergnes, M. Vincent, T. Budtova

**2:10** CELL **41.** Structure, properties, and stabilization kinetics of gel spun polyacrylonitrile/lignin blends toward carbon fiber. H.C. Liu, A. Chien, B. Newcomb, A. Bakhtiyari Davijani, S. Kumar

**2:35** CELL **42.** Properties of large amyloid fibers. J.R. Barone, D. Roth

**3:00** Intermission.

**3:30** CELL **43.** Green approaches to preparation of aqueous soy protein colloids and pure protein fibers. X. Liu, Y. Hsieh

**3:55** CELL **44.** Compositional, ultrastructural, and enzymatic efficiency changes of *eucalyptus* during the combination of ionic liquid and alkali treatments. H. Li, S. Sun, R. Sun

**4:20** CELL **45.** Physicochemical properties of cellulose-dissolving superbase ionic liquids. O. Kuzmina, T. Welton

**4:45** CELL **46.** Enhancing the function of graphene oxide nanosheets by crystallization control: Unexpected harvest of strength, ductility and thermal stability for poly(lactic acid) barrier films. H. Xu, D. Wu, X. Yang, Z. Feng, K. Adolfsson, L. Xie, M. Hakkarainen

### Section B

Marriott Marquis San Diego Marina  
La Costa

#### Lignin Refining, Functionalization & Utilization

#### Oxidative & Reductive Lignin Depolymerization

D. Argyropoulos, *Organizer*

C. Crestini, *Organizer, Presiding*

**1:20** CELL **47.** Oxidation depolymerization of lignin using metal-free catalysts. Z. Tong

**1:45** CELL **48.** Design of novel tri- and tetradentate Co-Schiff base complexes for selective catalytic cleavage of lignin. R. Key

**2:10** CELL **49.** Oxidative cracking of lignin with molecular oxygen for production of aromatics and organic acids under mild conditions. G. Lyu, C. Yoo, X. Pan

**2:35** CELL **50.** Depolymerisation of lignin by oxidation in ionic liquids. R. Prado, A. Brandt, X. Erdocia, J.P. Hallett, J. Labidi, T. Welton

**3:00** Intermission.

**3:30** CELL **51.** Withdrawn

**3:55** CELL **52.** Application of low temperature, low pressure hydrogenation to liquefy and stabilize lignin streams. M.R. Rover

**4:20** CELL **53.** *In-situ* and selective hydrodeoxygenation of lignin hydroxyolysis products via bimetallic FeMo phosphide catalyst. Y. Gao, D. Rensel, J.C. Hicks, M. Foston

**4:45** CELL **54.** Nitrate-intercalated layered double-hydroxide catalysts for lignin depolymerization. J. Kruger

### Section C

Marriott Marquis San Diego Marina  
Point Loma

#### New Horizons in Sustainable Materials Lignocellulosics

Cosponsored by DAC<sup>+</sup> and POLY

Financially supported by EPNOE

K. J. Edgar, P. R. Navard, *Organizers*

N. Robitaille Brown, *Presiding*

**1:45** CELL **55.** Comprehensive study on lignin-containing nanocellulose and their effect on properties of the materials made thereof. M.S. Peresin, E. Rojo, O.J. Rojas

**2:10** CELL **56.** From cells to bio-based materials: Dispersion and interfaces as a key to controlling physical properties. N. Le Moigne

**2:35** CELL **57.** Investigation of morphological changes to cellulose via interactions with lignin and clickable designer monogols. S. Basu, O. Ormadjela, C.T. Anderson, Y. Zhu, J.M. Catchmark, J. Zimmer, N. Robitaille Brown

**3:00** Intermission.

**3:30** CELL **58.** Syntheses of hemicellulose derivatives and their application as plastic material. Y. Enomoto-Rogers, N. Fundador, T. Danjo, Y. Oomomo, T. Iwata

**3:55** CELL **59.** Withdrawn.

**4:20** CELL **60.** Design of functionalized cellulose ethers for amorphous solid dispersion via olefin cross-metathesis. Y. Dong, L.I. Mosquera-Giraldo, L. Taylor, K.J. Edgar

**4:45** CELL **61.** NMR and rheological investigations of cellulose dissolution in 1-ethyl-3-methylimidazolium octanoate, as a comparison to cellulose in 1-ethyl-3-methylimidazolium acetate. S.M. Green, M.E. Ries, T. Budtova

### Section D

Marriott Marquis San Diego Marina  
Marina Salon G

#### Structure of Native Celluloses & Variety of Nano-celluloses That Can Be Formed from Them: Anselme Payen Award Symposium in honor of Akira Isogai

Financially supported by U.S. Forest Service

U. P. Agarwal, R. H. Atalla, *Organizers*

O. J. Rojas, J. Sugiyama, *Organizers, Presiding*

**1:15** Introductory Remarks.

**1:20** CELL **62.** Regenerating cellulose I from solution? T. Rosenau, M. Bacher, A. Poththast, F. Nakatsubo, A.D. French

**1:45** CELL **63.** Chemistry at 400 L: What it takes to prepare cellulose nanocrystals and the TEMPO grade of cellulose nanofibrils at pilot scale. A. Rudie, R.S. Reiner

**2:10** CELL **64.** Interactions of polyvinylamine-g-TEMPO with cellulose. R.H. Pelton

**2:35** CELL **65.** Cellulose biotemplates for advanced functional materials. P.E. Fardim, T.J. Heinze, L. Sobhana, C. Lange, K. Gabov, B. Vega, O. Grigoray

**3:00** Intermission.

**3:30** CELL **66.** Post-hydrolysis of birch paper-grade pulp to produce high-purity cellulosic fibers and xylo-oligosaccharides. M. Borrega, H. Sixta

**3:55** CELL **67.** TEMPO mediated oxidation of cellulose: At the cross-section of experimental research on cellulose microfibrils. Q. Li, M. Cho, S.H. Rennecker

**4:20** CELL **68.** Combination of nanocellulose and nanomaterials for functional applications. T. Kitaoka

**4:45** CELL **69.** Fibrillar assembly of bacterial cellulose in the presence of wood hemicelluloses. P.A. Penttilä, J. Sugiyama, T. Imai

### Section E

Marriott Marquis San Diego Marina  
Solana

#### Functional Lignocellulosics & Nanotechnology

#### Surface Interactions on Lignocellulosic Materials

Cosponsored by CARB

Financially supported by BioNavis; EPNOE

I. Filpponen, M. S. Peresin, *Organizers*

S. Spirk, T. Nypelö, *Organizers, Presiding*

**1:20** CELL **70.** Stimuli responsive cellulose nanocrystals hydrogel for smart applications. E. Gicquel, C. Martin, F. Pignon, B.R. Jean, J. Bras

**1:45** CELL **71.** Cellulose nanofibrils as templates for stimuli-responsive membrane materials. M. Hakalahti, A. Mautner, T. Hänninen, H. Setälä, E. Kontturi, A. Bismarck, T. Tammelin

**2:10** CELL **72.** Fabrication of cellulose structures via focused electron beam induced conversion: Approaching the nanoscale. H. Plank, B. Rumpf, T. Ganner, M. Eibinger, J. Sattelkow, B. Nidetzky

**2:35** CELL **73.** Lectin-polysaccharide interaction: An MP-SPR study. K. Niegelhell, E. Jantscher-Krenn, T. Ganner, C. Payerl, T. Wrodnigg, S. Spirk

**3:00** Intermission.

**3:30** CELL **74.** Surface modification of cellulose substrates by tailored latex nanoparticles for improvement of interfacial adhesion. J. Engström, F. Hattton, F. D'Agosto, M. Lansalot, E.E. Malmstrom, A.E. Carlmark

**3:55** CELL **75.** Bioinspired lignocellulosic materials as sensors for unravelling interaction features of enzymes. G. Paes, J. Berrin

**4:20** CELL **76.** Viscoelastic properties of nanocelluloses in liquid and dried states: Comparison of core-shell vs. surface-charged structures. R. Tanaka, T. Saito, T. Hänninen, Y. Ono, M. Hakalahti, T. Tammelin, A. Isogai

#### Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## SUNDAY EVENING

### Section A

San Diego Convention Center  
Halls B/C

#### General Posters

C. E. Frazier, *Organizer*

**6:00 - 8:00**

CELL **77.** On tailoring and validating the pore size distribution of nanocellulose based virus removal filter. S. Gustafsson, A. Mhraryan

CELL **78.** Adsorption of cationic malachite green using high specific surface cellulose nanofibrils aerogel. F. Jiang, D.M. Dinh, Y. Hsieh

CELL **79.** Effect of liquid-to-solid ratio on delignification efficiency of acid catalysis ethanol fractionation process. Y. Gao, Y. Shi, Q. Li

CELL **80.** Green and simple approach for one-pot preparation of an efficient palladium adsorbent based on functionalized 2,3-dialdehyde cellulose. C. Ruan, M. Strömme, J. Lindh

CELL **81.** Mechanical, thermal and barrier properties of methyl cellulose / carvacrol / montmorillonite nanocomposite films prepared as active food packaging material. T. Gurkan Polat, S. Tunç, O. Duman

CELL **82.** Spontaneous formation of 2,3-dialdehyde cellulose (DAC) beads via periodate oxidation and application of the beads as matrix material in protein purification. J. Lindh, D. Carlsson, M. Vall, M. Strömme, A. Mhraryan

CELL **83.** On the pore space of agarose-based chromatography media. D. Carlsson, J. Lindh, M. Strömme, J. Maloisel

CELL **84.** Analyses on hydrogen bonding in noncrystalline regions of regioselectively methylated cellulose films by a combination of vapor-phase deuteration and generalized two-dimensional correlation IR spectroscopy. Y. Hishikawa, T. Kondo

CELL **85.** Solidification of 3D printed cellulose nanofibrils. K.M. Haakansson, I.C. Henriksson, P. Gatenholm

- CELL 86.** Influence of deep eutectic solvent on structure and behaviour of wood based cellulose fibres. T. Tenhunen, T.A. Hänninen, M.K. Österberg, A. Harlin, T. Tammelin
- CELL 87.** Next generation fibers through energy dissipating linkage. P. Mohammadi, M. Linder
- CELL 88.** Cellulose synthase activity assayed in the living cell. S. Sun, Y. Horikawa, J. Sugiyama, T. Imai
- CELL 89.** Cellulose nanofibrils from agro-industrial waste: Raw materials selection, obtention and characterization. V. Fabiola, G. Chinga-Carrasco, C. Ciudad, R. Briones
- CELL 90.** Dynamics behaviors of a bacterial expansin on cellulose crystal surface. T. Yui, T. Uto, M. Takemoto, T. Imai
- CELL 91.** Low instrumented colorimetric paper-based photochromic UV sensor. W. Li, H. Schenderlein, M. Graf, S. Trosien, M.A. Biesalski
- CELL 92.** Surface activation of ACC-nanocellulose for chemical modification in an aqueous system. S. Yokota, A. Nishimoto, T. Kondo
- CELL 93.** Strategies to formulate polymeric nanocomposites from nanofibrillated cellulose. G.A. de Titto, A. Elisei Schichi, S. Perrone, M. Torres, P. Eisenberg
- CELL 94.** Ionic contaminant and dye removal from water using polysaccharide blended films. M. Li, G. Buschle-Dillier
- CELL 95.** Modified hemicelluloses as crosslinker towards tuning the gelling properties of nanocellulose dispersions. K. Markstedt, C. Xu, G. Toriz, P. Gatenholm
- CELL 96.** MDF fiber quality. M. Tasooji, C.E. Frazier
- CELL 97.** Transparent film from cellulose nano fiber prepared by phosphoric acid esterification. H. Fushimi
- CELL 98.** Easily dispersible wet powder from cellulose nanofiber prepared by phosphoric acid esterification. I. Homma
- CELL 99.** Cytocompatible approach toward biomimetic tissues and natural nanoparticles interactions. J. Gonzalez, J. Cubero, R. Gonzalez, J. Vega
- CELL 100.** Nanocellulose and xyloglucane for producing bio-based film with higher gas barrier properties. C. Reverdý, N. Bourry, D. Terrage, C. Moreau, A. Villares, B. Cathala, J. Bras
- CELL 101.** Assembled prolamin protein nanofabrics with greatly improved mechanical properties, three-dimensional shapeability, and resistance to fouling. Y. Wang, Z. Tian, L. Chen
- CELL 102.** Effect of lignin concentration in birch kraft pulp on fibre spinning from ionic liquid solutions. Y. Ma, J. Stubb, M. Hummel, H. Sixta
- CELL 103.** AVAP® Process: Conversion of lignocellulosics into value-added chemicals. X. You, A. Van Heiningen, H. Sixta, M. Iakovlev
- CELL 104.** Production of 2-isopropylmalate through bioengineered E. coli: A bio-based pathway toward conjugated dienes. S.N. Pham, J. Wang, K. Zhang
- CELL 105.** Polyethylenimine as homogeneous and heterogeneous catalysts for isomerization of glucose. Q. Yang, T. Runge
- CELL 106.** Interactions between cellulose surfaces and cellulases from different origins studied by QCM. J. Song, E. Jin, F. Yang, O.J. Rojas
- CELL 107.** Molecular dynamics of cellulose nanotubes predicted by theoretical study. T. Uto, T. Miyata, T. Yui
- CELL 108.** Microwave-assisted synthesis of cellulose carbamate: Structure and flow behaviour in dilute alkali. D.B. Lanieri, M.S. Peresin, M.G. Maximino
- CELL 109.** High strength and water absorbency hydrogels based on quaternized hemicelluloses and acrylic acid with biocompatibility. X. Qi, G. Chen, G. Fu, B. Zhang, Y. Niu, F. Peng, R. Sun
- CELL 110.** Extraction and characterization of cellulose nano crystals (CNC) from bamboo (*Bambusa vulgaris*) grown in Puerto Rico. M.I. Leon-Berrios, N. Grandia, W. Otaño, J. Vedrine, N. Ramos
- CELL 111.** Preparation of nanofibrillar cellulose-silicate composite aerogels by LiCl/DMSO cellulose solution. Z. Wang, L. Zhang, Y. Si, J. Ma, Y. Fan
- CELL 112.** Facile approach towards self-reinforced ZnO-cellulose composite. J. Ma, Z. Wang, S. Wu, X. Zhou
- CELL 113.** Preparation of  $\alpha$ -chitin nanofibers based hydrogels and composite hydrogels. L. Liu, H. Lv, Z. Wang, Y. Fan
- CELL 114.** Degradation of taste and odor compounds with cactus mucilage extraction: Applications for recirculating aquaculture systems. T. Peng, N. Alcantar, F. Guo, W. Zhao, S. Ergas, L. Gonzalez, R.G. Toomey
- CELL 115.** Spruce organosolv lignin derivate as hydrophobic material to use in wood treatments. O. Gordobil, R. Herrera, J. Labidi
- CELL 116.** Cellulose nanocrystals for drug delivery systems. A.M. Barbosa, E. Robles, E. Piva, N. Carreño, J. Labidi
- CELL 117.** Synthesis of 5-ethoxymethylfurfural from carbohydrates via a novel solid acid in  $\gamma$ -GVL co-solvent. Y. Bai, L. Xiao, R. Sun
- CELL 118.** Development of designer monolignols with new spectroscopic signals. R.E. Lamb, A.L. Tomasko, S.H. Kim, Y. Zhu
- CELL 119.** Contact lenses reinforced with nanocellulose. G. Tummala, A. Mhryanyan
- CELL 120.** Model compound study to characterize the development of acetoacetate functionalized resin derived from kraft lignin. E. Krall, D.C. Webster, T. Bader
- CELL 121.** Hierarchically structured nanoporous template based on balsa wood. Q. Fu, L. Berglund
- CELL 122.** Biocompatible bacterial nanocellulose hydrogel for 3D bioprinting of human tissue constructs. P. Gatenholm, A. Mantas
- CELL 123.** Determination of suitable parameters to produce activated carbons from Costa Rican residual woody biomasses. A.J. Martínez Brenes, M. Gudiño, J. Castro, J. Rodríguez, A. Puente-Urbina
- CELL 124.** Novel method to remove bacteria from drinking water using modified cellulose. A. Ottenhall
- CELL 125.** Conversion of lignocellulose facilitated by structural studies. M. Fortin, A. Lai, N. West, A. Sidorenko
- CELL 126.** Withdrawn.
- CELL 127.** Effect of monosaccharide composition in cellulose samples from corn husk and banana rachis on TEMPO-mediated oxidation. C. Gomez, J.A. Velasquez, A.M. Serpa Guerra, P. Posada, C. Castro Herazo, P. Gañán, R. Zuluaga Gallego
- CELL 128.** Effect of molecular weight reduction on surface activity of polysaccharide-based surfactants derived from pectin. Z. Mohd Aris, N. Tchirikova, R. Nagarajan
- CELL 129.** Gas-barrier properties of TEMPO-oxidized cellulose nanofibers. Y. Kumamoto, K. Mukai, Y. Yoshida, A. Isogai
- CELL 130.** Systematic study of the influence of nanocellulose processing methods on its physical and mechanical properties. M. Islam, D. White, C.J. Huntley, M.L. Curry
- CELL 131.** Structure and properties of nanocrystalline cellulose reinforced lignin based composite nanofibers. M. Cho, S. Rennecker, F.K. Ko
- CELL 132.** New approach of polymer reactive compatibilization. A. Rigoussen, P. Verge, F. Hassouna, J. Raguez, P. Dubois, Y. Habibi
- CELL 133.** Computational prediction of structure and self-assembly of plant cellulose synthase complex. A. Singh, Y. Yingling
- CELL 134.** Withdrawn.
- CELL 135.** Viscose filterability and fiber wall pore size as measures for pulp reactivity. E. Hartikainen, M. Borrega, H. Sixta
- CELL 136.** Low molecular weight cellulose produced by supercritical water treatment and its use as Pickering emulsion stabilizer. J. Buffiere, P. Tingaut, M. Borrega, T. Zimmermann, H. Sixta
- CELL 137.** High-purity pulp from paper-grade pulp by enzymatic treatment and post-extraction in caustic-borate solution. T. Toivari, L. Testova, M. Borrega, H. Sixta
- CELL 138.** Withdrawn.
- CELL 139.** Luminescent cellulose nanofibril composite films with high transparency, mechanical and oxygen-barrier properties. Q. Yang, Z. Shi, Z. Qi, T. Saito, C. Xiong, A. Isogai
- CELL 140.** Pretreatment and preparation of composite, smart fibers from perennial grasses for use in the production of biofuels. K.R. Bannister, J. Mendenhall

## MONDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Cardiff

### Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

M. L. Auad, J. Campos-Teran, O. El Seoud, O. J. Rojas, *Organizers*

D. Petri, *Organizer, Presiding*

S. H. Rennecker, *Presiding*

## 8:00 Introductory Remarks.

**8:05 CELL 141.** Adsorption of gold nanoparticles (NPau) and bovine serum albumin (BSA) complexes in algae cellulose films. D. Gómez-Maldonado, R. López-Simeon, I. Iñárritu, A. Topete, J. Campos-Teran

**8:30 CELL 142.** Evaluation of maltodextrin and poly-vinyl alcohol content in oven dried nanocellulose redispersability. J.A. Velasquez, P. Posada, A.M. Serpa Guerra, C. Castro Herazo, P. Gañán, B.E. Gomez, C. Gomez, R. Zuluaga Gallego

**8:55 CELL 143.** Properties of absorbents hydrogels prepared from different polysaccharides crosslinked with citric acid and bis(2,3-epoxypropyl)-N,N'-urea. P. Jimenez-Bonilla, H. Haber, M.L. Auad

**9:20 CELL 144.** Optimization of nanocellulose membrane using evolutionary algorithms. B.C. Sulbaran, V. Zuñiga, M. Perez, V. Osuna

## 9:45 Intermission.

**10:15 CELL 145.** Impact of bacterial cellulose nanocrystals charge density on the interaction with xyloglucan. D. Petri, C. Pirich, M. Sierakowski, R.A. Freitas

**10:40 CELL 146.** Can we make higher value, purer cellulose by synthesis rather than deconstruction? M. Pidcocke, M. Cho, J. Hu, J.N. Saddler, S.H. Rennecker

**11:05 CELL 147.** Protein-assisted interfacial adhesion in thermoforming of cellulose-based composites. A. Khakalo, I. Filpponen, O.J. Rojas

**11:30 CELL 148.** Micro-nano lignocellulosic fibrils (MNLFCF) aerogels from coconut and oil palm tree residuals and application for environmental remediation. A. Tripathi, A. Ferrer, S. Khan, O.J. Rojas

## Section B

Marriott Marquis San Diego Marina  
La Costa

### Lignin Refining, Functionalization & Utilization

## Lignin Utilization

D. Argyropoulos, C. Crestini, *Organizers*

D. Da Silva Perez, *Presiding*

**8:05 CELL 149.** Journey to polymeric materials composed exclusively of simple lignin derivatives. Y. Wang, Y. Chen, S. Sarkanen

**8:30 CELL 150.** Ultrasound driven self-assembly of natural polyphenols into microcapsules and nanoparticles for storage and delivery of hydrophobic molecules. C. Crestini, H. Lange, E. Bartzoka

**8:55 CELL 151.** Fibre spinning of lingo-cellulose biomass using ionic liquids. S. Rizal Vincent, R. Prado, A. Koutsomitopoulou, K. Potter, S.J. Eichhorn, O. Kuzmina, T. Welton, S. Rahatekar

**9:20 CELL 152.** Withdrawn.

## 9:45 Intermission.

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)



**10:15** CELL **153.** Performance of lignin-phenol-formaldehyde adhesives using various lignin sources. **J. Konnerth**, M. Ghorbani, H. Van Herwijnen, E. Budjav, F. Liebner

**10:40** CELL **154.** Synthesis of high performance lignin-phenol-urea-formaldehyde co-condensed resin under alkaline conditions. **S. Yang**, T. Yuan, R. Sun

**11:05** CELL **155.** Biogenic formaldehyde from lignin and its role in the wood-based composites industry. **G. Wan**, C.E. Frazier

**11:30** CELL **156.** Effect of market and technical parameter uncertainties on the optimal design of biorefineries. **A. Geraili**, J.A. Romagnoli

## Section C

Marriott Marquis San Diego Marina  
Marina Salon F

### New Horizons in Sustainable Materials

#### Glycoscience

Cosponsored by DAC $\ddagger$  and POLY  
Financially supported by EPNOE

K. J. Edgar, P. R. Navard, *Organizers*

M. Kipper, *Presiding*

**8:30** CELL **157.** Functional polysaccharide materials: From interface science to application. **R. Kargl**, S. Spirk, T. Mohan, K. Stana-Kleinschek

**8:55** CELL **158.** Novel cellulose derivatives as amorphous solid dispersion matrices for oral drug delivery. **X. Meng**, L.J. Mosquera-Giraldo, L. Taylor, K.J. Edgar

**9:20** CELL **159.** Compatible biomaterials from renewable resources. **M. Kipper**

**9:45** Intermission.

**10:15** CELL **160.** Targeting sugar antigens in cancer and heart diseases with glyco-nanoparticle. **V. Padler-Karavani**

**10:40** CELL **161.** Engineering a multi-zonal scaffold for cartilage tissue using cellulose nanocrystals. **J. Foster**

**11:05** CELL **162.** Quaternized hemicellulose-chitosan nanocomposite films for food packaging application. **G. Chen**, X. Qi, Y. Guan, F. Peng, C. Yao, R. Sun

**11:30** CELL **163.** Withdrawn.

## Section D

Marriott Marquis San Diego Marina  
Marina Salon G

### Structure of Native Celluloses & Variety of Nano-celluloses That Can Be Formed from Them: Anselme Payen Award Symposium in honor of Akira Isogai

Financially supported by U.S. Forest Service

U. P. Agarwal, R. H. Atalla, O. J. Rojas, J. Sugiyama, *Organizers*

P. E. Fardim, D. G. Gray, *Presiding*

**8:00** Introductory Remarks.

**8:05** CELL **164.** Nanocellulose-water interactions: From flat films to filaments from wet spinning. **M. Lundahl**, L. Wang, M. Vuoriluoto, G. Cunha, E. Rojo, H. Orelma, J. Arboleda, L. Johansson, M. Borghei, I. Filpponen, O.J. Rojas

**8:30** CELL **165.** Increased understanding of cellulose crystallinity. **A.D. French**, S. Nam, Y. Yue, Q. Wu, U.P. Agarwal, I. Simkovic, M. Santiago

**8:55** CELL **166.** Cellulose nanocrystals: Physical properties, dispersion and interfaces. **S.J. Eichhorn**

**9:20** CELL **167.** New design and fabrication of optical and magnetic functional films by ordered cellulose-inorganic hybridization. **Y. Nishio**

**9:45** Intermission.

**10:15** CELL **168.** Colloidal properties of cellulose nanofibrils. **L. Wågberg**, A. Fall, M. Nordenstrom

**10:40** CELL **169.** Thermal diffusivity in ultrahigh porosity solids of nanocellulose. **K. Sakai**, Y. Kobayashi, **T. Saito**, A. Isogai

**11:05** CELL **170.** Residual xylan desorption and re-adsorption on the cellulose microfibril. **L. Falcoz-Vigne**, L. Heux, Y. Nishiyama, k. Mazeau, V. Meyer, M. Petit-Conil

**11:30** CELL **171.** Source and process-linked nanocellulose structure, properties and self-assembling. **Y. Hsieh**

## Section E

Marriott Marquis San Diego Marina  
Temecula 1&2

### Functional Lignocellulosics & Nanotechnology

#### Lignocellulosic Nanomaterials & Their Applications

Cosponsored by CARB  
Financially supported by BioNavis; EPNOE

S. Spirk, T. Nypelö, *Organizers*

I. Filpponen, M. S. Peresin, *Organizers*,  
*Presiding*

**8:05** CELL **172.** Surface modification of lignocellulosic nanoparticles for functional materials. **M.K. Österberg**, M. Mattinen, J. Valle-Delgado, T. Leskinen

**8:30** CELL **173.** Augmenting the interfacial activities of lignins using controlled radical polymerization. **N. Washburn**, C. Gupta, K.M. Perkins, K. Silmore

**8:55** CELL **174.** Structure-property relation established by chemical mapping of cellulose nanofibril films containing renewable additives. **T. Nypelö**, C. Laine, U. Henniges, J. Konnerth, T. Tammelin

**9:20** CELL **175.** Lignocellulosic nanofibrils from neutral sulphite pulps. **S. Hanhikoski**, I. Solala, P. Lahtinen, K. Niemelä, T. Vuorinen

**9:45** Intermission.

**10:15** CELL **176.** Enhancing food security with nanocellulose. **J. Jung**, Z. Deng, Y. Zhao, J. Simonsen

**10:40** CELL **177.** Complete nanofibrillation of cellulose prepared by phosphoric acid esterification. **H. Fushimi**, I. Homma

**11:05** CELL **178.** 3D printing – a disruptive technology for innovative products based on lignocellulosics. **K. Markstedt**, G. Toriz, P. Gatenholm

**11:30** CELL **179.** Cellulose nanopapers as ion-exchangers for nitrate and heavy metal removal. **A. Mautner**, K. Li, A. Bismarck

### Glycosylases: Inhibition & Therapeutic Applications

Sponsored by CARB, Cosponsored by CELL

#### Is There a Crisis in Organic Chemistry Education?

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

## MONDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Cardiff

#### Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

M. L. Auad, J. Campos-Teran, D. Petri, O. J. Rojas, *Organizers*

O. El Seoud, *Organizer, Presiding*

F. Liebner, *Presiding*

**1:15** Introductory Remarks.

**1:20** CELL **180.** Impact of selected cellulose solvents on physico-chemical, morphological and mechanical properties of cellulose II aerogels. **N. Pircher**, S. Quraishi, M. Bacher, L. Carbajal-Galan, J. Nedelec, H. Renhhofer, H. Lichtenegger, T. Rosenau, **F. Liebner**

**1:45** CELL **181.** Influence of cation on the dissolution of cellulose in alkaline/urea system at low temperature and its mechanism. **A. Lu**

**2:10** CELL **182.** Xyloglucan-functional latex particles via RAFT-mediated emulsion polymerization for the modification of cellulose by physical adsorption. **F. Hatton**, M.C. Ruda, M. Lansalot, F. DAgosto, E.E. Malmstrom, A.E. Carlmark

**2:35** CELL **183.** Withdrawn.

**3:00** Intermission.

**3:30** CELL **184.** Diffusion rates of model metabolites through cell wall tissue: Toward understanding how chemical modification impacts decay resistance to wood. **C.G. Hunt**

**3:55** CELL **185.** How the flexibility properties of hemicelluloses are affected by the glycosidic bonds between different backbone sugars – A molecular dynamics study. **J. Berglund**, M. Bergenstråhle, F. Vilaplana, T. Angles d'Ortoli, G. Widmalm, M. Lawoko, G. Henriksson, M.E. Lindström, J. Wohlerk

**4:20** CELL **186.** Combined effects of sodium alginate and polyamideamine-epichlorohydrin on the wet strength development of cellulose sheets. **Y. Bai**, Y. Lei, L. Xiao, C. Yao, R. Sun

**4:45** CELL **187.** Probing cellulose acylation in mixtures of an ionic liquid with molecular solvents by chemical kinetics, viscometry, spectroscopy, and molecular dynamics simulations. **O. El Seoud**, H. Nawaz, P.A. Pires, E.P. Areas, N.I. Malek, T.C. Teixeira, T.A. Bioni

### Section B

Marriott Marquis San Diego Marina  
La Costa

#### Lignin Refining, Functionalization & Utilization

#### Structural & Analytical Aspects of Lignin Chemistry

D. Argyropoulos, C. Crestini, *Organizers*

S. Sarkanen, *Presiding*

**1:20** CELL **188.** From structural understanding to valorization: The structure of lignins from different isolation processes. **C. Crestini**, H. Lange

**1:45** CELL **189.** Lignosulfonate analysis: Improving the toolset. **P. Korntner**, I. Sumerskii, H.M. Amer, G. Zinovyev, T. Rosenau, A. Potthast

**2:10** CELL **190.** Quantifying lignin degradation products produced from alkaline pretreatment. **E. Karp**, C.T. Nimlos, D. Salvachua, S. Deutch, G. Beckham

**2:35** CELL **191.** Quantitative DFRC analysis of monolignols and monolignol conjugates incorporated into lignin. **M.R. Regner**, A.M. Bartuce, D. Padmakshan, Y. Li, S. Karlen, J. Ralph

**3:00** Intermission.

**3:30** CELL **192.** Where do thioacidolysis dimers come from? A model study. **F. Yue**, F. Lu, R. Sun, J. Ralph

**3:55** CELL **193.** Gradient elution moving boundary electrophoresis for analysis of alkaline pretreatment liquor. **M.S. Munson**, E. Karp, C.T. Nimlos, D. Salvachua, G. Beckham

**4:20** CELL **194.** Quantitation of triclin in grass lignins. **W. Lan**, F. Lu, J. Ralph

**4:45** CELL **195.** On the difficulty of applying 1064-nm Raman spectroscopy to investigate structures of kraft lignins. **U.P. Agarwal**, D. Argyropoulos, S. Ralph

## Section C

Marriott Marquis San Diego Marina  
Marina Salon F

### New Horizons in Sustainable Materials

#### Polysaccharide Materials

Cosponsored by DAC $\ddagger$  and POLY

K. J. Edgar, *Organizer*

P. R. Navard, *Organizer, Presiding*

**1:45** CELL **196.** Pushing the application limits for good old cellulose. **D. Reishofer**, M. Kaschowitz, R. Kargl, T. Griesser, G. Trimmel, H. Plank, **S. Spirk**

**2:10** CELL **197.** Smart materials based on sustainable cellulose. **K. Zhang**

**2:35** CELL **198.** Sustainability and nanocellulose: From process preparation to surface functionalization. **J. Bras**

**3:00** Intermission.

**3:30** CELL **199.** Cellulose photonics: From nature to applications. **S. Vignolini**

**3:55** CELL **200.** High-performance electrode materials fabricated from cellulose/polyaniline microspheres. **D. Xu**, J. Cai, L. Zhang

**4:20** Panel Discussion.

## Section D

Marriott Marquis San Diego Marina  
Marina Salon G

### Structure of Native Celluloses & Variety of Nano-celluloses That Can Be Formed from Them: Anselme Payen Award Symposium in honor of Akira Isogai

Financially supported by U.S. Forest Service

U. P. Agarwal, R. H. Atalla, O. J. Rojas, J. Sugiyama, *Organizers*

T. Rosenau, T. Vuorinen, *Presiding*

**1:15** Introductory Remarks.

**1:20** CELL **201.** Regioselective synthesis of polysaccharide derivatives. **K.J. Edgar**, S. Liu, R. Zhang, X. Zheng

**1:45** CELL **202.** Evolution of wood-cellulose native structure upon thermal and hydrothermal treatments. **U.P. Agarwal**

**2:10** CELL **203.** Highly permeable nanofibrous cellulose membranes for water purification. **B.S. Hsiao**, B.T. Chu

**2:35 CELL 204.** Construction of nanofibers from the unstable cellulose solution and their applications. **L. Zhang,** B. Duan, Z. Jiang, Y. Fang, D. Ye, D. Xu

**3:00** Intermission.

**3:30 CELL 205.** Internal structure of cellulose I fibril aggregates studied by a combination of structure and dynamics measurements. **T. Larsson,** L. Wågberg, P. Westlund, P. Karlsson

**3:55 CELL 206.** Development of silver nanoparticles bound by cellulose single nanofibers. **T. Isogai,** Y. Hayashi, H. Kameshima

**4:20 CELL 207.** Which was the first to appear,  $\beta$ -1,4 or  $\beta$ -1,3 glucans? **T. Kondo**

**4:45 CELL 208.** Longitudinal order on cellulose microfibrils in aquatic algae. **Y. Horikawa,** T. Imai, J. Sugiyama

## Section E

Marriott Marquis San Diego Marina  
Temecula 1&2

### Functional Lignocellulosics & Nanotechnology

#### Lignocellulosic Nanomaterials & Their Applications

*Cosponsored by CARB  
Financially supported by BioNavis; EPNOE*

I. Filpponen, M. S. Peresin, S. Spirk, *Organizers*

T. Nypelö, *Organizer, Presiding*

J. O. Zoppe, *Presiding*

**1:20 CELL 209.** Right nanofibrillated cellulose for the right application: Comparative study of the properties of three exciting nanofibrillated cellulose systems. **A. Naderi,** T. Lindström, J. Sundström, T. Pettersson, G. Flodberg

**1:45 CELL 210.** Use of phosphorylated cellulose nanofibrils in preparation of an all cellulose flame-retardant material. **M. Ghanadpour,** F. Carosio, P.T. Larsson, L. Wågberg

**2:10 CELL 211.** Molecular deformation in high performance cellulose fibres. **N. Wanasekara,** C. Zhu, S.J. Eichhorn, S. Rahatekar, T. Welton, A. Bismarck, K. Potter

**2:35 CELL 212.** Macro- and mesoporous spherical nanocellulose beads for use in energy storage devices. **J. Erlandsson,** H. Granberg, L. Wågberg

**3:00** Intermission.

**3:30 CELL 213.** Nano-fibrillated cellulose in high performance structural applications. **J. Read**

**3:55 CELL 214.** Heat-induced conversion of ionic bonds to amides or the way to improve the thermal stability of TEMPO-oxidized cellulose nanofibrils. **N. Lavoine,** J. Bras, T. Saito, A. Isogai

**4:20 CELL 215.** Functionalized nanocelluloses and their use in barrier and membrane thin films. **M. Visanko,** H. Liimatainen, J.A. Sirviö, O. Hormi, M. Illikainen

## Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**4:45 CELL 216.** Controlling colloidal stability in nanofibrillar systems by surface modification. **T. Kaldeus,** A.E. Carlmark, E.E. Malmstrom

### Diversity-Quantification-Success?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### Glycosylases: Inhibition & Therapeutic Applications

*Sponsored by CARB, Cosponsored by CELL*

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

C. E. Frazier, *Organizer*

**8:00 - 10:00**

77, 88, 101-102, 104, 107, 110, 113-114, 117, 120, 122-124, 127-129, 131-132. See previous listings.

## TUESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Cardiff

#### Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

M. L. Auaud, J. Campos-Teran, O. El Seoud, D. Petri, *Organizers*

O. J. Rojas, *Organizer, Presiding*

M. Ago, *Presiding*

**8:00** Introductory Remarks.

**8:05 CELL 217.** Valorizing lignin. **A.J. Ragauskas,** T. Wells, R. Khuu Le, P. Das

**8:30 CELL 218.** Phenolic resins modified with hydroxymethylated sodium lignosulfonate and kraft-type lignins and their application in decorative laminates. **M. Taverna,** V. Nicolau, **D. Estenoz**

**8:55 CELL 219.** Aggregation behavior of lignin in alkaline solutions studied by dynamic light scattering and rheology. **C. Fritz,** C.L. Salas, H. Jameel, O.J. Rojas

**9:20 CELL 220.** Supercritical carbon dioxide as a "green" catalyst for selective hydrothermal oxidation of alkali lignin. **A. Numan-Al-Mobin,** A. Kubatova, A. Smirnova

**9:45** Intermission.

**10:15 CELL 221.** To methylate or not to methylate polymeric materials with the highest attainable lignin contents. **Y. Chen,** Y. Wang, **S. Sarkanen**

**10:40 CELL 222.** Free-standing electrospun carbon network from lignin as a conductive electrode for super-capacitance. **M. Ago,** M. Borghei, O.J. Rojas

**11:05 CELL 223.** Withdrawn.

**11:30 CELL 224.** Effect of lignin on the material properties of chemically modified fibres by periodate oxidation and borohydride reduction. **V. Lopez Duran,** P. Larsson, L. Wågberg

### Section B

Marriott Marquis San Diego Marina  
La Costa

#### Lignin Refining, Functionalization & Utilization

##### Functionalization

D. Argyropoulos, C. Crestini, *Organizers*

M. Mattinen, *Presiding*

**8:05 CELL 225.** New functional lignin-based polymers: Synthesis and characterisation. **Y. Habibi**

**8:30 CELL 226.** Tailored lignin-protein heteroconjugates for bionanomaterial applications. **M. Mattinen**

**8:55 CELL 227.** Essential approaches to characterization of lignin following hydro-treatment. **A. Kubátová**

**9:20 CELL 228.** Modification of low molecular weight lignin model compounds for thermoset resin applications. **M. Jawerth,** M. Lawoko, S. Lundmark, C.M. Perez Berumen, M.K. Johansson

**9:45** Intermission.

**10:15 CELL 229.** Coupling and reactions of catechol monolignols. **L. Berstis,** T.J. Elder, G. Beckham, M.F. Crowley

**10:40 CELL 230.** New insights in bio-based benzoxazines. **Y. Habibi**

**11:05** Closing Remarks.

### Section C

Marriott Marquis San Diego Marina  
Presidio 1

#### Cellulose Nanocomposites Processing Development & their Structure Property Relations

*Financially supported by Bio4Energy, Sweden; Centre for Biocomposites and Biomaterials Processing at University of Toronto, Canada; GreenNano, Canada*

K. A. Oksman, *Organizer*

M. Sain, *Organizer, Presiding*

H. Liimatainen, *Presiding*

**8:00** Introductory Remarks.

**8:05 CELL 231.** Withdrawn.

**8:30 CELL 232.** Cellulose model probes for fundamental research on adhesion, swelling and adsorption. **P. Karlsson,** S.A. Pendergraph, T. Larsson, L. Wågberg

**8:55 CELL 233.** Nanocellulose production via green solvent pulping at low temperature and TEMPO-mediated oxidation. **S. Zhou,** T. Runge, D. Alonso, S. Hakim, J.A. Dumesic

**9:20 CELL 234.** Polyelectrolyte multilayers on differently charged cellulose surfaces. **T. Bensefelt,** J. Henschen, T. Pettersson, L. Wågberg

**9:45** Intermission.

**10:15 CELL 235.** Light scattering in cellulose nanofibre suspensions: Model and experiments. **Y. Aitomaki,** L. Berglund, T. Linder, T. Löfqvist, M. Noël, K.A. Oksman

**10:40 CELL 236.** Thermal stabilization of nanocellulose by chemical modification. **M.B. Agustin,** F. Nakatsubo, H. Yano

**11:05 CELL 237.** Understanding surface energy of nanocellulose for nano-enabled bioproduct. **J. Sameni,** M. Sain

**11:30 CELL 238.** Solvent-induced decrystallization and dissolution of cellulose for efficient biomass processing. **M. Ghasemi,** M. Tsiannou, **P. Alexandridis**

### Section D

Marriott Marquis San Diego Marina  
Marina Salon G

#### Structure of Native Celluloses & Variety of Nano-celluloses That Can Be Formed from Them: Anselme Payen Award Symposium in honor of Akira Isogai

*Financially supported by U.S. Forest Service*

U. P. Agarwal, R. H. Atalla, O. J. Rojas, J. Sugiyama, *Organizers*

T. Larsson, A. Potthast, *Presiding*

**8:00** Introductory Remarks.

**8:05 CELL 239.** From leveling-off degree of polymerization to cellulose nanocrystals. **E. Kontturi**

**8:30 CELL 240.** Cationic cellulose nanofibrils for smart applications. **J. Bras,** S. Saini, C. Yucel, L. Ciprian

**8:55 CELL 241.** Production of cellulose nanomaterials with good thermal stability, functionality, and tailored morphologies. **J. Zhu,** L. Chen

**9:20 CELL 242.** Uniaxial orientation of nanocelluloses in all-cellulose nanocomposite: The relationship between structure and mechanical properties. **S. Fujisawa,** E. Togawa, N. Hayashi, T. Saito, A. Isogai

**9:45** Intermission.

**10:15 CELL 243.** Nano-structures of native celluloses, their transformations upon isolation, and their implications for the production of nano-celluloses. **R.H. Atalla,** R.S. Atalla, U.P. Agarwal

**10:40 CELL 244.** Novel concept for nano-structuring of polymers. **T.J. Heinze**

**11:05 CELL 245.** Effect of synergistic reaction on the O<sub>2</sub>/laccase/TEMPO oxidation of cellulose and the preparation of nanofibers. **J. Jiang,** W. Ye, Y. Fan

**11:30 CELL 246.** Assessment of surface accessibility of nanocellulosic structures using surface sensitive methods. **T. Tammelin**

### Section E

Marriott Marquis San Diego Marina  
Miramar Room

#### Functional Lignocellulosics & Nanotechnology

##### Dispersions, Gels, Foams, Colloids, Films

*Cosponsored by CARB  
Financially supported by BioNavis; EPNOE*

I. Filpponen, S. Spirk, *Organizers*

M. S. Peresin, T. Nypelö, *Organizers, Presiding*

**8:05 CELL 247.** What next for device manufacturing: Synthetic molecular science or bio-nanotechnology? **M. Sain,** K. Nag

**8:30 CELL 248.** Functional materials with cellulose blocks: Synthesis and response properties. **R. Liu,** H. Kang, Y. Huang

**8:55 CELL 249.** Protein separation using magnetically responsive cellulose nanocrystals. **J. Guo,** I. Filpponen, O.J. Rojas

**9:20 CELL 250.** Structural analysis of the cellulose microfibrils from algae and higher plants via layer-by-layer peeling of their surface molecules. **R. Funahashi,** Y. Okita, H. Hondo, M. Zhao, T. Saito, A. Isogai

**9:45** Intermission.

**10:15 CELL 251.** Cationic cellulose nanocrystals as flocculants for harvesting *Chlorella Vulgaris* microalgae. **S. Eyley,** D. Vandamme, S. Lama, G. Van den Mooter, K. Muylaert, W. Thielemans

**10:40** CELL **252**. How to cationize lignocellulosics more efficiently. N. Odabas, H.M. Amer, U. Henniges, A. Potthast, T. Rosenau

**11:05** CELL **253**. Ambient-dried cellulose nanofibril aerogel membranes with high tensile strength and their use for aerosol collection and templates for transparent, flexible devices. M. Toivonen, A. Kaskela, O.J. Rojas, E. Kauppinen, O.T. Ikkala

**11:30** CELL **254**. Cellulose II nanogel consisting of spherical particles. M. Beaumont, M. Opietnik, A. Potthast, T. Rosenau

### Carbohydrate Research at Predominantly Undergraduate Institutions

Sponsored by CARB, Cosponsored by CELL

## TUESDAY AFTERNOON

### Section D

Marriott Marquis San Diego Marina  
Marina Salon G

### Structure of Native Celluloses & Variety of Nano-celluloses That Can Be Formed from Them: Anselme Payen Award Symposium in honor of Akira Isogai

Financially supported by U.S. Forest Service

R. H. Atalla, O. J. Rojas, J. Sugiyama, Organizers

U. P. Agarwal, Organizer, Presiding

A. D. French, Presiding

**1:15** Introductory Remarks.

**1:20** CELL **255**. Double modification of cellulose esters by olefin cross-metathesis and thiol-Michael addition reaction. X. Meng, K.J. Edgar

**1:45** CELL **256**. Nanomechanical properties of cellulose nanomaterials via the atomic force microscope. R. Wagner, R. Moon

**2:10** CELL **257**. Controlling the interactions within nanocelluloses for functional properties. O.T. Ikkala

**2:35** CELL **258**. Chemically treated cellulose nanofibrils by carboxymethylation or tempo-mediated oxidation and their sheet properties. K. Sim, H. Youn, J. Lee, Y. Jo

**3:00** CELL **259**. Estimation of the nanocellulose width from turbidity. M. Shimizu, T. Saito, Y. Nishiyama, H. Yano, A. Isogai, T. Endo

**3:25** Intermission.

**3:55** CELL **260**. Solid-state structure-dependent chemical modifications of celluloses at the molecular and microfibrillar levels under aqueous and non-aqueous conditions. A. Isogai

**4:45** Closing Remarks.

### Carbohydrate Research at Predominantly Undergraduate Institutions

Sponsored by CARB, Cosponsored by CELL

## WEDNESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Cardiff

### Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

J. Campos-Teran, O. El Seoud, D. Petri, O. J. Rojas, Organizers

M. L. Auad, Organizer, Presiding

C. G. Hunt, Presiding

**8:00** Introductory Remarks.

**8:05** CELL **261**. Using lignocellulosic aggregates for preparing concrete. P.R. Navard, L.T. Vo, L. Chupin, J. Girones, T. Cousin, E. Boix

**8:30** CELL **262**. Characterisation of pulp fibre fines and their technological properties. R. Eckhart, W.J. Fischer, R. Giner Tovar, L. Jagiello, M. Mayr, W. Bauer

**8:55** CELL **263**. Solubility and adsorption of wood biopolymers at model surfaces. S. Kishani Farahani, F. Vilaplana, P. Gatenholm, L. Wågberg

**9:20** CELL **264**. Value-added carbon products attained through microwave assisted hydrothermal treatment of cellulose and waste paper. K. Adolfsson, S. Hassanzadeh, M. Hakkarainen

**9:45** Intermission.

**10:15** CELL **265**. Synergistic catalytic effect of supercritical carbon dioxide and nickel oxide as a heterogeneous catalyst for lignin liquefaction and selective synthesis of phenolics. R. Bommadihallirajappagowda, A. Kubatova, A. Smirnova

**10:40** CELL **266**. Two-step pyrolysis process applied to used railroad tie. P. Kim

**11:05** CELL **267**. Possible by-products in spent liquors from neutral sulphite pulping of softwood. S. Hanhikoski, K. Niemelä, T. Vuorinen

**11:30** CELL **268**. Role of ethanol and temperature on the hydroxyl and carbonyl groups in the bio-oil produced by hydrothermal liquefaction of loblolly pine. Y. Celikbag, B. Via, S. Adhikari, G. Buschle-Diller, M.L. Auad

### Section B

Marriott Marquis San Diego Marina  
La Costa

### Cellulose Nanocrystal Fundamentals

Financially supported by BioNavis

E. D. Cranston, T. Tammelin, Organizers

E. Kontturi, Organizer, Presiding

**8:30** CELL **269**. Swelling of cellulose nanocrystal thin films in solvents and aqueous solutions. M.S. Reid, S. Kedzior, E.D. Cranston

**8:55** CELL **270**. Withdrawn.

**9:20** CELL **271**. Water vapor adsorption of 2D polysaccharide films to mimic the plant cell wall. E. Niinivaara, M. Faustini, T. Tammelin, E. Kontturi

**9:45** Intermission.

**10:15** CELL **272**. Quantitative assessment of water interactions of cellulose nanocrystals. T. Tammelin, E. Niinivaara, E. Kontturi

**10:40** CELL **273**. Cellulose-cellulose bonding in CNC aerogels. C. Buesch, J. Simonsen, S. Smith, J. Conley

**11:05** CELL **274**. Strengthening polymer thin films with cellulose nanocrystals. D. Grolman, C.S. Davis, J. Gilman, S. Kedzior, E.D. Cranston, A. Karim

**11:30** CELL **275**. Exploration of xyloglucan-cellulose nanocrystal complexes architecture by kinetic adsorption studies and enzymatic susceptibility. A. Villares, M. Celine, B. Cathala

### Section C

Marriott Marquis San Diego Marina  
Mission Hills

### Cellulose Nanocomposites Processing Development & their Structure Property Relations

Financially supported by Bio4Energy, Sweden; Centre for Biocomposites and Biomaterials Processing at University of Toronto, Canada; GreenNano, Canada

K. A. Oksman, Organizer

M. Sain, Organizer, Presiding

M. Illikainen, Presiding

**8:00** Introductory Remarks.

**8:05** CELL **276**. Dried nanofibrillated cellulose networks: Re-dispersion in different mediums and properties of prepared nanocomposites. M.L. Hietala, K.A. Oksman

**8:30** CELL **277**. Colloidal interactions in nanocellulose systems. M. Nordenstrom, L. Wågberg, L.G. Odberg

**8:55** CELL **278**. Sol-gel synthesis of cellulose nanofibrils/silica nanocomposite aerogels. F. Jiang, S. Hu, Y. Hsieh

**9:20** CELL **279**. Nanocellulose as dispersant for carbon nanotube suspensions. A. Hajian, S.B. Lindström, L. Berglund, L. Wågberg

**9:45** Intermission.

**10:15** CELL **280**. New perspectives for cellulose-based biocomposites. P.E. Fardim, J. Obradovic, C. Lange, J. Narewska, P.R. Navard

**10:40** CELL **281**. Free-standing antibacterial membranes based on biopolymers-silver nano-assemblies. P. Petkova, A. Francesco, M. Bakalova, T. Tzanov

**11:05** CELL **282**. Reinforcement of polymers with cellulose nanocrystals types having different aspect ratios. J. Sapkota, A. Shirole, J. Foster, J.C. Garcia, M. Lattuada, C. Weder

**11:30** CELL **283**. Catalytic paper reactor with a nano/micro hybrid porous structures. H. Koga, N. Namba, M. Nogi

### Section D

Marriott Marquis San Diego Marina  
Marina Salon G

### Biomedical & Drug Delivery Applications of Polysaccharide-Based Materials

### Pharmaceutical Applications

Cosponsored by CARB

V. Edwards, Organizer

M. Roman, Organizer, Presiding

**8:00** Introductory Remarks.

**8:05** CELL **284**. Isolation, characterization and pharmaceutical applications of polysaccharides from plants. S. Azeem

**8:30** CELL **285**. Inhibition of formation of amyloid  $\beta$ -protein fibrils using cactus mucilage. Z. Zeisi, E. Lobbens, L. Breydo, V. Uversky, D. Morgan, R.G. Toomey, N. Alcantar

**8:55** CELL **286**. Efficient, regioselective path to cationic polysaccharides for biomedical applications. S. Liu, K.J. Edgar

**9:20** CELL **287**. Designing cellulose esters for oral tuberculosis treatment. H. Arca, K.J. Edgar

**9:45** Intermission.

**10:15** CELL **288**. Development of a conjugate vaccine against *Cryptococcus neoformans* based on synthetic Capsular polysaccharide structures. S. Oscarson

**10:40** CELL **289**. Control release of nicotine from hydroxypropyl methylcellulose patches. D. Petri, G.D. Bloisi, P.L. Marani

**11:05** CELL **290**. Facile one-pot synthesis of hyaluronan nanoparticle for combination therapy. W. Zhang, C. Tung

**11:30** CELL **291**. Functional cellulose spheres for drug delivery and biochromatography. P.E. Fardim, J. Trygg, P. Trivedi

### Section E

Marriott Marquis San Diego Marina  
Leucadia

### Functional Lignocellulosics & Nanotechnology

### Dispersions, Gels, Foams, Colloids, Films

Cosponsored by CARB

Financially supported by BioNavis; EPNOE

I. Filpponen, S. Spirk, Organizers

T. Nypelö, M. S. Peresin, Organizers, Presiding

**8:30** CELL **292**. Future perspectives for functional materials from cellulose nanofibers. T. Zimmermann, H. Sehaqui, S. Josset, G. Siqueira, T. Geiger, P. Tingaut

**8:55** CELL **293**. Aerogels made from hydroxypropyl methylcellulose: Potential adsorbents for wastewater pollutants. D. Petri, P.O. Toledo, S.D. Novaes

**9:20** CELL **294**. Thermoresponsive supramolecular hydrogels of end-functionalized methylcelluloses as three-dimensional scaffolds for bio-inspired mineralization. H. Kamitakahara, M. Yamagami, R. Suhara, A. Yoshinaga, T. Takano

**9:45** Intermission.

**10:15** CELL **295**. Aqueous foam as the carrier medium for producing tailored fiber materials. J.A. Ketoja, A.M. Al-Qararah, T. Hjelt, A. Jäsberg, A. Koponen, A. Harlin

**10:40** CELL **296**. Effects of external conditions and chemical interactions on the behavior of aqueous cellulose-based foams. K.E. Salminen, T. Lappalainen, H. Kiiskinen, M. Sinkkonen, O.J. Rojas

**11:05** CELL **297**. Nanofibrillated cellulose dispersions at high solid contents and strong aerogels. H. Mertaniemi, O.T. Ikkala

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**11:30 CELL 298.** Protective wood coatings based on natural wax particles. **A. Lozhechnikova**, H. Bellanger, B. Michen, I. Burgert, M.K. Österberg

**Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Symposium in honor of Professor Sharpless's 75th Birthday**

*Sponsored by CARB, Cosponsored by CELL*

## WEDNESDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Cardiff

**Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems**

M. L. Auad, J. Campos-Teran, O. El Seoud, D. Petri, O. J. Rojas, *Organizers*

M. Esquivel Alfaro, G. Toriz, *Presiding*

**1:15** Introductory Remarks.

**1:20 CELL 299.** Synthesis and characterization of interpenetrating polymer networks (IPNs) using biomass derived materials. B. Sibaja, M.L. Auad

**1:45 CELL 300.** High performance carbon nanofibers derived from flax lignin. **M. Cho**, L. Ji, S. Potter, S. Mansfield, S. Renneckar

**2:10 CELL 301.** Effects of hydrothermal carbonisation (HTC) conditions on the morphology of hydrocarbon particles obtained from biomass mono/polysaccharides. **D. Da Silva Perez**, M. Guillot, M. Petit-Conil, S. Pellet-Rostaing, F. Goettmann

**2:35 CELL 302.** Full utilization of algal biomass by cyclic extraction. **M. Sterner**, U.M. Edlund

**3:00** Intermission.

**3:30 CELL 303.** Antibacterial hydrogels based on spruce xylan loaded with silver nanoparticles for biomedical applications. **G. Toriz**, N.A. González, M.A. Escalante, F.J. González, E. Delgado, P. Gatenholm

**3:55 CELL 304.** Surface functionalization strategies and viscoelastic properties of cellulose films for adsorption of inorganic photo-active nanoparticle/enzyme hybrid systems. **I. Iñarritu**, A. Topete, R. López-Simeon, E. Torres, **J. Campos-Teran**

**4:20 CELL 305.** Honeycomb porous films obtained with algae residue cellulose-polystyrene mixtures by breath figure technique. **R. Lopez-Simeon**, M. Hernandez-Guerrero, H.I. Beltran, **J. Campos-Teran**

**4:45 CELL 306.** Novel aqueous solvent for chitin and chitin-based materials thereof. **J. Cai**

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### Section B

Marriott Marquis San Diego Marina  
La Costa

**Cellulose Nanocrystal Fundamentals**

*Financially supported by BioNavis*

E. Kontturi, T. Tammelin, *Organizers*

E. D. Cranston, *Organizer, Presiding*

**1:45 CELL 307.** Film formation from sessile droplets of cellulose nanocrystal suspensions. **D.G. Gray**, X. Mu

**2:10 CELL 308.** Facile route for chiral plasmonic gold nanoparticle assemblies via templating with cellulose nanocrystals. **J. Majoinen**, J. Hassinen, J.J. Haataja, H.T. Rekola, E. Kontturi, M. Kostainen, R.H. Ras, P. Törmä, O.T. Ikkala

**2:35 CELL 309.** Amine-modified cellulose nanocrystals as cooperative chemocatalysts in acid-base catalyzed C-C bond forming reactions. **N.C. Ellebracht**, C.W. Jones

**3:00** Intermission.

**3:30 CELL 310.** Surface chemistry and characterization of modified cellulose nanocrystals. **S. Eyley**, W. Thielemans

**3:55 CELL 311.** Surface modification of cellulose nanocrystals using controlled radical polymerization. **S. Kedzior**, F. Hatton, J. Engström, A.E. Carlmark, E.E. Malmstrom, E.D. Cranston

**4:20 CELL 312.** Versatile surface functionalization of cellulose through modular chemistry. **J. Moran-Mirabal**

**4:45 CELL 313.** Nanocrystalline cellulose in biomolecular applications. **G.J. Westman**, K. Sahlin

### Section C

Marriott Marquis San Diego Marina  
Mission Hills

**Cellulose Nanocomposites Processing Development & their Structure Property Relations**

*Financially supported by Bio4Energy, Sweden; Centre for Biocomposites and Biomaterials Processing at University of Toronto, Canada; GreenNano, Canada*

M. Sain, *Organizer*

K. A. Oksman, *Organizer, Presiding*

M. L. Hietala, *Presiding*

**1:15** Introductory Remarks.

**1:20 CELL 314.** Melt processing of cellulose-based nanocomposites and high mechanical performance: Inherent incompatibility? **A. Dufresne**

**1:45 CELL 315.** Effect of functionalized cellulose on the thermal stability of abs and hips-reinforced composites. **C.J. Huntley**, K.D. Crews, M.L. Curry

**2:10 CELL 316.** Liquid assisted melt compounding of nanocomposites based on PLA: Processing and properties. **N. Herrera Vargas**, K.A. Oksman

**2:35 CELL 317.** Withdrawn.

**3:00** Intermission.

**3:30 CELL 318.** Bovine biomass based microfibrillated cellulose composites. **N. Mohd Kamal**, K. Lee, **A. Bismarck**

**3:55 CELL 319.** Manufacturing strong regenerated cellulose nano-composite fibres. **S. Rahatekar**, C. Zhu, S.J. Eichhorn, N.D. Wanasekara, O. Kuzmina, T. Welton, K. Potter

**4:20 CELL 320.** Orientation in uniaxially stretched plasticized polylactic acid/cellulose nanocomposites films. **A.A. Singh**, N. Herrera, K.A. Oksman

**4:45 CELL 321.** Enhancing the mechanical, thermal and biodegradability of thermoplastics through cellulose-based fillers. **K.D. Crews**, C.J. Huntley, M. Islam, D. White, M.L. Curry

### Section D

Marriott Marquis San Diego Marina  
Marina Salon G

**Biomedical & Drug Delivery Applications of Polysaccharide-Based Materials**

**Wound Care, Antimicrobial Surfaces, Point-of-Care Diagnostics**

*Cosponsored by CARB*

M. Roman, *Organizer*

V. Edwards, *Organizer, Presiding*

**1:20 CELL 322.** Peptide derivatized cellulose aerogel from cotton as a point of care diagnostic protease sensor. **K.R. Fontenot**, V. Edwards, N. Pircher, F. Liebner

**1:45 CELL 323.** Withdrawn.

**2:10 CELL 324.** Biointeractive fibers with antibacterial properties. **M.K. Ek**, J. Illergård, C. Chen, L. Wågberg

**2:35 CELL 325.** Monitoring human neutrophil elastase (HNE) in chronic wound. **A. Ferreira**, J. Cunha, A. Cavaco-Paulo

**3:00** Intermission.

**3:30 CELL 326.** Withdrawn

**3:55 CELL 327.** Porous electrospun nanocomposite mats based on cellulose/chitin nanocrystals for wound dressing. **N. Naseri**, A. Mathew, K.A. Oksman

**4:20 CELL 328.** Polysaccharide-based nanofibers as functional biomaterials: From biocatalysis to drug delivery. **S. Khan**

**4:45 CELL 329.** Development of structured polysaccharide based materials for biomedical applications. **R. Kargl**, T. Mohan, U. Mauer, L. Gradišnik, S. Spirk, S. Hribenik, M. Kurečić, **K. Stana-Kleinschek**

### Section E

Marriott Marquis San Diego Marina  
Leucadia

**Functional Lignocellulosics & Nanotechnology**

**Paper: Fundamentals & Applications**

*Cosponsored by CARB*

*Financially supported by BioNavis; EPNOE*

M. S. Peresin, T. Nypelö, *Organizers*

I. Filpponen, S. Spirk, *Organizers, Presiding*

**1:45 CELL 330.** Photo cross-linking paper sheets for modulation of mechanical properties in the wet state. **M.A. Biesalski**

**2:10 CELL 331.** Transparent oxygen-barrier films by conventional papermaking. **P.A. Larsson**, L. Wågberg

**2:35 CELL 332.** Cellulose fibers and bonds - Mechanical and morphological properties of the smallest constituents of the paper network. **W.J. Fischer**, M. Jajcinovic, U. Hirn, W. Bauer

**3:00** Intermission.

**3:30 CELL 333.** Understanding and designing the retention of model compounds in microfluidic paper devices. **S. Wendenburg**, M. Nachbar, A. Böhm, M.A. Biesalski

**3:55 CELL 334.** Cellulose nanofibrils as paper additives. **R. Hollertz**, L. Wågberg

**4:20 CELL 335.** Flame-retardant paper from wood fibers functionalized via layer-by-layer assembly. **O. Kökükaya**, F. Carosio, J.C. Grunlan, L. Wågberg

**4:45** Concluding Remarks.

**Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Symposium in honor of Professor Sharpless's 75th Birthday**

*Sponsored by CARB, Cosponsored by CELL*

## THURSDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Cardiff

**Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems**

M. L. Auad, O. El Seoud, D. Petri, O. J. Rojas, *Organizers*

J. Campos-Teran, *Organizer, Presiding*

P. E. Fardim, *Presiding*

**8:00** Introductory Remarks.

**8:05 CELL 336.** Morphological structure and chemical composition of willow (*Salix* sp.) inner bark. **J. Dou**, L. Galvis, U. Holopainen, T. Tamminen, T. Vuorinen

**8:30 CELL 337.** WOBAMA wood based materials based on bark. **M.K. Ek**, D. Li, M. Le Normand

**8:55 CELL 338.** Closed-loop strategy for valorization of starch and poly (lactic acid) into new materials. **D. Wu**, M. Hakkarainen

**9:20 CELL 339.** Polysaccharides as green binders for wood adhesives. **L. Fogelstrom**, E. Norström, P. Nordqvist, F. Khabbaz, E.E. Malmstrom

**9:45** Intermission.

**10:15 CELL 340.** New perspectives for valorisation of sugarcane bagasse using hydrotropes. **P.E. Fardim**, K. Gabov

**10:40 CELL 341.** Rapeseed straw extraction yields hemicelluloses for renewable materials. **A. Svard**, E. Brannvall, U.M. Edlund

**11:05 CELL 342.** Use of marine and agricultural waste for the obtaining of new materials. **M. Esquivel Alfaro**, G. Jiménez Villalta, S. Madrigal Carballo, J. Vega Baudrit, K. Ramirez Amador

**11:30 CELL 343.** Continuous laboratory scale hydrothermal reactor for biomass materials with high water contents. **J.F. Quesada-Kimzey**, P. Zúñiga, T. Gmelch

### Section B

Marriott Marquis San Diego Marina  
La Costa

**Cellulose Nanocrystal Fundamentals**

*Financially supported by BioNavis*

E. D. Cranston, E. Kontturi, *Organizers*

T. Tammelin, *Organizer, Presiding*

**8:30 CELL 344.** GIFT for the analysis of cellulose nanocrystals by SAXS. **H. Ehmman**, W. Binder, T. Mohan, K. Stana-Kleinschek, **S. Spirk**

**8:55 CELL 345.** Understanding crystallinity change upon production of CNCs. **U.P. Agarwal**, R.S. Reiner, C. Hunt, E. Foster, A. Isogai, J. Catchmark

**9:20 CELL 346.** Polymorphic and morphological changes of cellulose nanocrystals during mercerization. **J. Song**, E. Jin, J. Guo, F. Yang, O.J. Rojas

9:45 Intermission.

**10:15 CELL 347.** Allomorph transformation in cellulose nanocrystals from cellulose I to cellulose III on a 2D-surface submonolayer. R. Salminen, E. Kontturi

**10:40 CELL 348.** Na-cellulose complex dominates the dissolution of crystalline cellulose in precolloid aqueous NaOH/Urea solution. P. Chen, A.E. Ismail

**11:05 CELL 349.** Effective interactions in cellulose nanocrystals suspensions from 3D-RISM-KH molecular theory of solvation. A. Kovalenko, S.R. Stoyanov

**11:30 CELL 350.** Elastic and plastic deformation behaviour of cellulose crystal by atomistic simulation. Y. Ogawa, P. Chen, Y. Nishiyama, k. Mazeau

## Section C

Marriott Marquis San Diego Marina  
Mission Hills

### Cellulose Nanocomposites Processing Development & their Structure Property Relations

*Financially supported by Bio4Energy, Sweden; Centre for Biocomposites and Biomaterials Processing at University of Toronto, Canada; GreenNano, Canada*

K. A. Oksman, *Organizer*

M. Sain, *Organizer, Presiding*

S. Tanpichai, *Presiding*

8:00 Introductory Remarks.

**8:05 CELL 351.** Nanocellulose composites projects for structural applications from 2005 in Kyoto. H. Yano, F. Nakatsubo

**8:30 CELL 352.** 3D printing of a conductive ink based on cellulose nanofibrils and carbon nanotubes. K.M. Haakansson, C. de la Peña, V. Kuzmenko, P. Enoksson, P. Gatenholm

**8:55 CELL 353.** Cellulose based nanocomposites with outstanding dispersion produced by in-situ polymerization. S. Geng, M. Noël, P. Liu, K.A. Oksman

**9:20 CELL 354.** Comparative study on the reinforcing properties in rubber of cellulose nanocrystals and nanofibrils functionalized in water. B. Dhuique, G. Sebe

9:45 Intermission.

**10:15 CELL 355.** Cellulose fibers reinforced thermoset composites – micro vs nano. F. Ansari

**10:40 CELL 356.** All cellulose composites from nanocellulose networks by using green solvents. P. Pilttonen, M. Visanko, M. Illikainen, K.A. Oksman

**11:05 CELL 357.** Mechanical performance of 3D-printed porous nanocomposite bone scaffolds. J. Hong, M. Roman

**11:30 CELL 358.** Effect of cellulose nanocrystals on amaranth protein films properties. A.D. Blanco, S.O. Mendoza, K.A. Oksman

## Section D

Marriott Marquis San Diego Marina  
Marina Salon G

### Biomedical & Drug Delivery Applications of Polysaccharide-Based Materials

#### Hydrogels, Regenerative Medicine, Tissue Engineering

*Cosponsored by CARB*

V. Edwards, M. Roman, *Organizers*

K. R. Fontenot, *Presiding*

8:05 CELL 359. Withdrawn.

**8:30 CELL 360.** Nanocellulose reinforced contact lens for ophthalmic use. A. Mhryanayan

**8:55 CELL 361.** Engineering pH-responsive chitosan nanoparticles as a genetically specific nanoantibiotic. J.A. Edson, D. Ingato, Y.J. Kwon

**9:20 CELL 362.** High strength chitosan hydrogels fabricated in alkaline aqueous system. J. Duan

9:45 Intermission.

**10:15 CELL 363.** 3D bioprinting of living tissues and organs with polysaccharide based bioinks and human cells. P. Gatenholm, K. Markstedt, I. Tournier, D. Hägg

**10:40 CELL 364.** Design of biocellulose implants for first successful bile duct regeneration. D.O. Klemm, F. Rauchfuss, F. Kramer, K. Petzold-Welcke, T. Richter, C. Ruhe, A. Tannapfel

**11:05 CELL 365.** Biotechnologically designed biocellulose tubes as cardiovascular implants: Can they fulfill the challenge from surgeons' viewpoint? M. Wacker, J. Wippermann, M. Scherner, S. Reinhardt, D.O. Klemm, F. Kramer, K. Petzold-Welcke, T. Richter

**11:30 CELL 366.** Nanocellulose based materials for differentiating cell growth. M. Smyth, C. Fournier, C. Picart, J. Foster, J. Bras

### Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Symposium in honor of Professor Sharpless's 75th Birthday

*Sponsored by CARB, Cosponsored by CELL*

## THURSDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Cardiff

#### Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

M. L. Auaad, O. El Seoud, D. Petri, *Organizers*

J. Campos-Teran, O. J. Rojas, *Organizers, Presiding*

1:15 Introductory Remarks.

**1:20 CELL 367.** Valorization of agricultural residuals through biophysical transformation into an organic soil enhancer. Z. Samani, P. Bandini

**1:45 CELL 368.** Enzymatic synthesis of alkyl mannoside surfactants by  $\beta$ -mannanases. J. Morrill, A. Aronsson, A. Rosengren, E. Nordberg Karlsson, P. Adlercreutz, H. Ståhlbrand

**2:10 CELL 369.** Carbonize it? Simple test method to see whether carbonization is a good valorization choice for a material. J.F. Quesada-Kimzey

**2:35 CELL 370.** N/P dual-doped porous carbon synthesized from coconut husk and chitin as an efficient electrocatalyst for the oxygen reduction reaction. M. Borghei, N. Loacharen, E. Kibena, L. Johansson, J. Campbell, K. Tammeveski, O.J. Rojas

3:00 Intermission.

**3:30 CELL 371.** Valorization of renewable, plant-based proteins in advanced materials and surface modification. O.J. Rojas, C.L. Salas, K. Goll, M. Ago, J. Genzen

**3:55 CELL 372.** Evaluation of the cactus based-mucilage as an alternative natural dispersant to be incorporated in oil spill response strategies. F. Guo, D. Stebbins, T. Peng, W. Zhao, R. Falahat, S. Thomas, R.G. Toomey, N. Alcantar

**4:20 CELL 373.** Potential of corn husk to produce inorganic nanoparticles. C. Gomez, J.C. Cárdenas, P. Posada, A.M. Serpa Guerra, J.A. Velasquez, C. Castro Herazo, P. Gañán, R. Zuluaga Gallego

**4:45 CELL 374.** Protein-polysaccharide-based hydrogel microspheres as delivery systems for anthocyanins. I. Arroyo-Maya, D. McClements, J. Campos-Teran

## Section B

Marriott Marquis San Diego Marina  
La Costa

### Cellulose Nanocrystal Fundamentals

*Financially supported by BioNavis*

E. D. Cranston, E. Kontturi, T. Tammelin, *Organizers*

W. Thielemans, *Presiding*

**1:45 CELL 375.** Preparation of cellulose nanocrystals: Review, current status, and outlook. E. Kontturi

**2:10 CELL 376.** Benchmarking cellulose nanocrystals from various sources. M. Reid, M. Villalobos, E.D. Cranston

**2:35 CELL 377.** Ionic liquid-cellulose-in-oil microemulsions for directing morphology of cellulose nanoparticles. J.R. Alston, J.M. Mabry

3:00 Intermission.

**3:30 CELL 378.** Functional and highly thermal stable cellulose nanocrystals produced from a novel process with low cost. J. Zhu

**3:55 CELL 379.** Method for estimating the extent of tip broadening in AFM width measurements of cellulose nanocrystals. F. Navarro, R. Ramirez, M. Roman

## Section C

Marriott Marquis San Diego Marina  
Mission Hills

### Cellulose Nanocomposites Processing Development & their Structure Property Relations

*Financially supported by Bio4Energy, Sweden; Centre for Biocomposites and Biomaterials Processing at University of Toronto, Canada; GreenNano, Canada*

M. Sain, *Organizer*

K. A. Oksman, *Organizer, Presiding*

Y. Aitomaki, *Presiding*

1:15 Introductory Remarks.

**1:20 CELL 380.** Mechanical behavior of nanostructured cellulosic materials. L. Berglund

**1:45 CELL 381.** Tough, nanocomposites using cellulose nanocrystals: Interface modification and new multifunctional interface imaging probes. J.W. Gilman, J.W. Woodcock, C.S. Davis, M. Wang, J.A. Liddle, L.C. Brinson, X. Cheng, P.V. Kolluru, A. Karim, D. Grolman, S. Stranick, R. Beams, R.S. Rodriguez, M. Devillbliss, D. Fox

**2:10 CELL 382.** Micro or nanoscale cellulose reinforcement – does it matter? F. Vilaseca

**2:35 CELL 383.** Cellulose nanofibril/matrix interface structure – property relationships in polymer nanocomposites. H. Soeta, T. Saito, A. Isogai

3:00 Intermission.

**3:30 CELL 384.** Mechanical and thermal properties of cellulose nanocrystal reinforced poly(vinyl alcohol) hydrogels. S. Tanpichai, K.A. Oksman

**3:55 CELL 385.** Fundamental understanding of photoyellowing of NCC and NFC for durable applications. V. Pakharekno, S. Konar, M. Sain

**4:20 CELL 386.** Improving the interfacial and mechanical properties of short glass fiber/epoxy composites by coating the glass fibers with cellulose nanocrystals. A. Asadi, M. Miller, R. Moon, K. Kalaitzidou

**4:45 CELL 387.** Significant effects of TEMPO-oxidized cellulose nanofibril (TOCN) nanostructures on mechanical properties of TOCN/rubber composites. S. Fukui, T. Saito, A. Isogai

## CHED

### Division of Chemical Education

I. Levy, I. Black and D. Wicht, *Program Chairs*

#### OTHER SYMPOSIA OF INTEREST:

**Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences** (see IAC, Sun)

**Is There a Crisis in Organic Chemistry Education?** (see PRES, Mon)

**James Bryant Conant Award in High School Chemistry Teaching: Honoring Julia Winter** (see ORGN, Tue)

#### SOCIAL EVENTS:

**High School-College Interface Luncheon (Tickets Required)**, 12:00 PM, Sun

**Division Reception**, 5:30 PM, Sun

## SUNDAY MORNING

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom A

#### High School Program

*Cosponsored by SOCED*

*Financially supported by ACS Education Division*

J. L. Ball, S. B. Mitchell, *Organizers, Presiding*

8:00 Registration.

8:30 Introductory Remarks.

**8:35 CHED 1.** Energy, design and change with photo origami: 21st century engineering with shape memory polymers. E.W. Carpenter

**9:30 CHED 2.** The Albert Einstein Fellowship: Creating Connections for teachers. A. Artz

**9:50 CHED 3.** Computers in Chemistry: Breakthroughs in molecular spectroscopy. S. McQueen

10:10 Intermission.

**10:20 CHED 4.** Building mobile tools for chemistry. J. Winter

**11:00 CHED 5.** My high school chemistry teacher: Hero and the path to the golden egg. H. Freeze

**11:20 CHED 6.** Integrating the chemistry of climate science into high school classrooms. M.H. Towns, P.G. Mahaffy, M.M. Kirchoff, L.C. McKenzie, A. Versprille

**11:40 CHED 7.** Sip, spit, repeat: Learning the basics of assay development through evaluations of astringency in beverages. G.L. Sacks, L.F. Springer

## Section B

Manchester Grand Hyatt San Diego  
Mission Beach A/B

### Fall 2015 InterCollegiate Cheminformatics Course

*Cosponsored by CINP and MPPG*

S. J. Chalk, L. McEwen, *Organizers*

R. E. Belford, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:40 CHED 8.** Using cheminformatics to develop the next aspirin. J. Langenstein, J.H. Penn

**8:55 CHED 9.** Correlation of anti-cancer drug structure to efficacy. J. Turner, S.J. Chalk

**9:10 CHED 10.** Performing variable substituent chemical structure searches. J. House, R.E. Belford, S. Kim

**9:25 CHED 11.** Advanced database search. S. House, R.E. Belford, S. Kim

**9:40** Intermission.

**9:50 CHED 12.** pH and acid-base equilibria with cheminformatics. B.S. Brown, J.L. Muzyka

**10:05 CHED 13.** Aggregation of solubility data for quick access. P. Sharma, B.J. Davis, R.E. Belford, J.L. Muzyka, A. Lang, J. Cuadros

**10:20 CHED 14.** Cross-walking meta-data from the IUPAC-NIST solubility database to a new scientific data model. N. Gutierrez, S.J. Chalk

**10:35 CHED 15.** Semantic annotation of thermochemical data from the NIST-JANAF dataset. N. Azim, S.J. Chalk

**10:50** Intermission.

**11:00 CHED 16.** Integration of a spectral viewer for data stored in an open source electronic laboratory notebook. A.P. Cornell, R.E. Belford, D. Berleant, M.A. Bauer, O. Rothenberger, H. Bergwerf

**11:15 CHED 17.** Automated spectrum resolver with InChI enhanced lookup. A.H. Williams, J.L. Muzyka

**11:30 CHED 18.** LabPal: Chemical information for android. D.S. Graham, J.L. Muzyka

**11:45** Concluding Remarks.

## Section C

Manchester Grand Hyatt San Diego  
Solana Beach A/B

### NMR Spectroscopy in the Undergraduate Curriculum

*Financially supported by Bruker Biospin, JEOL USA*

L. J. Anna, D. P. Soulsby, A. S. Wallner, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 19.** Free radical chlorination of alkanes: Application of <sup>1</sup>H NMR and 1D TOCSY NMR spectroscopy to the analysis of reaction products. D.P. Soulsby

**8:55 CHED 20.** Preparing students to interpret NMR data from kinetics and thermodynamics experiments. C.S. Hamann, S.C. Young

**9:15 CHED 21.** Unequivocal structure proof using NMR spectroscopy in a first-year organic laboratory project. C.R. Butler, A.M. Schoffstall, R.K. Shoemaker

**9:35** Intermission.

**9:45 CHED 22.** Using NMR spectroscopy as an effective tool for promoting active learning in the introductory organic chemistry laboratory course. J.A. Cramer

**10:05 CHED 23.** Investigating molecular diffusion in aqueous media using experimental nuclear magnetic resonance (NMR) spectroscopy and computational molecular dynamics (MD): A modular undergraduate physical chemistry laboratory. B. Cherry, S.K. Davidowski, G. Gray, S. Amin, F. Thompson, J. Hillsten, A. Van Der Vaart, J.L. Yarger

**10:25 CHED 24.** There is more information in your proton NMR spectrum than you realized. D.D. Clarke, A.M. Baijja

**10:45** Concluding Remarks.

## Section D

Manchester Grand Hyatt San Diego  
Promenade A

### Undergraduate Research Papers

*Cosponsored by SOCED*

C. V. Gauthier, N. L. Snyder, *Organizers*

J. V. Ruppel, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 25.** Rapid synthesis of N-vanillylacetylacetamide. J. Choi, L.L. Bobyleva, M.M. Bobylev

**8:45 CHED 26.** Caffeic acid phenethyl ester analogues: Synthesis and optimization as xanthine oxidase inhibitors. L. Snider

**8:55 CHED 27.** Development of a continuous flow method with nitriles and amines substrates to form amides. A. Medina-Gonzalez, A. Julkowski, M. Turk, A. Pliesseis, M.T. Wentzel

**9:05 CHED 28.** Withdrawn.

**9:15** Intermission.

**9:25 CHED 29.** Synthesis and characterization of alkynylated porphyrins and bacteriochlorins. D. Dennis, R. Dolewski, M. George, B. Doornbos, B. Blough, N.L. Snyder, J.V. Ruppel

**9:35 CHED 30.** Synthesis of hyaluronic acid-based therapeutic conjugates for the diagnosis and treatment of glioblastoma multiforme. A.M. Ciancone, K.E. Gonzalez, E. Xu, R. Dolewski, D. Dennis, J.V. Ruppel, N.L. Snyder

**9:45 CHED 31.** Development and characterization of chemical tools for the identification of O-GlcNAcylated proteins. C. Brennan, M. Pratt

**9:55 CHED 32.** Drug delivery systems utilizing modified nucleobase hydrogels and polyamines. D. Johnson, C.M. Lawrence

**10:05** Intermission.

**10:15 CHED 33.** Iodination of the isoquinoline moiety of T-0632 to generate photolabile analogs. E. Yang, E.J. Nissen, D.R. Haines

**10:25 CHED 34.** Synthesis and evaluation of naphthoquinone derivatives as inhibitors for HER2-positive breast cancer. P. Tram, R. Schroeder, T. Stone, K. Nguyen, J. Geathers, J. Sridhar

**10:35 CHED 35.** Multifunctional polyurethane hydrogels for biomedical applications. C. Seitz, M. Nguyen-Kim, J. Borghs, J. Wallenborn, A. Böker

**10:45 CHED 36.** Design and synthesis of Janus dendrimers for drug delivery. N.D. Le, L. Ezell, D.G. Abebe, D. Watkins

**10:55** Concluding Remarks.

## Section E

Manchester Grand Hyatt San Diego  
Mission Beach C

### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

*Cosponsored by CCA, LSAC, SOCED and YCC*

E. S. Garcia Segal, *Organizer*

E. J. Brush, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 37.** Chemistry outreach from the perspective of a high school science teacher. K.A. Cavicchi, S. Wood

**8:55 CHED 38.** Analysis of axial ligation of N-methylimidazole to dirhodium tetraacetate catalyst. L.P. Ellis, A.E. Mangubat, S.C. Martin, M. Abernathy, Z.T. Ball

**9:15 CHED 39.** From bench to classroom then back to the bench: A quick, easy, and successful strategy for impacting high school science. M. Paulsen, J. Schoborg

**9:35 CHED 40.** Chemistry research used to bring inner city students into STEM careers. P. Bligh Glover, D.A. Schiraldi

**9:55** Intermission.

**10:10 CHED 41.** STEM outreach program designed to address attitudes of students about chemistry, math and other sciences that collaborates university faculty, local professionals and K-12 teachers on a year-long curriculum based research project. S.A. Brouet

**10:30 CHED 42.** Research experience for teachers program in polymers at the University of Akron: Activities, assessment, and best practices. K.A. Cavicchi

**10:50 CHED 43.** Inspiring innovation in material science education at the secondary level through a new polymer semiconductor kit. M.G. Walter, J. Enlow

**11:10 CHED 44.** Communicating chemistry in informal environments. M.M. Kirchoff

**11:30** Panel Discussion.

**11:50** Concluding Remarks.

## Section F

Manchester Grand Hyatt San Diego  
Promenade B

### The Two Year Guidelines: What's New

*Cosponsored by SOCED*

J. M. Sabourin, *Organizer*

S. M. Shih, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 45.** Chemistry-based technology programs in the 2015 ACS Guidelines for Chemistry in Two-Year College Programs. T.T. Duplessis

**8:55 CHED 46.** Importance of partnerships in two-year college chemistry programs. J.M. Sabourin

**9:15 CHED 47.** Safety in the 2015 two-year guidelines. J. Ellefson

**9:35** Panel Discussion.

**9:55** Intermission.

**10:05 CHED 48.** Student skills in the 2015 two-year guidelines. A.K. El-Ashmawy

**10:25 CHED 49.** Importance of student mentoring in the chemical sciences at the community college. A.M. Rivera Figueroa

**10:45 CHED 50.** Student transfer and the guidelines for chemistry in two-year college programs. M. Michalovic

**11:05 CHED 51.** Emerging trends in the two year college landscape. S.M. Shih

**11:25** Panel Discussion.

**11:45** Concluding Remarks.

## Section G

Manchester Grand Hyatt San Diego  
Ocean Beach

### Chemistry Education Research: Graduate Student Research Forum

A. G. Moon, C. L. Stanford, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 52.** Exploring collegiate students' ideas about the purpose and outcomes of chemistry outreach. J.M. Pratt, E.J. Yeziarski

**8:55 CHED 53.** Using the ACS climate science toolkit to improve the understanding of climate science among deaf and hard-of-hearing laboratory science technology students. A.D. Ross

**9:15 CHED 54.** Connections and conflicts students perceive between chemistry and molecular biology. K.P. Kohn, S.M. Underwood, M. Cooper

**9:35 CHED 55.** Curricular influences and design approaches in undergraduate inorganic chemistry. J.H. Torres King, E.J. Yeziarski

**9:55** Intermission.

**10:00 CHED 56.** Solved problem analysis to support student metacognition. D. Mlsna, N. Alexander, T. Linley

**10:20 CHED 57.** Creation of a homework program to improve test preparation metacognitive ability for low-performing students. B. Casselman, B. Ohlsen, C.H. Atwood

**10:40 CHED 58.** Item response theory as a tool to identify and improve difficult topics for individual students. B. Ohlsen, C.H. Atwood

**11:00** Concluding Remarks.

## Section H

Manchester Grand Hyatt San Diego  
Pier

### Cottrell Scholars Collaborative: Innovating the Integration of Research & Teaching

*Financially supported by Research Corporation for Science Advancement*

A. L. Feig, *Organizer*

R. Waterman, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 59.** Leadership training for teacher-scholars. R. Hernandez

**9:05 CHED 60.** Cottrell Scholars Collaborative New Faculty Workshop: A leg up for new chemistry faculty. R. Waterman, A.L. Feig, M.N. Stains

**9:35 CHED 61.** Integrating research and education in chemical biology. P.J. Beuning

**10:05** Intermission.

**10:20 CHED 62.** Building lifelong learners through course-based undergraduate research experiences (CUREs). J.M. Heemstra

**10:50 CHED 63.** Scholar, teacher, mentor: Using an Using an integrated portfolio of activities to promote positive institutional transformation. A.L. Feig

**11:20 CHED 64.** Integrating nanomaterials in and across the undergraduate curriculum. C.J. Murphy

**11:50** Concluding Remarks.

## Section I

Manchester Grand Hyatt San Diego  
Pier

### Cottrell Scholars Collaborative: Innovating the Integration of Research & Teaching

Financially supported by Research  
Corporation for Science Advancement

A. L. Feig, R. Waterman, *Organizers*

**8:30 - 10:30 CHED 65.** From research lab to classroom: A multi-faceted high school outreach program. D.G. Emmerson, T.B. Clark

### Undergraduate Teaching at the Frontiers of Inorganic Chemistry

#### Framing the Future

Sponsored by INOR, Cosponsored by CHED

### Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored  
by CHED, PROF and YCC

#### Ethics 101

Sponsored by PROF, Cosponsored  
by CHED, CINF and ETHC

## SUNDAY AFTERNOON

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom A

#### High School Program

Cosponsored by SOCED  
Financially supported by ACS Education Division

J. L. Ball, S. B. Mitchell, *Organizers, Presiding*

**1:00 CHED 66.** Atomic particles: Helping students gather data to understand the particles inside the atom. L.E. Slocum

**2:00 CHED 67.** Let's revel in the periodic table. E.R. Scerri

**3:00** Intermission.

**3:10 CHED 68.** Very practical chemistry of materials. J.M. Newsam

**3:30 CHED 69.** Encouraging focused student talk through lab structure in high school chemistry. J.L. Ball

**3:50 CHED 70.** Teachers as species: Survive, interact, adapt, and thrive. P.L. Daubenmire, D.G. Herrington

**4:10 CHED 71.** I'm a pack rat! Simple activities to teach chemistry with things found in your junk drawer. S.C. Rukes

**4:30** Concluding Remarks.

### Section B

Manchester Grand Hyatt San Diego  
Mission Beach A/B

#### Fall 2015 InterCollegiate Cheminformatics Course

Cosponsored by CINF and MPPG

S. J. Chalk, L. McEwen, *Organizers*

R. E. Belford, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:40 CHED 72.** Future intercollegiate course management systems: Under the hood of the Cheminformatics OLCC. J.L. Holmes, R.E. Belford

**2:00 CHED 73.** Future intercollegiate course management systems: Part 2 - An extensible nodal network of TLOs (Teaching and Learning Objects). R.E. Belford, J.L. Holmes

**2:20 CHED 74.** Better data habits for better science: Chemical information literacy in the digital era. K. Briney, Y. Li, L. McEwen

**2:40 CHED 75.** Talking about cheminformatics to undergraduate chemistry majors. S. Kim, E. Hepler-Smith, L. McEwen, A. Clark

**3:00** Intermission.

**3:10 CHED 76.** Facilitators perspective on teaching chemical informatics as part of the Online Collaborative Chemistry (OLCC) course. S.J. Chalk

**3:30 CHED 77.** Cheminformatics directed study with OLCC. J.L. Muzyka

**3:50 CHED 78.** Reviewing PubChem laboratory chemical safety summaries for different user types. B. Murphy, R. Stuart, R.E. Belford, L. McEwen

**4:10** Panel Discussion.

## Section C

Manchester Grand Hyatt San Diego  
Solana Beach A/B

### NMR Spectroscopy in the Undergraduate Curriculum

Financially supported by Bruker  
Biospin, JEOL USA

L. J. Anna, D. P. Soulsby, A. S. Wallner, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 79.** Liquid CO<sub>2</sub> extraction and NMR characterization of anethole from fennel seed: A general chemistry laboratory. B.R. Bodsgard, N.R. Lien, Q.T. Waulters

**1:55 CHED 80.** Identification of *Arabica* and *Robusta* varieties of green coffee beans by proton NMR based principle component analysis: A laboratory in NMR metabolomics for an undergraduate instrumental analysis course. P.O. Sandusky

**2:15 CHED 81.** Incorporation of scaffolding into the teaching of NMR in the organic laboratory. C. Gabel

**2:35** Intermission.

**2:45 CHED 82.** Assessment of NMR teaching and learning strategies in organic undergraduate labs. S.M. Schelble, J. Trate, K. Murphy

**3:05 CHED 83.** Interventions in laboratory instruction for using NMR based on assessments. S.M. Schelble, J. Cook

**3:25 CHED 84.** Evolution of teaching NMR in the undergraduate organic chemistry curriculum: Fifty years of changes. F.J. Matthews

**3:45** Concluding Remarks.

## Section D

Manchester Grand Hyatt San Diego  
Promenade A

### Undergraduate Research Papers

Cosponsored by SOCED

J. V. Ruppel, N. L. Snyder, *Organizers*

C. V. Gauthier, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 85.** Synthesis of chalcone derivative's ferrocene polymers for potential multi-functional materials. G. Rodriguez Diaz, J. Fajardo, Y. Enriquez Gonzalez, A.R. Guadalupe Quinones, I. Montes

**1:45 CHED 86.** Bis(imino)acenaphthenes (BIAN) complexes of vanadium. G. Risica, N. Tsamchoe, N. Onishi, J. Niklas, J.D. Gordon, C.D. Abernethy

**1:55 CHED 87.** Cyclic voltammetry study of ruthenium oxide nanostructured electrode. L. Douglas, C.L. Arnold, A. Navulla, L. Meda

**2:05 CHED 88.** Synthesis, characterization, and study of the interactions with DNA of ruthenium (II) polypyridyl complexes with ferrocenyl thiosemicarbazones. F.A. Beckford, D. Blach

**2:15** Intermission.

**2:25 CHED 89.** AFM based fabrication of gold nanowires through electroless deposition. H. Ashberry, C.L. Berrie, S. Ulapane, J. Tolleben

**2:35 CHED 90.** Synthesis of gold-carbon nanoparticles and evidence of gold-carbon bond. C.E. Mullen, J. Ford, A.L. Hernandez, Y. Pajouhafsar, J.J. Borski, C.R. Witkowski, A. Mohamed, H. Abdou

**2:45 CHED 91.** Interaction of partially green double reduced gold nanoparticles with lead. A. Cruz Torres, R. Noriega Rivera, C. Osorio Cantillo, E.J. Ferrer Torres, J.I. Ramirez Domenech

**2:55 CHED 92.** Synthesis, characterization, and reactivity of iridium(I) complexes containing chelating diphosphine ligands. S.H. Schreiner, K. Olsen

**3:05** Intermission.

**3:15 CHED 93.** Luminescent analysis and anion sensing studies of urea and amidothiourea based rhenium (I) complexes. N. Vecchio, J.M. Bachor, M.O. Odago

**3:25 CHED 94.** Synthesis of N-H based ligands for luminescent anion recognition. N. LaScala, M.O. Odago

**3:35 CHED 95.** Predictive design principles for earth abundant mononuclear water oxidation catalysts via *ab initio* calculations. K. Hunter, J. Alvarado, E.A. Jarvis

**3:45 CHED 96.** Nickel oxide nanospheres and their exceptional lithium-ion storage capacity. C.L. Arnold, A. Dangerfield, L. Meda

**3:55** Concluding Remarks.

## Section E

Manchester Grand Hyatt San Diego  
Mission Beach C

### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Cosponsored by CCA, LSAC, SOCED and YCC

E. J. Brush, *Organizer*

E. S. Garcia Segal, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 97.** Dialogue with the Centers for Chemical Innovation: Pioneering chemistry outreach and education. M. DeBoever, C. Parsons, J. Henderson, M. Ruffin, B. Hames, M. Krause, E. Pererra, D. Watt, H. Weizman

**2:05 CHED 98.** Open lab night outreach education at Bridgewater State University: Design and logistics. S. Nellutla

**2:25 CHED 99.** Open lab night outreach education at Bridgewater State University: Part II - learning objectives, metrics and assessment. E.J. Brush, S. Nellutla

**2:45 CHED 100.** ACS Chemoji: Harnessing social media to create a buzz. J.M. Morrison

**3:05 CHED 101.** Exciting or educational? Finding a balance between entertainment and educational demonstrations. J. Meyer

**3:25** Intermission.

**3:40 CHED 102.** High school chemistry teacher workshops as educational outreach. E.S. Garcia Segal

**4:00 CHED 103.** Students learning science through a sustained network of teachers: Professional development for high school chemistry teachers in southwestern Illinois. S. Khazaeli, E.J. Voss, W.J. Hunter, E. Osthoff

**4:20 CHED 104.** Impact of NECT, New England Association of Chemistry Teachers, on the professional development of chemistry teachers in schools and colleges in New England. M. Govindan, M. Christian-Madden

**4:40 CHED 105.** Science outreach for adult learners: Designing a hands-on science experience for students in G.E.D. and adult literacy courses. A. Komor, N. Gagnon

**5:00** Panel Discussion.

**5:20** Concluding Remarks.

## Section F

Manchester Grand Hyatt San Diego  
Promenade B

### Perspectives on Climate Change Literacy & Education: Local to International

Cosponsored by CEI

G. P. Foy, K. E. Peterman, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 106.** Climate change and development: Global perspectives on the role of developed nations in mitigating the effects of climate change. P. Shrestha, G.P. Foy, K.E. Peterman

**1:55 CHED 107.** Climate change and poverty: Global inequalities. C. Jackson, G.P. Foy, K.E. Peterman

**2:15 CHED 108.** Climate change and protests: The personal side of policy. N.D. Diklich, G.P. Foy, K.E. Peterman

**2:35** Intermission.

**2:45 CHED 109.** The unheard voice: Indigenous peoples' role in COP 21. J. Leaness, G.P. Foy, K.E. Peterman

**3:05 CHED 110.** Comparative perspectives of France and the US in climate change negotiations. G.D. Vial, G.P. Foy, K.E. Peterman

**3:25 CHED 111.** Water's role in climate literacy. G. Margida, G.P. Foy, K.E. Peterman

**3:45** Intermission.

**3:55 CHED 112.** Air quality and climate change interactions. W. Marrero, G.P. Foy, K.E. Peterman

**4:15 CHED 113.** Deployment of low-cost, carbon dioxide sensors throughout the Washington metropolitan area: The capital climate initiative. K. Caine, D. Bailey, J.H. Miller

**4:35 CHED 114.** Chemistry and sustainable practices: Completing the idea before large-scale implementation. T. Di Nardo, G.P. Foy, K.E. Peterman

**4:55 CHED 115.** Striving for climate change literacy in "The Age of Disinformation". G.M. Bodner

**5:15** Concluding Remarks.

## Section G

Manchester Grand Hyatt San Diego  
Ocean Beach

**Chemistry Education Research:  
Graduate Student Research Forum**

A. C. Moon, C. L. Stanford, *Organizers,  
Presiding*

1:30 Introductory Remarks.

1:35 CHED 116. Withdrawn.

1:55 CHED 117. Deconstructing constructivism: Modeling causal relationships between constructivist learning environment factors and student outcomes in introductory chemistry. R. Komperda, D. Bunce

2:15 CHED 118. Investigation of the discrepant achievement between non-TRIO and TRIO students in undergraduate general chemistry. L. Fox, G. Roehrig

2:35 Intermission.

2:40 CHED 119. Comparing different approaches to the implementation of a new chemistry curriculum. Y. Hou, V. Talanquer

3:00 CHED 120. Exploring students' understanding of macroscopic energy in solution formation. O. Judd, M. Cooper

3:20 CHED 121. How does students' prior knowledge influence their understanding of a common external representation of a voltaic cell? M.M. Wu, T.J. Bussey

3:40 Concluding Remarks.

## Section H

Manchester Grand Hyatt San Diego  
Pier

**Molecular Modeling at the  
Undergraduate Level**

*Cosponsored by MPPG*

C. H. Jaworek-Lopes, *Organizer*

F. Ryykin, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 122. Molecular visualization and computation early, often, and as an upper-level elective. K. Range

1:55 CHED 123. Development of higher order thinking skills: Application of simulations and molecular modeling to instruction in physical and organic chemistry. E.N. Ndip, G.C. Nwokogu, C.M. Bump, M.K. Waddell

2:15 CHED 124. Synergy between computation and experiment: Determining the major conformer of a Diels-Alder reaction product. J.E. Hanson

2:35 Intermission.

2:45 CHED 125. Molecular modeling with Wavefunction's Spartan and Odyssey programs in the advanced inorganic chemistry course. T. Gardner

3:05 CHED 126. Novel approach to molecular modeling using line drawings, molecule kits, and found materials. S. Burchett, J.L. Hayes, K.H. Woelk

3:25 CHED 127. Designing an introductory molecular modeling course for undergraduate students. F. Ryykin

3:45 Concluding Remarks.

**Safety Begins in the Classroom:  
Demonstrations, Awareness  
& Pre-Lab Planning**

*Sponsored by CHAS, Cosponsored  
by CCS and CHED*

**Discussions with the President's  
Task Force on Employment**

*Sponsored by PRES, Cosponsored by  
BIOL, BMGT, CARB, CELL, CHED, CINP,  
COLL, COMSCI, DAC, GEOC, I&EG,  
IAC, INOR, MEDI, ORGN, PHYS, PMSE,  
POLY, PROF, SCHB and WCC*

**Going Global with International  
Scientific Training: An Undergraduate  
Perspective of International  
Research Experiences**

*Sponsored by IAC, Cosponsored  
by CHED and YCC*

**Preceptors of Chemistry**

*Sponsored by HIST, Cosponsored by CHED*

## SUNDAY EVENING

## Section A

San Diego Convention Center  
Hall D

**General Posters**

I. J. Levy, *Organizer*

7:00 - 9:00

CHED 128. Philatelic table of the elements. L.G. French

CHED 129. Girls in STEM: Who stole the painting? S. Hubbard

CHED 130. Society for women in graduate studies in chemistry & biochemistry: Fostering an inclusive and empowering environment for all graduate students. M.L. Clark, K.A. Nadler, A. Sasayama, L. Adamiak, S. Brydges

CHED 131. Design and implementation of an on-line alchemy course. M. Harrison

CHED 132. Chemical vignettes. F.J. Torre

CHED 133. Flexible capstone experiment introducing elements of multiregression analysis and experimental design. P.A. Snetsinger, A. Alayyafi, Y. Almadani, M. Basaeed

CHED 134. Evaluation of technology-enhanced peer-led team learning and homework in organic chemistry. J.E. Haky, T.S. Sempertegui Plaza, E.M. Rezier, L. Deacon

CHED 135. Designing a two-semester inorganic chemistry curriculum. C.M. Zaleski

CHED 136. Investigation of student attitudes and understanding in inorganic chemistry. L. Ley, R.M. Theisen

CHED 137. Impact of supplemental instruction on conceptual understanding and learning attitudes in organic chemistry. S. Li, J. Leister

CHED 138. Designing for sustained adoption. C.L. Stanford, R.S. Cole, C. Henderson, J. Froyd, R. Khatri, D. Friedrichsen

CHED 139. Overcoming resistance to change: Stated and enacted inquiry practices of four high school chemistry teachers. J.M. Pratt, S.E. Nielsen, E.J. Yeziarski

CHED 140. Effect of the "dropped" exam on the student performance and overall grade in the organic chemistry course. E.N. Kadnikova, A.P. Thome

CHED 141. Organic chemistry students' understandings of the relationship between stability and reactivity in the context of bonding. M. Popova, S. Bretz

CHED 142. Educational features essential for a successful scholarship program for students at varying stages of degree progress. A. Kubatova, R. Simmons, D. Pedersen

CHED 143. Impact of a university-secondary school partnership on the communication skills of STEM graduate students. J.E. Haky, D. Louda, N. Romance, A. Campbell, D. Chameily Wiik

CHED 144. Integrating departmental and institutional resources for peer tutoring in organic chemistry. W.E. Brenzovich, W.G. Hollis

CHED 145. Teaching organic synthesis using game-based learning. P.A. Sibbald

CHED 146. Application of the Arachno™ technology inside educational fields: Introduction of parallel synthesis concepts inside an undergraduate lab. M.L. Lolli, A. Moreo, A. Barge, D. Boschi, A. Costale, F. Dosio, L. Stevanato

CHED 147. Expansion of the science resource center into a STEM resource center. S. Richards, P.J. Iles, D. Saunders, L.D. Giddings, R. Holcomb, J. Lusk

CHED 148. STEM-SIRE: STEM student self-involvement, regulation and efficacy. N. Zhao

CHED 149. Undergraduate research outcomes: Does gender matter? C.D. Bruce, G. Lacueva, B. Mellis, P. Soto, A.M. Wilson

CHED 150. Development of teaching and learning materials for cognition accelerating science classes for lower elementary students. Y. Kong

CHED 151. Effects of erythrytol on *Drosophila melanogaster*: An undergraduate research study performed by students not majoring in chemistry. B. Budy, J. Minbiole, M. Feng, P. Kohl, M. Ladis

CHED 152. Barriers to the implementation of inquiry-based instruction for high school chemistry teachers participating in long-term professional development. J.H. Torres King, E.J. Yeziarski

CHED 153. Essentials of chemistry: An alternative starting point for at-risk STEM majors. B.A. Davis

CHED 154. Addressing the gender gap in STEM through an after-school program for middle school girls. E.E. Hardy, C.D. Tutson, M.M. West, A.E. Gorden

CHED 155. Investigation of student understanding of solution chemistry through the lenses of enthalpy and entropy. T.N. Abell, S. Bretz

CHED 156. Multi-regression Factors influencing textile dye adsorption on activated carbon in a continuous flow reactor. E. Alkhatib, A. Alobaidi, R. Alharbi, S. Rajeh

CHED 157. Three question self-assessments. J.A. Parr

CHED 158. Inverted instruction for problem-solving in a GOB course. B.J. Chitester, W. Tallmadge

CHED 159. Hands-on activity using the three levels of representation to teach buffers. J.B. Padilla, J. Ortiz, Z. Medina

CHED 160. Flipped classroom application in the university basic chemistry class. Z. Own

CHED 161. Does screencast length impact student viewing? D.B. King

CHED 162. Business of chemistry: Using 2nd generation biofuels as an interdisciplinary project in scientific literacy. C. Reid, M. Gravier

CHED 163. Electron configuration board game: A new way to teach the pattern of electron configuration. S. Burchett, J.L. Hayes, K.H. Woelk

CHED 164. Student understanding of atomic interactions: Impact of simulation vs. screencast use. D.G. Herrington, R.D. Sweeder, J.R. Vandenplas

CHED 165. Conjugated mechanisms in textbooks: Kinetic control of the addition of hydrogen halides to conjugated systems. D.J. Oostendorp, J. Painter, O. Anibire

CHED 166. Carnival of chemistry: A public celebration at the University of Kansas. R.S. Black, C. Appelman

CHED 167. Using cartoon characters to represent chemical structures involved in nutrition and vitamins. R.J. Schroeder

CHED 168. Quantitative analytical chemistry as a writing intensive course. A.B. Ormond

CHED 169. Click here! The role of clickers in class preparation for general chemistry. A. Kahl

CHED 170. Teaching with technology: Waste of class time or effective incentive for active learning? M. Ilies

CHED 171. Teaching UNIX based molecular modeling in upper division undergraduate chemistry. R. Nori, A.C. Jungong, K.A. Thomasson

CHED 172. 3D printing in chemical education: Incorporating orbital isosurfaces into molecular models of calculated geometries. F.A. Carroll, D.N. Blauch

CHED 173. Flipped classroom modules for large enrollment general chemistry courses: Increasing active learning and improving student performance. J.F. Eichler

CHED 174. Creating chemistry with algebra: How a learning community helps students be more successful. M. Adrian

CHED 175. Multi-year study on using first-day assessments to determine math readiness for general chemistry. D.S. Heroux, C. Chant

CHED 176. Using peer learning to strengthen basic math skills in the general chemistry lab. H.B. Miller, M.C. Srougi, M. Knippenberg

CHED 177. Curie-us interactions: Increasing student engagement and retention in general chemistry and physics. N.N. Tahmazian, E. Li

CHED 178. Slope statistics: An Instrumental Analysis experiment to study the reliability of calibration curves obtained from different visible absorption methods. S.L. Hiley

CHED 179. Investigation of experiential learning approach in quantitative chemical analysis laboratory. S. Gamagegara, J.M. Bowen

CHED 180. Implementing POGIL in a first-year biochemistry course for pharmacy students. R.D. Hills, E. Erpenbeck

CHED 181. Experimental approach to teaching renal concentration and Gibbs-Donnan equilibrium using osmometry. M.S. McAfee

CHED 182. Research-based laboratory course examining the structure and function of alcohol dehydrogenase improves student confidence in common biochemical techniques. A. Krzysiak, M. Huff

CHED 183. Purification of lactate dehydrogenase from mammalian blood: Using a non-traditional source in a multi-week protein purification biochemistry laboratory experiment. L.S. Brunauer

Technical program information  
known at press time.

The official technical program  
for the 251st ACS National  
Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)



**CHED 184.** Utilization of guided-inquiry to correct biochemistry students' misconceptions. **E. Humphreys**, K.J. Linenberger

**CHED 185.** Ocean acidification and acid-base chemistry a student experiment. **B. Budy**, **M. Hoffman Trotter**, J. Paddack, E. Rhea, M. Sosis

**CHED 186.** Environmental chemistry as an interdisciplinary course in the undergraduate curriculum. **E.C. Sylvester**, B. Stout, M.E. Railing

**CHED 187.** Maximizing environmental chemistry research projects at a PUI. **M.E. Railing**, J. Fuller

**CHED 188.** Do ACT scores really matter in organic chemistry? **J.A. Jensen**

**CHED 189.** Displacement quantization in the simple harmonic motion. **A.A. Hasanien**, **Y.R. Elmarassi**, **B.A. Ali**, **E.N. Madi**

**CHED 190.** Students' ideas about electron structure with regards to probability and energy quantization. **Z.R. Allred**, S. Bretz

**CHED 191.** Using lanthanides to illustrate Hund's rule. **S.N. Natoli**, D.R. McMillin

**CHED 192.** Use of substituent constants for correlating molecular properties: A valuable instructional tool in the undergraduate classroom. **D. Rillema**, S. Stoyanov, A.J. Cruz, H. Nguyen

**CHED 193.** Flipping physical chemistry. **K.E. Anderson**

**CHED 194.** Investigation of the glycosidic bond energy of disaccharides through bomb calorimetry. **T. LaBelle**, **A. Baxter**, S.E. Hayik

**CHED 195.** Intersystem crossing and fluorescence saturation: A physical chemistry experiment. **M.C. Gelabert**, R.K. Lammi

**CHED 196.** Measurement of heating value of manure by bomb calorimetry. **H. Bascal**, J.L. Frye

**CHED 197.** Refining a combustible dust explosion apparatus. **S.D. Wiediger**, B. Mollvoy

**CHED 198.** One-dimensional transport of colloidal silver nanoparticles in a saturated porous media: A laboratory experiment for chemistry and engineering students. **S. Brittle**, S.R. Kanel, J. Dagher, A.J. Meyerhoefer, I.E. Pavel Sizemore

**CHED 199.** Art forensics and Raman spectroscopy: Undergraduate research projects. **I.S. Butler**, D.F. Gilson, E. von Aderkas, J.W. Riddle, J.M. Bayne, J. Yu, G. Beaulieu-Houle, K. Karim

**CHED 200.** Enhancing the undergraduate chemistry curriculum using Raman spectroscopy and related techniques. **E.M. Rezler**, J.E. Haky, A.C. Terentis, S. Hyvarinen

**CHED 201.** Service learning in an analytical chemistry laboratory: Analysis of wastewater effluent and wetlands water polishing. **D. Valenti**, A. Garbou, M. Rex, J. Harper, E. Heider

**CHED 202.** Purification of river water: An open-inquiry experiment for the undergraduate teaching laboratory. **A.J. Lacy**, C. Cross, J.G. Nguyen

### Undergraduate Teaching at the Frontiers of Inorganic Chemistry

Sponsored by INOR, Cosponsored by CHED

### My Comments to the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

### My Experience with & Advice for Improving Diversity in Chemistry

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

### My Experiences in & Advice for Organic Chemistry Courses

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

## MONDAY MORNING

### Section A

Manchester Grand Hyatt San Diego Harbor Ballroom A

### GSSPC: Resolving the Big Picture: Bringing Molecules into Focus

Cosponsored by ANYL†, MPPG and PROF†. Financially supported by Purdue University Chemistry Department; Purdue Graduate Education Advisory Board (GEAB); Dow Agrosiences; ACS Indiana Local Section

S. Ayrton, Organizer

S. D. Banziger, K. E. Gettys, C. Schnoebelen, H. Schoonover, A. Tomaine, Organizers, Presiding

9:00 Introductory Remarks.

9:05 **CHED 203.** Shedding lights on diseases with dark material. **Z. Cheng**

9:45 **CHED 204.** Molecules for multiscale imaging, against cancer, or for long-term memory storage. **R.Y. Tsien**

10:25 Intermission.

10:35 **CHED 205.** Imaging mass spectrometry: Molecular microscopy for biology and medicine. **R.M. Caprioli**

11:15 **CHED 206.** Mass spectrometry in surgical diagnostics and in organic synthesis. **R.G. Cooks**

11:55 Concluding Remarks.

### Section B

Manchester Grand Hyatt San Diego Mission Beach A/B

### ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Symposium in honor of Avi Hofstein

H. Sevia, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **CHED 207.** Exploiting all senses in chemistry laboratories: Novel adaptations of sensory activities for laboratory instruction. **M. Oliver-Hoyo**

9:00 **CHED 208.** Measuring meaningful learning in the undergraduate chemistry laboratory. **S. Bretz**, K.R. Galloway

9:25 **CHED 209.** Course-based Undergraduate Research Experiences as a "CURE" for what ails science education for the 21st Century. **G.C. Weaver**

9:50 **CHED 210.** Looking at the ACS strategic plan from the perspective of the concept of relevance. **G.M. Bodner**

10:15 Intermission.

10:25 **CHED 211.** Science writing Heuristic-aligned laboratory teaching within an implementation of the the 6th edition of *Chemistry in the Community*. **D.J. Wink**, N. Hike, S. Hughes-Phelan

10:50 **CHED 212.** Accomplished practice of chemistry teachers through evidence-based continuous professional development: A workshop focusing on the inquiry approach in the chemistry laboratory. **R. Mamluk-Naaman**

11:15 **CHED 213.** Target Inquiry: Transforming teachers' ideas about laboratory instruction. **D.G. Herrington**, E.J. Yeziarski

11:40 Intermission.

11:50 Introduction of Award Recipient. **J. Shymansky**.

11:55 **CHED 214.** Award Address (ACS Award for Achievement in Research for the Teaching and Learning of Chemistry sponsored by Pearson Education). Development of "skills for life" in the high school chemistry laboratory. **A. Hofstein**

### Section C

Manchester Grand Hyatt San Diego Solana Beach A/B

### Chemists Helping Teachers Incorporate Next Generation Science Standards (NGSS) into Their K-12 Classrooms

M. Brock, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **CHED 215.** Development of a distributed teacher-led professional development program for incorporating the NGSS into high school science. **D.J. Wink**, M. Snow, C. James, J. Sarna

8:55 **CHED 216.** Discovery learning approach to atomic structure and the periodic table: Training current and future teachers what really matters in NGSS. **A. Jordan**, N. Yates

9:15 **CHED 217.** Pre-service K-8 teacher preparation course in chemistry: Roles of IHE content faculty in translating science standards into practice. **M. Brock**

9:35 **CHED 218.** Chemistry as the crosscutting connection for secondary science teacher professional development. **D.I. Del Carlo**, S.B. Boesdorfer

9:55 Intermission.

10:10 **CHED 219.** Challenges of introducing science teachers to effective guided-inquiry activities. **M. Dewane**, T.J. Greenbowe

10:30 **CHED 220.** College readiness in NGSS: A presentation of metric conversions background preparation for introductory college courses in the physical sciences. **S. Raju**

10:50 **CHED 221.** Chemistry education for gifted students with the next generation science standards (NGSS). **S. Nagarajan**

11:10 Concluding Remarks.

### Section D

Manchester Grand Hyatt San Diego Promenade A

### Undergraduate Research Papers

Cosponsored by SOCED

C. V. Gauthier, J. V. Ruppel, Organizers  
N. L. Snyder, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **CHED 222.** Towards the concise syntheses of selenium- and tellurium-containing tryptophan analogs for the elucidation of protein structure and function. **R. Agh**, A. Rice, R. Marti-Arbona, L.A. Silks, D.M. Hatch

8:45 **CHED 223.** Understanding aging biology: The role of *mir-34* in sarcopenia. **C. Torres Caban**, C. Ibanez-Ventosa, M. Driscoll

8:55 **CHED 224.** Neuroprotective multi-domain peptide hydrogel in traumatic brain injury. **S. Shi**, V.A. Kumar, J.D. Hartgerink

9:05 **CHED 225.** *Cryptosporidium parvum* has functional amyloids that impact adhesion and infection. **D.R. Lee**, C.X. Chan

9:15 Intermission.

9:25 **CHED 226.** Mutagenesis studies of phosphorylated lipid droplet protein HSD17b13 in hepatocytes. **T. Ritter**, S. Khan, D. Mashek, A. Stoekman

9:35 **CHED 227.** Effects of simulated microgravity on the microbial physiology of *Ralstonia pickettii* isolates from the International Space Station. **S.J. Fergione**

9:45 **CHED 228.** Dermatological phantom study of pigment yellow 74. **H. Butman**

9:55 Intermission.

10:05 **CHED 229.** Vibrational normal mode analysis of uracil and its methylated derivatives. **A. Al-Enaizan**, M.A. Morsy

10:15 **CHED 230.** Molecular dynamics simulations of ion transport through bent carbon nanotubes. **C. Jackson**, T.D. Shepherd

10:25 **CHED 231.** Solar spectral filtration using nanoparticles for photovoltaic cells. **M. Muni**, E. Tunkara, D. DeJarnette, A. Saunders, K. Roberts, T. Otanicar

10:35 **CHED 232.** Kinetics and mechanism of the oxidation of  $[\text{Co}(\text{dmgBF}_2)_2(\text{OH})_2]$  by bromine and sodium hypochlorite in aqueous media. **L.S. Joseph**, M.J. Celestine, A. Holder

10:45 Concluding Remarks.

### Section E

Manchester Grand Hyatt San Diego Mission Beach C

### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Cosponsored by CCA, LSAC, SOCED and YCC

E. J. Brush, E. S. Garcia Segal, Organizers

S. Nellutu, Presiding

8:30 Introductory Remarks.

8:35 **CHED 233.** Engaging our undergraduate students in conversations on the teaching and learning of science. **S. Brydges**

8:55 **CHED 234.** It's elementary: Serving to learn. **K. Stone**

9:15 **CHED 235.** Chemistry day at Payson High School. **M. Rustagi**

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or to stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from ACS.

9:35 CHED 236. Promoting STEM education through BSU chemistry club outreach. K. Dooley, P. Kurriss, E.J. Brush, S. Nellutla

9:55 Intermission.

10:10 CHED 237. Chemical circus: Integrating service learning into the organic chemistry curriculum. D.M. Solano

10:30 CHED 238. Breaking stereotypes: Developing a 30-week program to encourage middle school girls to pursue STEM studies. S.S. Grathoff, M.R. Wilhelm

10:50 CHED 239. Sustainable chemistry: A series of laboratory field trips for high school students. K. Aubrecht, L. Padwa

11:10 CHED 240. Chemistry Science Saturday: Engaging pre-college students through a real laboratory experience. E.A. Alemán, S.L. Phillips, M. Gordon, M.D. Drake

11:30 CHED 241. OCTET & BIOTEC: A model of a summer intensive designed to cultivate the future generation of young leaders in STEM. J. Donnelly, F.E. Hernandez

11:50 Panel Discussion.

12:10 Concluding Remarks.

## Section F

Manchester Grand Hyatt San Diego Promenade B

### Strategies Promoting Success of Two-Year College Students

L. J. Anna, T. B. Higgins, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 242. Partnerships and collaborations that impact community college student outcomes in STEM research programs. C.J. Foley, N. Leonhardt

8:55 CHED 243. College students get excited about whiskey: The accidental creation of an independent student research program at a two year community college. R. Silvestri, A. Thompson, C. Kazee

9:15 CHED 244. Early career undergraduate research experience (eCURE) at Pasadena City College. V.I. Jaramillo, J. Blatti, J. Ashcroft

9:35 Intermission.

9:45 CHED 245. Promoting success of two-year college students through collaboration. J.L. Hayes, S. Burchett

10:05 CHED 246. Synergistic efforts to support early STEM students. K.S. Owens, A. Murkowski

10:25 CHED 247. Community college undergraduate research initiative model: A case study for national collaboration. P. Powers

10:45 Intermission.

10:55 CHED 248. Improving understanding on limiting reagent in chemistry I students through an inquiry-based lab. A. Vagle

11:15 CHED 249. On the suitability of computational tools to enhance the general chemistry sequence at two-year colleges. O.E. Raola, S.M. Dalton

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

11:35 CHED 250. Developing a departmental assessment program to measure student success. J. Ellefson-Kuehn, R. House

11:55 Concluding Remarks.

## Section G

Manchester Grand Hyatt San Diego Ocean Beach

### Chemistry Education Research

#### New & Noteworthy in 2014-2015

K. J. Linenberger, J. R. Raker, *Organizers*

S. Pazicni, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 251. Experience sampling methodology to facilitate measuring general chemistry students' study habits. L. Ye, R. Oueini, A.P. Dickerson, S.E. Lewis

9:15 CHED 252. Influence of PBL on students' self-efficacy beliefs in chemistry. M.G. Kowalske, L. Mataka

9:55 Intermission.

10:10 CHED 253. Self-explaining effect in general chemistry instruction: Eliciting overt categorical behaviors by design. A. Villalta-Cerdas

10:50 CHED 254. Stemming the diffusion of responsibility: A longitudinal case study of America's chemistry teachers. G.T. Rushton, G. Ray, S.J. Polizzi, B.A. Criswell

11:30 Discussion.

### Is There a Crisis in Organic Chemistry Education?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

### Preparing for the Real World: Challenges Faced by Young Investigators

### Choosing Grad Research Advisors & A Career in Academia or Industry

*Sponsored by MPPG, Cosponsored by CHED, CINF, COMP, PHYS and YCC*

## MONDAY AFTERNOON

### Section A

Manchester Grand Hyatt San Diego Harbor Ballroom A

### GSSPC: Resolving the Big Picture: Bringing Molecules into Focus

*Cosponsored by ANYL†, MPPG and PROF†. Financially supported by Purdue University Chemistry Department; Purdue Graduate Education Advisory Board (GEAB); Dow Agrosiences; ACS Indiana Local Section*

S. Ayrton, *Organizer*

S. D. Banziger, K. E. Gettys, C. Schnoebelen, H. Schoonover, A. Tomaine, *Organizers, Presiding*

2:00 Introductory Remarks.

2:05 CHED 255. Imaging intracellular redox chemistry: Spatially-resolved sensing of hydrogen peroxide in living cells. C.K. Payne

2:45 CHED 256. *In vivo* vibrational spectroscopic imaging: Emerging platform for biology and medicine. J. Cheng

3:25 Intermission.

3:35 CHED 257. Near-IR uncaging chemistry: Discovery and applications. M.J. Schnermann, R.R. Nani, A.P. Gorka

4:15 CHED 258. Making the brain light-up (in cultures): New small quantum dots and super-resolution microscopy. P.R. Selvin

4:55 Concluding Remarks.

## Section B

Manchester Grand Hyatt San Diego Mission Beach A/B

### Integration of STEM & the Liberal Arts

C. J. Foley, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 259. Instructor perceptions of undergraduate STEM education. L. Fox, G. Roehrig

1:55 CHED 260. Space Cowboys: A course that weaves art, history, and science through stories and movies. S.L. Hiley

2:15 CHED 261. The bomb: Nuclear chemistry and history. R.E. Rosenberg

2:35 CHED 262. Contextualizing analytical chemistry in chemical weapons non-proliferation. U.J. Williams

2:55 Intermission.

3:05 CHED 263. Teaching a broad non-science major audience using the science of food and cooking. K.L. Colabroy, J.J. Provost, B.S. Kelly, M.A. Wallert

3:25 CHED 264. Telling the story of chemical evolution: How physical chemistry topics align with the narrative of natural history. B.J. McFarland

3:45 CHED 265. Gaining STEAM: Establishing a campus 3D printing and fabrication center to explore cross-disciplinary collaboration and innovation in STEM and the liberal Arts. L.A. Porter

4:05 CHED 266. Teaching chemical instrumentation through analysis of oil paintings. D. O'Donnell

4:25 Concluding Remarks.

## Section C

Manchester Grand Hyatt San Diego Solana Beach A/B

### Chemists Helping Teachers Incorporate Next Generation Science Standards (NGSS) into Their K-12 Classrooms

M. Brock, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 267. Connected chemistry curriculum and the next generation science standards. S.C. Ryan, M. Stieff

1:55 CHED 268. Partnering with high school teachers to develop chemistry activities well-aligned with NGSS. M. Brock

2:15 CHED 269. Incorporating NGSS by utilizing green chemistry innovations in the classroom. K. Anderson, M. Enright, A.S. Cannon

2:35 Intermission.

2:50 CHED 270. Enhancing conceptual and visual understanding of nuclear chemistry in high school general chemistry courses. J. Ellis, P. Jones, C. Barnett

3:10 CHED 271. Withdrawn.

3:30 CHED 272. Active learning-based integrated project between high schools and the University: Analysis of bioethanol fuel and its blends with synthetic gasoline. O. El Seoud, L.P. Novaki, A.M. Chinelatto

3:50 Concluding Remarks.

## Section D

Manchester Grand Hyatt San Diego Promenade A

### Undergraduate Research Papers

*Cosponsored by SOCED*

C. V. Gauthier, J. V. Ruppel, *Organizers*

N. L. Snyder, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 273. Withdrawn.

1:45 CHED 274. Comprehensive comparison of nicotine and other minor components in tobacco products. K.A. McCarthy, A.S. Dutton

1:55 CHED 275. Simultaneous determination of bisphenol A and bisphenol S in methanol:water (1:1) samples using UV/VIS spectrophotometry. J. Benecyo, S. Hubbard

2:05 CHED 276. Establishing giant brown kelp as biosentinel of environmental mercury. R.T. Pratt, K. Skinner, S. Aloisio

2:15 Intermission.

2:25 CHED 277. Optimized microalgae lipid extraction for the production of fuels. C. McKeleph, E. Santillan-Jimenez, M. Crocker

2:35 CHED 278. Remnant lipoprotein size distribution profiling via dynamic light scattering analysis. K. Garza, R. Chandra

2:45 CHED 279. Chromatographic investigation of the interaction between a polymorphic compound and tailored surfaces. T.A. Watts, R.E. Sours

2:55 CHED 280. Thermal and chemical modification of activated carbon for increased urea adsorbivity. K.M. Humrichouse, B.J. Winters, K.E. Rohly, M. Berens

3:05 CHED 281. Monitoring surface water of Lake Sinclair in Georgia. J. Olmstead, C.H. Lisse

3:15 Intermission.

3:25 CHED 282. Examination of biomarkers used in archaeology and consideration of potential degradation products and their implications for archaeological biomarkers. A.D. Bravenec, T.J. Ward, S.M. Barker, A.R. Kaminski, C. Quach, H. Lam, T. Patterson, T. Tian

3:35 CHED 283. Characterization of halogen bond-driven assemblies of thiophene and furan-based building blocks. S. Nguyen, J.L. Wilson, J. Williams, J.W. Jurss, N. Hammer, G.S. Tschumper, D. Watkins

3:45 CHED 284. Expanding on the adaptability and sustainability of an inquiry-based polymer experiment for the teaching laboratory through inclusion of simple mechanical testing, degradation of the product, and microwave reactions. Z. Swingen, C. Blaquiere, G. Fahnhorst, J. Kempf, J.E. Wissinger, M.T. Wentzel

3:55 CHED 285. CHEM scholar: The efficacy of a new board game to learn chemical nomenclature. J. Wood, M.L. Golden

4:05 CHED 286. Using simulation for stoichiometry in organic chemistry laboratory. Z.P. Ziolkowski, T. Gupta, A. Mehta, G. Albing

4:15 Concluding Remarks.

## Section E

Manchester Grand Hyatt San Diego Mission Beach C

### Research on Learning in the Lab

S. Sandi-Urena, *Organizer, Presiding*

M. J. Chrzanowski, *Presiding*

1:30 Introductory Remarks.

- 1:35 CHED 287.** Effect of real samples on student attitude and learning in a chemistry laboratory course. J. Haan, K. Roell
- 1:55 CHED 288.** Flipping the general chemistry laboratory: Increasing student engagement by enhancing self-directed learning. R.M. Theisen, J.A. Halfen
- 2:15 CHED 289.** First-year chemistry majors' experiences in a general and descriptive chemistry laboratory course. H. Arce Rojas, S. Sandi-Urena
- 2:35** Intermission.
- 2:50 CHED 290.** Exploring argument from evidence in the general chemistry laboratory. R. Sansom, J.L. Reynolds, N.T. Humphries
- 3:10 CHED 291.** Joys and challenges to laboratory reform: An instructional design analysis. J. Walker, A.G. Van Duzor
- 3:30 CHED 292.** Student learning outcomes in a project-based laboratory: Generic skills. S.R. Mooring, N.L. Burrows
- 3:50 CHED 293.** Reform in general chemistry laboratory instruction: How do students experience change? S. Sandi-Urena, M.J. Chrzanowski, I. Chopra, R. Pancho, J. O'Connor
- 4:10 CHED 294.** Transformation of a large enrollment general chemistry laboratory sequence. J.H. Carmel, J.S. Ward, A. Pollock, L.A. Posey, M. Cooper
- 4:30** Discussion.

## Section F

Manchester Grand Hyatt San Diego  
Promenade B

### Communicating Chemistry Through Social Media

Cosponsored by MPPG

L. Jones, C. Sorensen-Unruh, *Organizers, Presiding*

#### 1:30 Introductory Remarks.

- 1:35 CHED 295.** Communicating chemistry through social media: A whirlwind tour of some options. L. Jones, C. Sorensen-Unruh
- 1:55 CHED 296.** Periscoping your way through general chemistry. A.T. Griffin
- 2:15 CHED 297.** What place does Facebook have in the chemistry curriculum? T. Gardner
- 2:35** Intermission.
- 2:45 CHED 298.** When  $1+1+1 = \text{More than three}$ : Collaboration in teaching chemistry. J.K. Murray, M.J. Castaldi, D. Kosciuszko
- 3:05 CHED 299.** Optimizing student engagement through social media. B. Burd, C. Sorensen-Unruh
- 3:25 CHED 300.** Green chemistry innovation portal. D.J. Constable, C. Briddell
- 3:45** Discussion.
- 4:05** Concluding Remarks.

## Section G

Manchester Grand Hyatt San Diego  
Ocean Beach

### Chemistry Education Research

S. Pazioni, J. R. Raker, *Organizers*  
K. J. Linenberger, *Organizer, Presiding*

#### 1:30 Introductory Remarks.

- 1:35 CHED 301.** Analyzing chemistry students' decision making in realistic contexts. V. Talanquer

- 1:55 CHED 302.** Thinking Like a chemist: Development of a chemistry card-sorting task to probe conceptual expertise. F. Krieter, R. Julius, K. Tanner, S. Bush, G.E. Scott
- 2:15 CHED 303.** Investigation into how students make connections that cross the disciplinary boundaries of chemistry, biology, and physics. S.M. Underwood, V. Sawtelle, R. Matz, C. Anderson, E. Scott
- 2:35 CHED 304.** How experienced chemistry teachers evaluate student thinking in chemistry. H. Sevian
- 2:55** Intermission.
- 3:10 CHED 305.** Using surveys and interviews to measure general chemistry and biochemistry students' understanding of intermolecular forces. C.J. Luxford, K.A. Shaw
- 3:30 CHED 306.** Nonresponse bias in survey research: A case study from a national survey of postsecondary chemistry faculty. J.R. Raker, S. Villafane-Garcia, M.N. Stains, K.L. Murphy, E. Laga, J. Leon
- 3:50 CHED 307.** Examining student performance without the whole test: Analyzing the validity of subset norms using ACS Exams. J.J. Reed, J.R. Raker, K.L. Murphy
- 4:10 CHED 308.** Applying the taxonomy of biochemistry external representations to biochemistry textbooks. K.J. Linenberger, C. House, W. Medina
- 4:30** Discussion.

## Section H

San Diego Convention Center  
Halls D/E

### Undergraduate Research Posters

#### Agricultural & Food Chemistry

Cosponsored by AGFD and SOCED

N. Di Fabio, *Organizer*

#### 12:00 - 2:00

- CHED 309.** Determination and variation of organic acids, caffeine and ethanol during green tea kombucha fermentation by high-performance liquid chromatography. Z. Huang, L. Benedict
- CHED 310.** Yew tree extract as a natural insecticide against tobacco hornworms. B. Nhan, A. Hoffman, J. Yun
- CHED 311.** Cuticular hydrocarbon analysis of *Drosophila athabasca*: Identification, quantification, and synthesis. B. Gay, L. Vo, T. Harvey, R. Yukilevich, J.D. Kehlbeck
- CHED 312.** Isolation and identification of biologically active secondary metabolites from a fungal endophyte of alfalfa. A. Harnagel, A. Jordan, D. Foster-Hartnett
- CHED 313.** Analysis of organic vs conventional produce: Diphenylamine and kresoxim-methyl in apples and cp4 epsps gene found in frozen corn. M. Snider, T. Sivy
- CHED 314.** Determination of cocoa liquor provenance using fatty acid and trace element signatures. S. Maloney, P. Sudol, R. Khalsa, S.E. Stitzel, R.E. Sours
- CHED 315.** N-Linked carbohydrate conjugated antioxidants. A. Oles, A. Petek, M. Cook, R. Petek, E. Kemboi, M. Hunsen
- CHED 316.** Determination of capsaicin and related compounds from complex matrices. J.W. Peschke, S. Chakraborty
- CHED 317.** Hop flavoring in beer through GC-MS and chemometric analysis. J.D. Espinosa, K.J. Sorauf
- CHED 318.** Novel bioactive compounds produced by endophytes extracted from *Fragaria vesca*. J. Ross, M.D. Halling
- CHED 319.** Novel compounds extracted from endophytes isolated from *Lycium barbarum*. S. Goasind, M.D. Halling
- CHED 320.** Use of ESI MS to characterize metabolites of citrus leaves. N. Ramazani, Z. Woydziak
- CHED 321.** Evaluation of the concentration of iso- $\alpha$ -acids as Bitterness Units, at different profiles throughout the liquid column of beer samples. L. Benedict, R. Michaud
- CHED 322.** Depth profiling of heterocyclic amines in meat formed during cooking. J.C. Sessums, A. Le
- CHED 323.** Depth profiling of capsaicinoid migration into meat during preparation. L. Riley, A. Le
- CHED 324.** Quantification of polyphenols and assessment of antioxidant activity of polyphenols present in organic and non-organic raspberries from different sources. S. Elmaliki, K.A. Daus
- CHED 325.** Ex vivo characterization of tissue browning products using apple (*Malus spp.*) as a model system. E. Lotkowska, S. Chakraborty
- CHED 326.** Analysis of essential oils in centennial hops grown in different types of soil. N. Bryant, D. Clark, J.A. Trishman
- CHED 327.** Investigating tissue browning using polyphenol oxidase mediated oxidation of phenolic compounds *in vitro*. A.T. Steele, S. Chakraborty
- CHED 328.** DNA adduct formation and detection in crop plants from pesticide exposure. T. Cunningham, D.W. Boerth
- CHED 329.** Quantitation of antioxidants using silver nanoparticles. C. Knight, A. Smalley
- CHED 330.** Behavior of polyphenols and sulfur-containing compounds in relation to the flavor stability of beer, wine, tea, and juices. N. Fleckenstein, L.A. Curry
- CHED 331.** Spectroscopic analysis of secondary metabolites from extracts of *Alternaria metachromatica*. M. Exline, A. Jordan, D. Foster-Hartnett
- CHED 332.** Synthesis of a water-soluble radicinin derivative for use as an antibacterial agent in grapevines. L. Semmler, J. Sawada, M. Steinhaus, J. Reader, P.E. Rolshausen, C. Roper, J. Rapicavoli, K.N. Maloney

## Section H

San Diego Convention Center  
Halls D/E

### Undergraduate Research Posters

#### Analytical Chemistry

Cosponsored by ANYL and SOCED

N. Di Fabio, *Organizer*

#### 12:00 - 2:00

- CHED 333.** Withdrawn.
- CHED 334.** Electrochemiluminescent quenching of calcein blue by TNT in aqueous solution. J. DeVincent, K.D. Sienerth
- CHED 335.** Exploring quenching of electrochemiluminescence by RDX in aqueous solution. C.E. Burton, K.D. Sienerth
- CHED 336.** Relationship of phenolics with antioxidant activities in different bee propolis extracts. E.E. Mojica, K. Symczak, A. Javornik, N. Evans
- CHED 337.** Vibrational and electronic properties of chloramphenicol. T. Batte, A. Kuptsov, E.E. Mojica
- CHED 338.** Development of luminescent metal-organic frameworks for use as oxygen sensors. G. Yankelevich, K. Hess, K. Kneas, J.A. Rood
- CHED 339.** Monitoring the interaction of nanomaterials with catalase using optical spectroscopy. K. Chhe, T. Nolan, E.E. Mojica, N. Abbas
- CHED 340.** Thin layer chromatography-digital image analysis (TLC-DIA) for quantitative determination of creatinine. E. Kerr, C.L. West, S. Kradtap Hartwell
- CHED 341.** Quantitative determination of 4-hydroxybenzoate and related biomarkers in urine by high performance liquid chromatography with diode array detection. T. Yen, Z. Hassan, S. Gamedgara
- CHED 342.** Quantification of isomerized  $\alpha$ -acid extraction efficiencies in beer using high performance liquid chromatography. E.J. Dompkowski, R.A. Hunter
- CHED 343.** Analysis of a series of silver coins of King Azes via energy dispersive x-ray fluorescence spectroscopy (EDXRF). G. Nguyen, J. Pothoof, M.A. Benvenuto
- CHED 344.** Investigation of biodiesel-diesel blends using GCMS and PCA. R.R. Dean, C.D. Brown, A.M. Hupp
- CHED 345.** Cloud point extraction for electroanalysis: Anodic stripping voltammetry of lead. M. Warren, C.A. Rusinek, W.R. Heineman, A.F. Bange, I. Papautsky
- CHED 346.** Comparative statistical analysis approach for seven alkyl chloroformates. R. Dina, A. Jefferies, M.J. D'Souza
- CHED 347.** Analysis of electrolyte changes between male and female athletes using ICP-OES. C.C. O'Hara, G. Geme, G. White, R. Smith, J. Killsgaard
- CHED 348.** Historical organic pigments: The challenge and opportunity of the nearly forgotten. T.J. Moore, J.F. Lomax
- CHED 349.** Investigation of the rod transition in micelles of 12-3-12 and 12-4-12 Gemini surfactants using chemical trapping. D. Carothers, S.J. Bachofer
- CHED 350.** Analysis of mercury concentration in cigarettes as a viable source of human absorption of the top two brands sold in the United States. K. Malloy, S. Aloisio, S.L. Freitag, M.J. Soriano
- CHED 351.** Comparison of trace metals in tattoo inks with isolated dry pigments using CEM MARS 6 microwave and Agilent ICP MP-AES. C. Kelly, H. Butman, R. Philibert, C.H. Jaworek-Lopes
- CHED 352.** Analysis of calcium phosphate mineralization in microfluidic platforms with variable dimensions. A. Sanford, A.E. Gerdon
- CHED 353.** 3-D printed chromatography: Fast performance liquid chromatography (FPLC). B. McCarthy Riley, D. Dilworth, K. Cissell, M. Champion
- CHED 354.** Chemical analysis of ancient paintings: AMS radiocarbon dating of binders & x-ray diffraction of pigment. S.L. Petty, K.L. Steelman
- CHED 355.** Refining a solid phase micro-extraction method for the multisampling of *trans*-resveratrol in red wines by orbital agitation and subsequent HPLC analysis. J. Bascaran, C.E. Thornton, J.A. Boiani
- CHED 356.** Extraction of capsaicin and parallel quantitative analysis. N.S. Jackson, A.R. Schroeder, C.A. Simpson, C. Nicholson, K.S. Molek

- CHED 357.** Analysis of a group of possibly counterfeit ancient coins via energy dispersive x-ray fluorescence spectroscopy (EDXRF). J. Pothoof, R. Wong, S. Maurice, G. Nguyen, S. Tinawi, J. Payne, J. Roehl, M.A. Benvenuto
- CHED 358.** Identification of chemotypes of commercial thyme products. S. O'Neill, C. Bowers
- CHED 359.** Development of the chemical based semi-conductive electrodes (multi-potential ion guide) and their adaptation to the quadrupole ion mass spectrometer and time-of-flight ion mass spectrometer. D. Kravchuk, M. Flesch, J. Nederhoff, C. Hanson
- CHED 360.** Analysis of x-ray fluorescence spectroscopy on Fort Union glass trade beads. K. Springer, H. Karlovich, N. Grabow, D. O'Donnell
- CHED 361.** Electrochemical characterization of ferritin. M. Hennessy, S. Olubajo, D.C. Zapien
- CHED 362.** Electrochemical monitoring and correlated fluorescence imaging of single *Escherichia coli* and *Bacillus subtilis* bacteria using ultramicroelectrodes. A.T. Ronspees, S.N. Thorgaard
- CHED 363.** Single-pot approach to preparation of hydrophobic sol-gel monolithic capillary columns for reversed-phase liquid chromatography. M. Abdallah, T. Silva Campos, R. Hernandez, Z. Zajickova, F. Svec
- CHED 364.** Determination of pharmaceutical residues in water samples of the Housatonic River Valley Region by solid phase extraction (SPE) and gas chromatography-mass spectrometry (GC-MS). J. Sima, Y. Mei-Ratiff
- CHED 365.** Effect of molecular ligands on platinum electrocatalytic activity. M. Ma, K. Wong, E.C. Landis
- CHED 366.** Surface-enhanced Raman scattering based optical fiber sensors. D. Myers, L. DeGraaff, S.R. Emory
- CHED 367.** Development of a chemical-based electrode for reflection time-of-flight mass spectrometry. J. Nederhoff, D. Kravchuk, M. Flesch, C. Hanson
- CHED 368.** Development of a semiconductor-based quadrupole mass analyzer. M. Flesch, D. Kravchuk, J. Nederhoff, C. Hanson
- CHED 369.** Fluorescent properties of a novel chemosensor for metal ions. C. Sanchez, S. Plummer Oxley
- CHED 370.** Investigation of quality control and analysis for small breweries. B. Gomez, B.D. Gilbert
- CHED 371.** Reactive nitrogen compounds emitted in the exhaust of on-road vehicles. M.B. Anderson, V. Aguirre, S.A. Churchman, R. Fanter, J.A. Moss, M.M. Baum
- CHED 372.** Synthesis of nanostructured thermoelectrics. L. Presson, G. Szulcowski, T. Sutch
- CHED 373.** Quantitative elemental analysis of tires with x-Ray spectroscopy. M. Rooney, R. Walsh, L. Huang
- CHED 374.** How energy drinks affect human enamel. J.M. Campbell, B.A. Davis
- CHED 375.** Effect of pH on physical properties of an amphiphilic leucine valine molecule. F.H. Billiot, s. Vera, Z. Ramos, K.F. Morris, C. Lewis, E. Billiot
- CHED 376.** Quantitative mineral and nutrient analysis of *Moringa oleifera* leaves. R.W. Schaeffer, L.E. Coleman, P. Leiphart
- CHED 377.** Method to selectively analyze the antibacterial compounds of natural products. M. Martin, J.A. Gurak, S. Bhawal, F.W. Foss, L. Mydlarz, K. Schug
- CHED 378.** Chromatographic comparison of penicillin residues in conventional and organic eggs. J. Kalal, J.L. Franz
- CHED 379.** Development of a method for monitoring ATP and its metabolites as biomarkers for traumatic brain injuries by capillary electrophoresis. E. Abbi, S. Gunawardhana, S.M. Lunte
- CHED 380.** Self-assembled monolayers on zinc selenide for use in *in vitro* cellular studies. A. Love, A.R. Noble
- CHED 381.** Formation of immunosensors using self-assembled monolayers on zinc selenide. S. Zwart, A.R. Noble
- CHED 382.** To benchtop NMR or not to benchtop NMR? S. Strenge, J.A. Goodnough
- CHED 383.** Optimization of 2D-LC conditions in the separation of furanocoumarins in plant extracts. M. Burnham, J.M. Danforth, D.C. Harnes, D.R. Stoll, D. Cook, S.C. Rutan
- CHED 384.** Determination of acetone, butanol and ethanol fermentation products in *Clostridium beijerinckii* by GC-FID. C. Olumba, S. Riedel, W. Lin, G.A. Barding
- CHED 385.** Deep eutectic solvents as medium for biphasic biocatalytic esterification. H. Chatelaine, D.E. Raynie, S. Asare
- CHED 386.** Investigation of the kinetics of electrochemically modulated separation of dysprosium. E. Velasquez, S. Anderson, M. Nilsson, E. Kalu
- CHED 387.** Study of the developmental metabolome of *Xenopus laevis* by capillary electrophoresis-mass spectrometry. D. Boley, J. Arceo, N. Schiavone, R. Wojcik, S. Sarver, E. Peuchen, N.J. Dovichi
- CHED 388.** NMR investigation of micelle formation by a chiral dipeptide surfactant. T. Witzleb, F.H. Billiot, E. Billiot, K.F. Morris
- CHED 389.** NMR Investigation of the effect of pH on aggregation, counterion binding, and amide proton exchange in amino-acid-based surfactants. B. Hughes, F.H. Billiot, E. Billiot, K.F. Morris
- CHED 390.** Molecular dynamics simulation study of the binding of chlorthalidone enantiomers to a chiral molecular micelle. J. Ingle, F.H. Billiot, E. Billiot, Y. Fang, K.F. Morris
- CHED 391.** Quantitative water testing using API kits. A. Obert, V.P. McCaffrey
- CHED 392.** In depth analysis of the relationship between allicin, an organosulfur compound, and its ability to mitigate the production and development of carcinogenic compounds, such as PhIP, MeIQ and MeIQx, within cooked meats. J.C. Sessums, A. Le
- CHED 393.** Photoreactivity of 2-methoxy-4-(2-phthalimidinyl)phenylsulfonfyl chloride. T. Cleary, P. Sibbald
- CHED 394.** Caries and periodontal disease: Trace metal ion analysis of human dentin using inductively coupled plasma mass spectrometry. L. Schaller, A. Hoang, J. Thomas, M.B. Jacobs
- CHED 395.** Analyzing *Saint Peter* with a manually built Raman spectrometer. L. Ostrosky, S.J. Gravelle
- CHED 396.** Interfacing GC-MS with a catalytic testbed for analysis of aerogel materials. S. Kleinberg, M.K. Carroll, A.M. Anderson, B.A. Bruno
- CHED 397.** Optimizing microsphere whispering gallery mode resonators for sensing. J. Flores, S. Wildgen, R. Dunn
- CHED 398.** Variations in volatile organic compounds released by organic versus non-organic habanero peppers and shishito peppers. B. Elizan, M. Kopecki Fjetland
- CHED 399.** Analysis of phytogetic volatile organic compounds released by herbivore-induced damaged, mechanically damaged, and intact leaves of *Solanum lycopersicum*. R. Park, M. Kopecki Fjetland
- CHED 400.** Stability-indicating UPLC-MS/MS assay for 1960's era pharmaceuticals in dosage forms. C. Quinn, P. Orr, T.R. Rybolt, S. Symes
- CHED 401.** Selective digestion of glyphosate and AMPA using flow injection analysis (FIA). A.K. Perry, A.F. Bauer, A.R. Roerdink
- CHED 402.** Attenuation of matrix effects during biomonitoring of trace metals by ICP-MS: Quantification of Na, Mg, Ca, and K in human matrix. E. Ness, P. Jannetto, D.L. Murray, A. Bluhm
- CHED 403.** Characterization of the advantages and limitations of the use of handheld x-ray fluorescence for the analysis of ceramics. H.R. Munro, J.R. Hornak, C.C. Deibel, M.A. Deibel
- CHED 404.** Studies on SPE-GC-MS for isolation, identification and quantitation of alkaloids in frog skin. A.R. Morris, R.W. Fitch
- CHED 405.** Remnant lipoprotein size distribution profiling of serum samples of varying metabolic disorders via dynamic light scattering analysis. R. Chandra, S.A. Hameed, J.M. Jurica
- CHED 406.** Evaluation of antioxidant protection in human serum via a ferric reduction assay. R. Chandra, C. Chidi
- CHED 407.** Method development in assessing DNA damage in model bacterium by engineered nanoparticles. T. Nguyen, L.M. Jacob, C.J. Murphy, C.L. Haynes, V. Feng
- CHED 408.** Analysis of trace materials on bullets and their ballistic terminal pathways. B.J. Karns, M. Cipoletti
- CHED 409.** Cyclic voltammetric analysis of 1-methyl-4-nitroimidazole under biological conditions. A.D. Nguyen, D.K. Smith
- CHED 410.** Determining the effectiveness of sol-gels as vessels for controlled release of fragrances. K. Ehret, C.H. Lisse
- CHED 411.** Absorbance properties of a novel chemosensor for metal ions. S. Lizarraga, S. Plummer Oxley
- CHED 412.** Using HPLC to determine the effects of pH on the decomposition of heroin in the blood. B. Baumgarten, C. Saner
- CHED 413.** HPLC analysis of  $\alpha$ - and  $\beta$ -Acids from hops in beer. J.A. Rountree, M.D. Schuder
- CHED 414.** Development of liquid chromatography-mass spectrometry methods for forced degradation studies. S. Kurtovic, S. Zoma, K.C. Lapworth, D. Alton, M. Smalley, B.L. Dymm, K.R. Evans
- CHED 415.** Coffee quality determination by chlorogenic acid content using HPLC analysis. C. Gates, E.A. Baldauff
- CHED 416.** Using HPLC to further analyze caffeine content of Blackbird coffee. T.L. Self, K. Cossey
- CHED 417.** Spectroscopic monitoring of nutrient competition between *Dunaliella salina* and *Nannochloropsis oculata*. N. Dunn, F. Vogt
- CHED 418.** Electrochemical reduction of aromatic nitro compounds: Strategies for LC-EC analysis of Sanger tagged analytes. P. Guerrero, J. Becker, H. Sun, M.D. Koppang
- CHED 419.** Selection of DNA aptamers for rapid detection of *Renibacterium salmoninarum*. B. Mandella, A. Olivo, T. Keochokalee-Look, A.G. Cavinato
- CHED 420.** Detection of small molecules using redox active enzyme triggers. D. Daley, J. Grennell, C. Dunlock, S. Sitaula, M.F. Ali
- CHED 421.** Ethanol extraction from gasoline using zeolites. T. Bromenschenkel, H.J. Fletcher
- CHED 422.** Comparison of metal ion selectivity of fluorophore 1,4-bis(2-quinolyl)-2,3-diaza-1,3-butadiene in THF/water and acetonitrile. C.A. Flahin, B.N. Norris
- CHED 423.** Analysis of urine organic acids via GC/MS-based metabolomics to determine the effect of diet on urine composition. J.L. Minnick, C.H. Lisse
- CHED 424.** Selection of protein-binding DNA aptamers for bacterial detection in salmon. E. Clow, K.M. Harris, A.G. Cavinato
- CHED 425.** Using multi-step synthesis for the production of hydrogels with adhesive properties. J. Deardorff, C.H. Lisse
- CHED 426.** Examination of the effect of acid- and base-catalyzed silica sol-gels, xerogels, and aerogels containing silver nanoparticles on 4-mercaptobenzoic acid using surface-enhanced Raman spectroscopy. T. Corrado, E.J. Atkinson, B.D. Gilbert
- CHED 427.** Detection and comparison of eutrophication levels of surface water in lakes in Maine and Georgia using HACH and YSI surface water kits. K. Hachat, C.H. Lisse
- CHED 428.** Is the water safe? Monitoring the water quality near an EPA superfund site. K. Miller, C.H. Lisse
- CHED 429.** Detection of lead in soil samples collected throughout Berks County, Pennsylvania, using flame atomic absorption spectroscopy. K. Schubert, R. Cupo, R. Chinni
- CHED 430.** Let-7i binding signaled by enzyme reactivation. A. Gee, N. Hughes, S. Sitaula, M.F. Ali
- CHED 431.** Optimization of a standard method to analyze ammonium ion in salt water. E. Pinedo Escobedo, S. Storm
- CHED 432.** Quantitative identification of volatile organic compounds present in electronic-cigarette vapor via GC/MS detection. E. Smith, C.H. Lisse
- CHED 433.** Qualitative identification of residual pesticides present in Houston County, Georgia waterways via HPLC and GC/MS detection. I. Filer, C.H. Lisse
- CHED 434.** Analyses of archaeological biomarkers to examine diet and identify ingredients used in ritualistic practices. A.R. Kaminski, S.M. Barker, A.D. Bravenec, C. Quach, H. Lam, T. Tian, T. Patterson, T.J. Ward
- CHED 435.** Design and characterization of a sol-gel glucose biosensor. M. Alcantar, S. Moore, C.H. Lisse
- CHED 436.** Identification of volatile organic compounds present in cigarette smoke via purge-n-trap coupled with GC/MS. P. Skersick, C.H. Lisse
- CHED 437.** Development of an amperometric biosensor for the detection of urea in human urine. J.J. Soto Perez, M. Morales, C.R. Cabrera
- CHED 438.** Qualitative determination of the adherence of VOCs to building materials. J. Turner, C.H. Lisse
- CHED 439.** Evaluation of a portable gas chromatograph for environmental monitoring of pollutants. K. Evans, D. Hughes, R.J. Noll

- CHED 440.** Analysis of  $\alpha$ - and  $\beta$ -acids of hops found in three regions of the United States. **J.E. Zawacki, M.D. Schuder**
- CHED 441.** Food adulteration detection methods for maple syrup. **A. Horowitz, R.M. Hyde**
- CHED 442.** Effect of nitrate on the release of glucose into the hemolymph of crayfish *Procambarus clarkii*. **A. Flores, L.B. Kats, D.B. Green, G.M. Bucciarelli**
- CHED 443.** Analysis of polyacrylamide as a calibration material. **D. Roberts, L.M. Goss, T. Murphy, J.J. Pak**
- CHED 444.** Effect of temperature on the generation of carbonyl compounds from e-liquids containing flavor additives. **P. Torres, L.A. Curry**
- CHED 445.** Infrared optical measurements of hyperbolic metamaterials. **C. Harris, D. Wei, S. Law**
- CHED 446.** Probing heparin-CXCL14 interactions using capillary electrophoresis and NMR spectroscopy. **A. Schrader, A.K. Korir**
- CHED 447.** Characterization of key odorants in coffee by headspace solid phase microextraction and gas chromatography-mass spectrometry. **J.J. Kyle, E.A. Baldauff**
- CHED 448.** Photophysical processes in measurements of natural organic matter using multidimensional fluorescence spectroscopy with parallel factor analysis. **N. Pannullo, M. Bida, J. Kenny, T.E. Pagano**
- CHED 449.** Quantification of fluoride levels in toothpaste. **K. Green, R. Fietkau**
- Section H**
- San Diego Convention Center  
Halls D/E
- Undergraduate Research Posters**
- Biochemistry**
- Cosponsored by BIOL and SOCED*
- N. Di Fabio, *Organizer*
- 12:00 - 2:00**
- CHED 450.** Synthesis and use of biotinylated NAADP's for the affinity purification of the NAADP receptor. **N.N. Olmeda, T. Walseth**
- CHED 451.** Mutagenesis studies of phosphorylated lipid droplet protein PLIN2 in hepatocytes. **A. Dahlgren, S. Khan, D. Mashek, A. Stoekman**
- CHED 452.** Combining kinase inhibition and oxidative stress to treat erbB2 driven cancer. **A.E. Walter, C.J. Kuhnheim, D. Jones, C.E. Taylor**
- CHED 453.** Carbonic anhydrase: A model for matrix metalloproteinase inhibition. **D. DeGenova, R. Patel, G. Reed, A. Forchione, A. Plonski, R. Venna, W. Richert, S. Al-Abdul-Wahid, D.L. Tierney**
- CHED 454.** Topology and conformational changes of the chloroplast twin arginine protein, HCF106, as revealed by site-directed spin label and electron paramagnetic resonance spectroscopy. **A. Habtemichael, P. New, G.M. Thomas, C. Dabney-Smith**
- CHED 455.** Characterization of a putative antimicrobial peptide from the hemolymph of the American lobster, *Homarus americanus*. **G. Vu, P. Dickinson, A. Christie, E.A. Stemmler**
- CHED 456.** Inhibition of  $\beta$ -sheet formation by a short, random coil peptide. **S. Michelhaugh, S. Petty**
- CHED 457.** HmuT protein in the heme uptake pathway of *Corynebacterium diphtheriae*. **C.S. Keutcha, E. Bennett, M.P. Schmitt, D.W. Dixon**
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- CHED 623.** Buffer standards of tris(hydroxymethyl)aminomethane (TRIS) for the physiological pH range at  $I = 0.16 \text{ mol}\cdot\text{kg}^{-1}$ . **T. Wehmeyer**, K. Hundley, L.S. Tebbe, C. Smith, Y. Kang, L. Roy, R.N. Roy
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- CHED 625.** Natural antisense RNA plays a role in *Arabidopsis thaliana* growth and development. **A. Simoni**, C. Makaroff
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- CHED 634.** Efforts towards engineered luciferases with optimized function. **E. Warner**, A. Leconte
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- CHED 637.** Utilization of discovery-based proteomics to study the role of the HGPRT gene in yeast. **M. van der Horst**, E. Cooper, C. Minogue
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- CHED 639.** Modulating back electron transfer between guanine radicals and 2-aminopurine by variations in separation distance and local sequence in duplex DNA. **D. Galindo**, **P. Garcia**, M. Safaeipour, M. Marquez, Z.A. Esguerra, E. Stemp
- CHED 640.** Using 3D printing to model disturbed flow through arteries. **N. Mburu**, M. Richardson, L. Bellan
- CHED 641.** New chemical methods developed on prototypes with hopes to improve gas exchange within respiratory devices. **J. Nguyen**, A. Malkin, W. Federspiel
- Section H**  
San Diego Convention Center  
Halls D/E
- Undergraduate Research Posters**  
**Chemical Education**  
*Cosponsored by SOCED*
- N. Di Fabio, *Organizer*
- 12:00 - 2:00**
- CHED 642.** NMR studies conducted on five coordinate Co(II) compounds. **C.N. Worley**, D.L. Tierney, J.H. Carmel
- CHED 643.** Development of an interactive dynamic simulation for the limiting reactant concept. **S. Santos**, E. Ortiz Nives, Z. Medina Torres
- CHED 644.** Kinetic isotope effects and dynamics for Friedel-Crafts acylation. **A. Sanchez**, Y. Nieves, D. Singleton
- CHED 645.** Exploring amine nanotethers: New routes to functionalized CdSe nanoparticles. **A.S. Tysoe**, K.A. Bolduc, D.J. Jackson, J.D. Kehlbeck, M.E. Hagerman
- CHED 646.** Development of a green multi-week synthesis for the organic lab: Total synthesis towards calarene. **R. Petit-Homme**, D.C. Bromfield-Lee
- CHED 647.** Assessing students' understanding of intermolecular forces through representations of small molecules and large biological structures. **K.A. Shaw**, C.J. Luxford
- CHED 648.** Assessing working memory load during logical thinking by measuring the task-evoked pupillary response. **R.C. Zahran**, N. Barrows, J.R. Vandenplas
- CHED 649.** Synthesis and characterization of cannabinoid metabolites for drug detection. **G. Ellis**, T. Herbelin
- CHED 650.** Adulterated orange juice: An introduction to analytical chemistry through use of high performance liquid chromatography (HPLC) and the case study approach. **G. Johal**, J. Congioli, P.M. Schaber
- CHED 651.** Measuring changes in self-efficacy, interest, engagement, and facility with the chemistry triplet in general chemistry lab. **J.L. Reynolds**, N. Garlick, R. Sansom
- CHED 652.** Real-time analysis of aspirin synthesis using Arduino based microprocessors. **C.B. Hall**, F. Iqbal, C.E. Stilts
- CHED 653.** Expanding instrumentation access through the incorporation of portable x-ray fluorescence spectrometry into the curriculum. **A.W. Jarnot**, **A. Mansfield**, K.H. Bennett, C.J. Stromberg
- CHED 654.** Practical method for examining the dynamics of a three molecule system for use in a physical chemistry curriculum. **J. Meyer**, **Z. Crandall**
- CHED 655.** Various genetic changes compensate for a lacZ  $\alpha$  insertion in a sensitive area of the M13 bacteriophage genome. **E.M. Zygiel**, C.L. Carroll, M.A. Cerezo, R.J. Aprile, C.R. Hebert, K.A. Noren, C.J. Noren, M.F. Hall
- CHED 656.** Student-led reimagining of the Barnard College general chemistry laboratory curriculum. **N. Patel**, A. Scorese, R.L. Starr, **J.S. Alexander**
- CHED 657.** Green revolution: Reactive iron-containing minerals and prebiotic metabolism. **V. Aguirre**, S. Churchman, M.M. Baum, L.M. Barge, J.A. Moss
- CHED 658.** Analysis of the concentration of mercury in rice to determine if it can be a significant source of mercury to humans. **T.M. Goodman**, S. Aloisio, C.F. Mayhew
- CHED 659.** VFL2 and wild type centrin-Sfi1p21 complex crystallization screenings. **M. Lu-Diaz**, B. Pastrana-Rios
- CHED 660.** Microwave-assisted synthesis of KTp\* and the corresponding Ni complex as an undergraduate inorganic chemistry experiment. **E.M. Helm**, R.M. Tarkka
- CHED 661.** Green metal extraction using monocarboxylic acid and dicarboxylic acid ligands. **H. Drake**, A. Schoffstall, R.M. Henry
- CHED 662.** Copper-catalyzed multicomponent approach to  $\beta$ -lactams. **A. Bosse**, A.K. Isaacs, t. Correia
- CHED 663.** Synthesis of *N*-Tosyl-4-iminoquinolizines. **A.K. Isaacs**, **L. Lauchert**, **G. Tsougranis**
- CHED 664.** Puerto Rico coffee characterization: An instrumental analysis course research project. **A. Acosta**, J. Jusino, **M. Martinez-Mercado**, **A. Rodriguez-Perez**, J. Santiago-Feliciano, G. Signorelli, E. Velez-Avila, A. Zapata Feliciano, A.M. Gonzalez
- CHED 665.** Using essential oils to teach chromatography and separation techniques in undergraduate organic chemistry labs. **H.S. McFall-Boegeman**, M. Zhu, B. Lybbert
- CHED 666.** In pursuit of a novel ruthenium carborane catalyst: A novice organometallic chemist report in poster and video format. **M. Wirth**, A. Larsen
- CHED 667.** Using C-H/ $\pi$  interactions for the synthesis of dipeptide based hydrogels. **D. Reigner**, C.R. Forbes, G.P. Yap, N.J. Zondlo
- CHED 668.** Comparative study in TCNQ reduction techniques for bulk synthesis of TCNQ radical anion salts. **N. Medina Berrios**, G.N. Gonzalez, D. Pinero
- CHED 669.** Distal heme coordination in ferric cytochrome c'. **Z. Nilsson**, B. Mandella, J.P. Bard, K. Hamann, M. Evans, C. Anderw
- CHED 670.** Free energy changes of magnesium ions in water clusters using quantum molecular dynamic simulations. **K. Spirak**, J.D. Madura, S. Upadhyay, R.J. Workman
- CHED 671.** Engineering a recombinant east coast fever vaccine from the tobacco mosaic virus and *Theileria parva* Tp1(03) antigen. **J. Grotts**, L. Grill, A. Gochi, E. Henderson
- CHED 672.** Glycosylated monoterpenoids: Miticides to protect honey bee colonies. **W.R. Collins**, **M. Walker**
- CHED 673.** Physical properties of mixed CTAB/Octyl-valine based surfactants. **S.I. Subnaik**, D. Georgiadis, J. Georgiadis, C. Lewis, K.F. Morris, E. Billiot, F.H. Billiot
- CHED 674.** Determination of illicit drug metabolites in wastewater by liquid chromatography mass spectroscopy. **G.D. Vial**, G.P. Foy
- CHED 675.** Faculty expectations for students' cognitive and affective learning in the undergraduate chemistry laboratory. **J. Orzel**, **E. Gross**, K.R. Galloway, S. Bretz
- CHED 676.** Implementing a critical thinking schema in a general chemistry II class. **L. Schaller**, C. Gabel
- CHED 677.** Development of a chemistry laboratory manual for blind and low-vision students. **W. Abraham**, **E. Miller**, A.A. Hill, C.A. Supalo
- CHED 678.** Tactile concept based labs for the visually impaired: A world of untapped potential. **A.E. Neybert**, P. Morehouse
- CHED 679.** Development of experimental flow chemistry methods. **J. Bard**, R.B. Kelley
- CHED 680.** Structural and electrochemical investigation of  $[\text{Cu}^{\text{II}}(\text{Me}_6\text{TREN})\text{Cl}][\text{Cl}]$  complex in the presence of weak nitrogen containing bases. **M.C. Wasson**, G.J. Pros, T. Pintauer
- CHED 681.** Bioactivity of compounds produced by endophytes found in Utah willow trees. **R. Toomey**, M.D. Halling
- CHED 682.** Investigating the stability of novel nano-vehicles in model biological fluid. **A.W. Cheema**, N.T. Flynn, A. Webb
- CHED 683.** Expanding the scope of mechanochromic porphyrin synthesis. **Q. Su**, T.D. Hamilton
- CHED 684.** Does thinking about thinking influence chemical thinking? **J.R. Pollard**, **J. Tashiro**

- CHED 685.** Crosslinking of the antibody anti-human IL 13R alpha 2 peptide IgY to FITC via PDPH. **R.A. Beck, L.C. Esmeralda, J.P. Thompson, J.M. Fautch, K.M. Halligan**
- CHED 686.** 15 letters. **C. Amster, J. Allison**
- CHED 687.** Card sorting inventory to describe the organizational thought processes between novices and experts in the field of chemistry. **F. Krieter, R. Julius, K. Tanner, S. Bush, G.E. Scott**
- CHED 688.** Ferritin in arthropods: A phylogenetic analysis. **C. Lowrance, E. Ragan**
- CHED 689.** Synthesis of a polyhydroxylated pyrrolidine from a D-glucose derivative. **A. Harney, L.J. Liotta**
- CHED 690.** Enhancing elementary STEM education through a two-year partial immersion model. **S. Hollinshead, R.C. Nangreave**
- CHED 691.** Study of reactions of transition metal oxides with NaOH, Na<sub>2</sub>O, Na<sub>2</sub>O<sub>2</sub> and KOH at high temperatures. **D.A. Habboush, J.W. Barbar, S.L. Bergman**
- CHED 692.** Study of reactions of transition metals with their respective divalent metal halides at high temperature. **D.A. Habboush, K.M. Campos, F.E. Divisconti, S.C. Jareb**
- CHED 693.** Determination of sulfate by conductometric titration: An undergraduate laboratory experiment. **J. Garcia, L.D. Schultz**
- CHED 694.** Withdrawn.
- CHED 695.** Determining the inhibitory effect of heme-*artemisinin*-lipid metabolites on enzyme activity. **E. Auwarter, C. Hartwig**
- CHED 696.** Synthesis of (2R,3S,4S)-2-(Hydroxymethyl)pyrrolidine-3,4-diol from  $\alpha$ -Methyl-D-galactopyranoside. **M.J. Smith, L.J. Liotta**
- CHED 697.** Direct probing of the reversible self-assembly of amyloid beta peptide oligomers over nanoscale metal colloidal surfaces. **E. D'Ambrosio, N. Ralbovsky, K. Yokoyama**
- CHED 698.** Expansion of molecular orbital theory: Application of Dirac's theory. **B. Barrett, J. Lacy**
- CHED 699.** Probing the diffusion rate and internal peptide dynamics: Temperature and pH-dependence studies of a fluorescein-tagged amyloid beta peptide and thioflavin T in a sol-gel matrix. **J. Chapman, K. Yokoyama, K. Chung**
- CHED 700.** Effect of copper imbalance in cell viability of the budding yeast *Saccharomyces cerevisiae*. **J.O. Strubbe, Y. Velez-Burgos, J.F. Rodriguez Quinones**
- CHED 701.** Using small molecule pyridine-based compounds to extract Ca<sup>2+</sup> and Sr<sup>2+</sup> from aqueous solutions then to be used as a nutrient source for soil bacteria. **K. Page, M. Porter, A. Richardson, C. Sobraske, S.G. Tajc**
- CHED 702.** Bioremediation of water soluble aluminum with dipicolinic acid. **E. Luta, S.G. Tajc, C. Sobraske, K. Page**
- CHED 703.** From students to scholars: The development of a student lead undergraduate lab using stain-blocking polymers. **N.E. Huddleston, A. Allred, A. Shupert, J. Holland, J. Konzieman**
- CHED 704.** Analysis of vitamin D3 using FT-IR. **C. Gregori, S.M. Yochum**
- CHED 705.** VSEPR: Virtual reality experience for general chemistry students. **S.K. Hall, J.G. Coonce**
- CHED 706.** Cationic gemini surfactants for enhanced oil recovery. **A.X. Woods, K.A. Daus**
- CHED 707.** Target Inquiry: Changing the way teachers think about science instruction in their classrooms. **R. Dumitrache, S. Tanis, D.G. Herrington, S.F. Bancroft**
- CHED 708.** Optimization and exploration of four-membered ring formation. **S. Johnston, L.J. Tilley**
- CHED 709.** Development of a copper catalyzed enantioselective allylic oxidation reaction using chiral amino acid ligands. **N. Khubchandani, P.J. Lombardi**
- CHED 710.** Effects of steric bulk on silyl bridging in the synthesis of trifluoromethylbicyclobutane. **L. Macary, L.J. Tilley**
- CHED 711.** Measuring the time diffusion of a colored gas in a small enclosed container. **F. Reachy Guadarrama, V. Castro, M. Ballester**
- CHED 712.** Progress towards the synthesis of novel N-heterocyclic carbene ligands. **M.D. Crawford, P.J. Lombardi**
- CHED 713.** Synthesis of cyanobicyclobutane via the gamma silyl effect. **M. Poto, L.J. Tilley**
- CHED 714.** Investigation into the reactivity of chlorosilanes with N-heterocyclic carbene ligands. **M. Golding, P.J. Lombardi**
- CHED 715.** Withdrawn.
- CHED 716.** Synthesis of all-*trans* cyclobutyl systems. **M. Wolf, L.J. Tilley**
- CHED 717.** Porphyrin basicity competition studies of octa alkyl substituted porphyrins with H<sub>2</sub>TPP. **A. Lam**
- CHED 718.** Project FORCE: A community of peer-learning coaches in STEM at NKU. **R. Kline, R. McLane, A.J. Onate, S. Emery, J. Filaseta, B.V. Bowling, D. Maureen, B. Brooke, P.M. Hare**
- CHED 719.** Exploring the interactions of polyethylene glycol-coated magnetic nanoparticles with lysozyme. **J.J. Freemark, A. Fazal**
- CHED 720.** Effects of hydraulic fracturing. **B. Ivan, A. Claffey, C. Kriley**
- CHED 721.** Synthesis of novel quercetin derivatives for targeting of mouse cancer cell lines T3HA and T2A. **A. Abel, B. Ivan, A. Claffey, C. Kriley**
- CHED 722.** Towards porphyrin-walled metal-organic polyhedra. **C.N. Molina, T.D. Hamilton**
- CHED 723.** Nitro as an electron-withdrawing group to enhance gamma-silyl elimination for the production of bicyclobutane derivatives. **A. Hunt, L.J. Tilley**
- CHED 724.** Dye sensitized solar cells utilizing polyethylenedioxythiophene (PEDOT) cathodes and a new light-absorbing dye complex. **K.L. Digan, C.A. Sweet, C.J. Timpson**
- CHED 725.** Second harmonic generation production via BBO crystal for artificial photosynthesis. **S. Desmarais, H. Patel, E. Pacheco, C.S. Schnitzer**
- CHED 726.** Application of adapted supplemental instruction program to chemistry education. **E.N. Reale, A.M. Reeve**
- CHED 727.** Comparing the levels of lead in stormwater runoff before and after bioretention. **K. Greeley, C.D. King**
- CHED 728.** Extraction of oil and grease contaminants from stormwater samples in order to facilitate nutrient testing. **D. Lewis, C.D. King**
- CHED 729.** From CAD to reality: A simple and inexpensive 3D printed colorimeter for laboratory and outreach activities. **B.M. Washer, M.H. Hakim, L.A. Porter**
- CHED 730.** Design and fabrication of a 3D printed fluorometer: A low-cost tool for student exploration of instrument design and performance. **C.A. Chapman, J.A. Alaniz, L.A. Porter**
- CHED 731.** Research toward the development and implementation of an online chemistry/mathematical tutorial. **E. Rwanuzza, A. Stebbins, F.M. Yarbbery, L. Christman**
- CHED 732.** BioBrick assembly of metal biosensors as a student research experience in biochemistry teaching labs. **M.J. Duckwall, L. Gwyn**
- CHED 733.** Investigation of the biological activity and mechanism of action of novel heterocyclic imines. **E. Segrist, A. Delawder, K. Liles, D. Dopp, M. Manpadi**
- CHED 734.** Preparation of  $\alpha$ - and  $\beta$ -acid standards for hops. **A.E. Gasow, C.J. Knutson, B.E. Sturgeon, M.R. Prinsell**
- CHED 735.** Searching for a strategy: Examining H-NMR spectroscopy in textbooks. **W. Ong, S. Anderson, E. Offerdahl**
- CHED 736.** Evaluating a class of click chemistry-based techniques for fluorescent detection of DNA-Pt adducts. **A.M. Wallum, A.D. Moghaddam, V. DeRose**
- CHED 737.** Analysis of anthocyanins in red wine: Development of a separation science lab for organic chemistry students. **W. Adrian, A.E. Fischer**
- CHED 738.** Synthesis of magnetite nanoparticles with applications for drug target delivery medicines and environmental water treatment removal of endocrine disrupting compounds. **J. Olmeda Russo, V. Fernandez-Alos, F.R. Roman, O. Perales**
- CHED 739.** Designing a new system for studying long range oxidation in DNA. **M. Safaiepour, K. Hernandez, P. Lee, E. Stemp**
- CHED 740.** Monitoring freshwater microbial contamination with qPCR rapid testing and source tracking methods. **E.M. Greeson, T. Sivy**
- CHED 741.** Structure-activity relationship study on histone deacetylase (HDAC) inhibitors derived from Santacruzamate. **E. Hogle, A.J. Onate, J. Tucker, R. LeDuc, T.D. Do, R. Klein, F.S. Thowfeik, E.J. Merino, L. Ma**
- CHED 742.** Obtaining electricity from solar energy utilizing household products. **D. Romero, E. Zuniga, A. Calderon, E. Stemp, R. Senter**
- CHED 743.** Malonic acid monoesters for the synthesis of xanthine oxidase inhibitors. **N. Brusman, E. Hogle, R. Kline, L. Snider, J. Tucker, T.D. Do, S. Paula, L. Ma**
- CHED 744.** Enaminone synthesis via mechanochemical accelerated eschenmoser coupling reaction. **E. Lopez Quiroz, S.R. Hussaini**
- CHED 745.** Development of a rogue's gallery that illustrates practical errors in the use of Schlenk flasks. **S. Ike, A. Rodriguez, J. Barro, R. Lopez de la Vega, J.M. Quirke**
- CHED 746.** Translation among multiple representations in chemistry: Examining student ability and response time. **T. Weiss, S. Vitale, J.R. Vandenplas**
- CHED 747.** Molecular docking of histone deacetylase (HDAC8) inhibitors. **R. Kline, N. Brusman, L. Snider, L. Ma**
- CHED 748.** Effect of computational chemistry software on student's comprehension of molecular properties. **W. Epps, H.M. Bevsek**
- CHED 749.** Development towards a copper-catalyzed asymmetric reduction of aryl 2*H*-azirines. **T.J. Mathews, J. Unger**
- CHED 750.** Using UV spectroscopy to follow exonuclease-induced hyperchromicity in the undergraduate biochemistry lab. **M. Ackerman, C. Ricciardi, A. Chant, D. Weiss, C. Chant**
- CHED 751.** Path integral Monte Carlo simulation of lithium nanoparticle aggregation. **M. Denchy, J. Kegerreis**
- CHED 752.** Calculation of position autocorrelation functions dampened with cyclic invariance for a system coupled to a harmonic bath. **C. Daly, J. Kegerreis**
- CHED 753.** Inquiry-based lab for the investigation of Michaelis-Menten kinetics. **G.H. Jones, E.V. Iski**
- CHED 754.** Simple no-heat, no-stir synthesis of butylmethylimidazolium bromide. **M. Acker, A. Primrose**
- CHED 755.** IR spectroscopic tracking of PbS and CdS quantum dot formation in fully dehydrated Nafion membranes. **D. Diawara, E.S. Smotkin, J.H. Doan, N. Nasirova, N. Loupe**
- CHED 756.** Detecting instructional change: Capturing teacher-student interactions and teacher moves in high school chemistry classrooms before and during professional development. **L. Vu, C. Sandvick, S.E. Nielsen, E.J. Yezierski**
- CHED 757.** Modifying the dehydration of cyclohexanol so as to become student centered. **A.S. Koch, E.H. Bresslour-Rashap, L.R. Eller**
- CHED 758.** Assessing correlation between VARK learning modalities and science majors. **K.M. Page, S.K. Hamilton**
- CHED 759.** Biochemistry question-guided derivation of a potential mechanism for HbA1c formation in diabetes mellitus leading to a data-driven clinical diagnosis. **B. Park, R.W. Holman, T. Slade, M.E. Murdock, K. Rodnick, A. Swislocki**
- CHED 760.** Ordered polytetrafluoroethylene thin-films for columnar liquid crystal alignment. **M. Van Winkle, J.J. Reczek**
- CHED 761.** Investigation of math preparedness for student success in general chemistry. **J. Lingen, A. Thompson, J. Zemke**
- CHED 762.** Aspirin synthesis and pharmacokinetic studies. **E. Robinson, R.V. Macri**
- CHED 763.** Exploiting the action of copper on nitric acid to generate atmospherically relevant nitrogen-containing gases: A physical-atmospheric chemistry laboratory project. **A. Li, M.D. Gribble, J.A. Ganske**
- CHED 764.** Investigating cellular metabolism to preferentially target cancer cells with deregulated p27. **K.B. Chancellor, R. Sheaff**
- CHED 765.** Exploiting <sup>1</sup>H-<sup>15</sup>N two-dimensional nuclear magnetic resonance correlations in the characterization of alkaloids in an advanced organic spectroscopy course. **J.K. Tran, T.P. Dang, J. Carroll**
- CHED 766.** Halobacteria as a source of food coloring pigments. **C. Detrés-Román, D. Pérez-Pardo, C.R. Ruiz-Martinez, J.M. Planas-Rivera**
- CHED 767.** Synthesis and analysis of 2,2,2-trichloro-*N*-(1-phenylprop-2-en-1-yl)acetamide through overman rearrangement. **J.K. Murray, H. Low**
- CHED 768.** Anti-carcinogenic effects of quercetin derivatives in metastatic mouse cells. **D. Greenfield, J. Ostrowski, C. Kriley, D. Ray**
- CHED 769.** Cellular internalization and cytocompatibility of direct water synthesized cadmium selenide quantum dots. **O.D. Rivera, M. Rodriguez-Torres, C. Velez, B. Zayas, O. Primera-Pedrozo**



- CHED 770.** Synthesis of silver nanoparticle films: The search for the green color. **H.E. Skipper, M. Roca**
- CHED 771.** Undergraduate laboratory experiment to investigate surface areas of nanoscale materials. **J. Denhardt, D.S. Heroux**
- CHED 772.** Does science education affect college students' perceptions of harm and of availability of prescription opioids. **M. Blackburn, M. Rohan, H. Kraus, M.E. Railing**
- CHED 773.** Measuring learning outcomes in chemistry outreach in kindergarten through 6th grade elementary school students. **S. Quintero, A. Doong, C. Carr, N. Pham, H. Hsieh, D. West, C. Carter, N. Patel, S. Denton, G. Rydaldh, N. Al-Dulaimi, R.V. Valcarce, P.J. Iles, L.D. Giddings, N.R. Bastian, M. Alvarez, S. Richards, R. Holcomb**
- CHED 774.** Using "Drug of the Week" to educate chemistry students about prescription drugs and their abuse. **H. Kraus, M. Blackburn, M. Rohan, M.E. Railing**
- CHED 775.** Community-based learning on campus: A partnership between Department of Chemistry & Biochemistry and dining services. **K. Hess, K. Kneas, E.C. Turzai**
- CHED 776.** Genetic engineering and expression of functional fusion protein serving as biological modification on silica nanofibers for neural tissue engineering. **A.M. Masroujeh, A. Augustine, S. Brennan, S. Johnson, W. Chen, Y. Chen-Yang, M. Yang**
- CHED 777.** Heavy metal content analysis of wines produced in the U.S. using inductively coupled plasma-optical emission spectroscopy. **K. Craven, G.P. Foy**
- CHED 778.** Investigation of the relative migratory aptitude of phenyl and substituted phenyl groups in the Baeyer-Villiger reaction. **J. Killen, B. Withrow, M. Bissell, D.L. Dillon**
- CHED 779.** Synthetic investigation of highly substituted cyclohexene compounds via Diels-Alder reactions. **L. Soong, J. O'Sullivan, K. Cetto Bales**
- CHED 780.** Synthesis and catalytic properties of Ir (I) NHC nitro complexes. **S. Kacsok, E. Rajaseelan**
- CHED 781.** Ethanol induces mitochondrial biogenesis in rats fed ethanol and a low-fat diet. **A. Jivan, A.A. Caro**
- CHED 782.** Greener procedure for the regioselective hydration of alkenes: Use in the undergraduate organic laboratory. **E. Fjellstad, I.R. Commins, L.J. O'Donnell, A. Swartzel, M. Paul, I.J. Levy, K. Van Kirk**
- CHED 783.** Synthesis of deep eutectic solvents from biodiesel waste glycerol. **A. Valceschini, L. Ott**
- CHED 784.** Effects of time delay between sample collection and extraction of wastewater samples for amphetamine and opioid analysis. **W. Parker, T.H. Boles**
- CHED 785.** Studying amyloid peptide oligomer dynamics over nanometer-interface. **H. Chen, M. Luce, K. Yokoyama**
- CHED 786.** Development of a rogue's gallery that illustrates practical errors in distillation. **S. Ike, L. San Miguel, M. Exposito, J.M. Quirke**
- CHED 787.** Progress toward a polyphenol releasing bare metal stent. **W. Owen, J.A. Harris, J. Gigliotti, C.M. Jones, N. Widstrom**
- CHED 788.** Extraction of an active component (mitragynine) from Kratom leaves. **L. Tran, K. Ng**
- CHED 789.** Modification of P27 by human transglutaminase. **E. Wilson, R. Patel, R. Shearf, W. Crawford, L. Zhang**
- CHED 790.** Development of an organic laboratory experiment: An old school characterization of ketones and aldehydes. **J. Cleland, K. Cossey**
- CHED 791.** Detection of methamphetamines in medium and low velocity bloodstain patterns. **J. Roy, G.P. Foy**
- CHED 792.** Electrochemical properties of imine candidates for organic light emitting diodes. **M. Seidel, N. Rosenfeld, N. Capra, J. Bennett**
- CHED 793.** Quantum dots. **H. Ruiz, C. Edwards**
- CHED 794.** Kinetics of indigo bleaching: Reflectance versus absorbance. **E. Stopler, J. Bennett**
- CHED 795.** Probing the profile of volatile organics in American bourbon using a student grade gas chromatograph. **D. Medrano, D.G. Patel**
- CHED 796.** Fluorescent spectroscopy studies of complex formation between porphyrin H<sub>2</sub>TPP and fullerene-like nanoparticle PCBM. **E. Parsons, H.A. Stretz**
- CHED 797.** Characterization of the p250GAP messenger RNA and interactions with the fragile X mental retardation protein. **A. Williams, M. Mihalescu**
- CHED 798.** Separation and detection of phenytoin and chemotherapeutic drug and extraction of phenytoin from a biological sample. **K. Ng, M. Arnot, A. Vu**
- CHED 799.** Design of an automated visual system for demonstration of acid base reactions. **K. Ng, T. Lim, D. Monsivaiz, E. Nicolas**
- CHED 800.** Antimicrobial activity against *Bacillus cereus* and *Escherichia coli*: Acetylugenol and eugenol from clove oil. **D. Brown, J. Wilson, C.J. Stromberg, P. Wood, D.J. Ellis**
- CHED 801.** Capillary electrophoresis of a protein mixture. **N.S. Sundo, L.H. Rickard**
- CHED 802.** Assessment of variability in a kinetic isotope effect experiment based on a biphasic oxidation. **R.A. Wyatt, R.J. Noll, R.W. Fitch**
- CHED 803.** Investigating arson accelerants: An instrumental methods discovery approach to gas chromatography. **M. Comiskey, A.M. Hupp**
- CHED 804.** Designing an ELISA for biochemistry laboratory students to study immunochemistry in biotechnology. **M. Pereira Marques Leal, W.L. Swanson, S.G. Garrett**
- CHED 805.** Expression of a recombinant enzyme. **N.J. Beyer, N. Cordes**
- CHED 806.** Success in early chemistry classes. **J.M. Dallman, K.M. Elliott, S. Wuerz**
- CHED 807.** Flash and the bang in chemical education: Magic shows, explosions, and other dramatic effects. **E.M. Fauglid, J.M. Dallman, S. Wuerz**
- CHED 808.** Quality of drinking water and public understanding of water quality. **K.J. Morland, E.M. Fauglid, S. Wuerz**
- CHED 809.** Chemical safety and public perceptions in home and laboratory. **K.M. Elliott, K.J. Morland, S. Wuerz**
- CHED 810.** Synthesis and antimicrobial activity of benzohydrazides substituted at the aryl and N' positions. **A. Mason, S. Thompson, D. Caprioglio, J. Steel, D.L. Dillon**
- CHED 811.** Quantification of pseudouridine modifications through uridine specific cleavage of RNA. **A. Aninweze, P.A. Limbach, B. Addepali**
- CHED 812.** Optimization of hydrothermal synthesis of lithium vanadyl phosphate. **E. Cassidy, Y. Chung, N. Chernova, F. Omenya, M.S. Whittingham**
- CHED 813.**  $\alpha$ -Synuclein misfolding and  $\beta$ -sheet aggregation in Parkinson's disease. **M. Stuckey, S. Petty**
- CHED 814.** Flexible photoremovable protecting groups (PRPGs) for efficient photorelease. **A. Aremu, A. Gudmundsdottir**
- CHED 815.** Synthesis of a chloride chemosensor by ligand structure manipulation. **N. Brocius, J.M. Fautsch**

## Section H

San Diego Convention Center  
Halls D/E

## Undergraduate Research Posters

### Computational Chemistry

*Cosponsored by COMP and SOCED*

N. Di Fabio, *Organizer*

### 12:00 - 2:00

- CHED 816.** Structure and stability of DNA duplexes with dangling ends and a central mutation in a model microarray system. **B.R. Rivard, J.M. Stubbs**
- CHED 817.** Renewable energy insights through hydrogen sulfide oxidation. **M. Wilkinson, J. Herr, J. Talbot, S. Floris, R. Steele**
- CHED 818.** New method for determining the interfacial tension of spherical liquid/liquid interfaces using molecular dynamics simulations. **E. Sanchez, S.O. Nielsen**
- CHED 819.** Utilization of numeric analytical continuation to study node evolution in the Sech wave packet. **C. Lechak, B.A. Rowland**
- CHED 820.** Deriving a group additivity scheme for organics in aqueous solution. **V. Vargas, J. Kua**
- CHED 821.** Constructing a free energy map for HCN, formamidic acid and formamide in aqueous solution. **K. Thrush, J. Kua**
- CHED 822.** DFT study of chiral organic superbase. **A.E. Andrews, S.M. Bachrach**
- CHED 823.** MD/QM excited-state approach to predicting tryptophan fluorescence in proteins. **E.B. Kofke, K.M. Vorwerk, W. Kennerly**
- CHED 824.** Computational study on the ground state of silaethynyl. **D. Corey, A. Shah, A. Seitz, J. Song**
- CHED 825.** Computational study on reaction mechanism of the formation of levoglucosan. **A. Shah, D. Corey, L. Aebbersold, D. Wang, B.N. Leja, J. Henry, A. Seitz, J. Song**
- CHED 826.** Computational determination of mechanism for aldehyde insertion into *N*-acylphthalimides to form *N*,*O*-acetals. **C. Tan, J. Scanlon, P. Willoughby**
- CHED 827.** Exploring wider ExBox<sup>+</sup> analogs. **C. Tallant, A.E. Andrews, S.M. Bachrach**
- CHED 828.** Effects of residue mutations on the enantiospecificity of CYP2C9. **T. Meece, G.P. Miller, M.D. Perry**
- CHED 829.** Computational investigations of enantiospecificity of mutated CYP2C9. **L. Bond, G.P. Miller, M.D. Perry**
- CHED 830.** Monte Carlo simulations of the adsorption of alkane and alcohol mixtures near an explicit platinum surface. **J.H. Barfield, T. Stoneham, K.E. Anderson**
- CHED 831.** Computational studies of oxygen bond weakening with group-10 metal clusters. **D. Gray, M. Paul**
- CHED 832.** Investigation of oxo-substituted peroxy radicals reacting with HO<sub>2</sub> in the atmosphere. **M.P. DeVault, K.T. Kuwata**
- CHED 833.** Computational studies on the decomposition pathways of vinylhydroperoxide. **K. Huang, K.T. Kuwata**
- CHED 834.** Characterization of carbon-deuterium vibrational probes as reporters of protein binding. **Y. Arnouk, P. Edwards, C. Miller**
- CHED 835.** Core electron binding energy shifts in transition metal hydrides. **J.L. Wells, C.M. Morales**
- CHED 836.** Comparison of density functional methods for initial SN2 and SN2' reactions of guanine with activated arylamines. **J. Bautista, S. Shrestha, A.S. Dutton, A. Leach**
- CHED 837.** In silico development of novel isoform selective LXR agonist ligands. **M. Ndukwe, K. Riley, J. Sridhar**
- CHED 838.** Insight into asymmetric catalysis of aqueous asymmetric Mukaiyama aldol reactions by dinuclear zinc semi-crown ligand. **A. Ahmed, B. Vernier, J.D. Evanseck, J. Rohde**
- CHED 839.** Construction and molecular dynamics of a SMA nanodisc for membrane protein simulation. **R. Franklin, J.E. Curtis, K. Edler**
- CHED 840.** Predicted ensemble of 3D structures for human olfactory receptor hOR1A1-4. **C. Seitz, S. Kim, W.A. Goddard**
- CHED 841.** Computational modeling of the kinetics of the reaction of hypochlorous acid with resorcinol. **B.H. Frohock, G.H. Purser**
- CHED 842.** Ground state stabilization of carbamoyl phosphate by hydration "buckle". **L.R. Andreola, I. Pathiraja, A. Tamez, S.M. Firestone, J.D. Evanseck**
- CHED 843.** On the connection between excited quantum states and a multiply-mapped 1-sphere: A heuristic derivation of the Pauli-exclusion sphere. **L.C. Jake, E. Curotto**
- CHED 844.** Computational study of the decomposition of 2-azido-2-nitropropane radical anion. **W.J. Kelly, D. Ramirez**
- CHED 845.** Nature of the anti-electrostatic hydrogen bond. **R.C. Rudisell, P.R. Cheek, E.D. Glendening**
- CHED 846.** Computational chemistry modeling of copper-based drugs to DNA oligomers. **K. Kim, L.A. Tyler, J.S. Anderson**
- CHED 847.** Confined diffusion of monovalent electrolytes. **A. Dominguez, T.D. Shepherd**
- CHED 848.** Rutile 110 quantum surface models for carboxylic and phosphonic acid binding. **A.L. Gagliardi, A. Carlson, E.S. Gawalt, J.D. Evanseck**
- CHED 849.** Computer modeling of transition states for the greener hydration of alkenes. **L.J. O'Donnell, I. Commins, E. Fjellstad, A. Swartzel, M. Paul, I.J. Levy, K. Van Kirk**
- CHED 850.** Computational modeling of the <sup>235</sup>U temporary anion of CO<sub>2</sub> using the stabilization method. **N.D. Reilly, M.F. Falcetta**
- CHED 851.** Computational study of azaphosphole dimers. **S. Warren, J.N. Woodford**
- CHED 852.** How does the quality of the electrostatic potential depend on the size of the basis set used? **K. Tran, K. Riley**

- CHED 853.** Computational studies of methane and methyl radical reactions with selected hydrocarbons that are of relevance to atmospheric chemistry and astrochemistry. **D.M. Gardner**, W.K. Gichuhi
- CHED 854.** Role of kinesin-13 in the depolymerization of microtubules. **T. Reeves**, C. Shulman, D. Merz, R. Dima
- CHED 855.** Oxidation of hydrated hydrogen sulfide. **S. Floris**, M. Wilkinson, J. Herr, R. Steele
- CHED 856.** Computational study of protonated methionine thermochemistry and dissociation mechanism. **A. Zhanseerkeev**, J. Johnston, P.B. Armentrout
- CHED 857.** Investigation of polymerized molecular micelle formation with molecular modeling and NMR. **C. Lewis**, E. Billiot, F.H. Billiot, K.F. Morris, Y. Fang
- CHED 858.** Quantum excited-state structure of indole fluorescence. **K.M. Vorwerk**, **W. Kennerly**
- CHED 859.** Mechanistic investigation of the origin of reactivity and stereoselectivity in tandem cross metathesis-coupled reactions. **W.C. Bell**, P. Liu, R.H. Grubbs, P.K. Dornan, G. Lu
- CHED 860.** Importance of methanol absorption thermodynamics to the flexibility of caffeine: Halide-nitrobenzoic acid cocystal. **J. Rumley**, A.H. Shutt, H.K. Hernandez-Soto, A.B. Singaraju, I. Nessler, L.L. Stevens, M.J. Schnieders
- CHED 861.** RNA G-quadruplex topology and stability. **J.A. Imperatore**, R.J. Workman, J.D. Madura
- CHED 862.** Computational studies on the realkylation of aged acetylcholinesterase (AChE) by quinone method precursors (QMPs). **R.J. McCauslin**, R. Dummermuth, R. Dicken, C.S. Callam, C.M. Hadad, R.J. Yoder
- CHED 863.** Predicting catalytic potential: The accessibility and energetics of metal-based electron density for group 10 diphosphinito complexes, interpreted based on density functional theory. **M. Ellis**, **L. Patrick**, **K. Downey**
- CHED 864.** From precursor to catalyst: A density functional analysis of ligand substitution and catalytic activation in group 10 metallo-organic phosphinito complexes. **K. Downey**, **M. Ellis**, **L. Patrick**
- Section H**
- San Diego Convention Center  
Halls D/E
- Undergraduate Research Posters**
- Environmental Chemistry**
- Cosponsored by ENVR and SOCED*
- N. Di Fabio, Organizer**
- 12:00 - 2:00**
- CHED 865.** Synthesis of hybrid materials of silver nanoparticles decorated-graphene and polyamide: With sorption evaluation. **A.S. AlJameel**, T.A. Saleh
- CHED 866.** Atmospheric aerosol sampling and analysis by GC/MS. **J. Higgins**, D. Hughes, C.D. Hatch
- CHED 867.** Traces of heavy metals in Carraizo Reservoir and Sergio Cuevas Water Treatment Plant in Puerto Rico. **E. Estrada**, G. Infante
- CHED 868.** Comparison of the determination of metal ions in water samples by rotating disk voltammetry and atomic absorption spectroscopy. **S. Kennedy**, L.H. Rickard
- CHED 869.** Analysis of the open limestone channel at the Swank 13 abandoned coal mine. **D.R. Mosier**, J. Krug, C.J. Weyant, L.J. Stern, D.K. Wolfe, C.D. Spellman, W.H. Strosnider, J. Bandstra, E.P. Zovinka
- CHED 870.** Use of naturally occurring minerals to remove phosphorus from water in the Saginaw Bay watershed. **M.A. Dobulis**, D.S. Karpovich
- CHED 871.** Using mixtures of trans-decahydronaphthalene and 1,2,3,4-tetrahydronaphthalene to model the properties of hydrodepolymerized cellulosic diesel fuel. **B. Lee**, D.J. Luning Prak
- CHED 872.** Antibiotic resistance in surface drinking water sources and finished tap water. **M. Andreone**, C. Heiling, S. Beck, T. LaPara, K.H. Wammer
- CHED 873.** Mercury bioaccumulation in otters of Lake DeGray: Multiple tissue analysis. **M. Davis**, D. Bateman, **A. Surf**, R. Tumilson
- CHED 874.** Prudent practices in the storage, handling, and disposal of laboratory chemicals. **L. Neff**, **K. Mitchell**, K. Roeske, M.J. D'Souza
- CHED 875.** Solvent reactions of chloroformates and carbonyl tosylates. **D. Williams**, M.J. D'Souza
- CHED 876.** Quality of water and soils in the subterranean ecosystems of Puerto Rico. **A. Rodriguez Velazquez**, L. Delgado-Vega, K.D. Ortiz
- CHED 877.** Photoreduction of Hg(II) and photodemethylation of methylmercury: The key role of thiol sites on dissolved organic matter. **J. Jeremiason**, **J. Portner**, D.E. Latch, G. Aiken
- CHED 878.** Biosorption of metal ions by *Neochloris minuta* and *Neochloris oleoabundans* algae grown in Bristol and nitrogen depleted media. **S.A. Rodriguez**, K. Fins, D.G. Giarikos
- CHED 879.** Regiospecific rates and steric effects of phenyl ether bromination by aqueous free bromine. **G.A. Taggart**, J.D. Sivey
- CHED 880.** Investigating pyrene levels in water and sediment samples in presence of bioturbators. **F. Louka**, A. Cazan, **S. Osman**, P. Morandi, M. Hoag, P. Klerks
- CHED 881.** Characterization of uranium and arsenic in soil and sediment collected from southwestern Navajo reservation. **B. Dalton**, T. Rock, J.C. Ingram
- CHED 882.** Optimization of a paper-based fluidic device for nitrogen detection. **J.A. Luthardt**, E. DeShano, K. Cissell
- CHED 883.** Metals in mushrooms of western Pennsylvania. **K.M. Gresko**, K.A. Wozniak
- CHED 884.** Interaction of lipids with natural surfactants from soils. **D.M. Blanchard**, J.S. Shore, J.A. Rice, G. Chilom
- CHED 885.** Surfactant content of mineral soils: Effect of depth and treatment. **D. Reidhead**, A. Fackler, S. Osborne, G. Chilom
- CHED 886.** Effect of soil surfactant-lipid composites on the water repellency of soils. **A. Fackler**, D. Reidhead, S. Osborne, G. Chilom
- CHED 887.** Influence of often-overlooked free chlorine and free bromine species on regiospecific halogenation rates of salicylic acid. **M.A. Broadwater**, J.D. Sivey
- CHED 888.** Identification of *Medicago truncatula* genes involved in symbiosis with *Sinorhizobium*. **B.M. Soriano**, M. Sadowsky, M. Nelson, C.L. Chun
- CHED 889.** Ensuring environmental health by assessing and monitoring water quality at Georgia Southern University Campus. **J. Ahweyevu**, A. Saha
- CHED 890.** Phosphate adsorption to soil upon addition of natural soil amendments. **K.L. Keel**, D.S. Karpovich
- CHED 891.** Effects of ozone on standards representing molecular components of epicuticular waxes in plant leaves. **M. Riches**, T. Kochar, A. Teller-Radzat, D.P. Soulsby, T.L. Longin
- CHED 892.** Characterization of aqueous glyoxal oxidation in the presence of salts using quartz crystal microbalance. **L. Rusch**, C.M. Strollo
- CHED 893.** Particulate matter formation in response to reduced sulfur-alkyl amine reactions. **L. Connor**, J. Dulla, A. Godoy, T. Zunguze, D.J. Price, P. Van Rooy, D. Cocker, K. Purvis
- CHED 894.** Analysis of ground turmeric samples with a handheld x-ray fluorescence analyzer. **S. Baghaie**, **S.L. Thomas**, **M.Y. Wu**, M.A. Benvenuto, E. Roberts-Kirchhoff
- CHED 895.** Investigation of the environmental impact and legacy of pressure treated wood on marine organisms. **R. Phelps**, J. Hugger, S.K. O'Shea
- CHED 896.** Measurement of lead by atomic absorption spectroscopy from soil at an airport and gas station in Taney County, Missouri. **S.M. Seaman**, K.E. Garrison
- CHED 897.** Determining the viability of ozone as a treatment method for eliminating antibacterial activity of clarithromycin. **D. Webb**, C. Fuerste, K.H. Wammer
- CHED 898.** Origin of atmospheric mercury deposition to Pacific Northwest alpine lakes. **W.F. Erickson**, R.H. Thirkill, F.M. Dunnivant
- CHED 899.** Extraction of lead ions from bulk water supplies using ionophore-embedded organic membranes. **K.M. Sheetz**, K.A. Mies, N.S. Green
- CHED 900.** Binding group II cations with DPA-amino acid complexes. **S.A. Fuentes**, **M.J. Leverich**, J. Moose, S.G. Tajc
- CHED 901.** XRF analysis of the otolith: A potential environmental bioindicator of salinity and toxic metal exposure. **J. Hugger**, R. Phelps, S.K. O'Shea
- CHED 902.** Rhodium catalyzed hydrogenation of fluoroarenes in mild condition. **T.J. Dick**, A.M. Luke, A.A. Peterson
- CHED 903.** Rh/Al<sub>2</sub>O<sub>3</sub> catalyzed hydrodehalogenation of TCE under mild conditions. **Z.M. Brown**, M.G. Lerick, G. Gorman, K. Kaiser, K. Lauer, A.A. Peterson
- CHED 904.** Quantifying THC-COOH as a tracer of cannabis use in wastewater from a residential treatment plant using LC-MS/MS. **R. Carpenter**, D. Westerman, D.A. Burgard
- CHED 905.** Biodiesel synthesis & purification analysis. **H. Black**, C. Edwards
- CHED 906.** Comprehensive characterization of the contribution from on-road light duty vehicles to environmental concentrations of carbonyl containing compounds. **A. Castonguay**, R. Fanter, A. Pesta, M. Anderson, J.A. Moss, M.M. Baum
- CHED 907.** Indirect effects of hemlock woolly adelgid on metal nutrient content of soil water. **K. Tallman**, J. Bains, Z. Balogh-Brunstad
- CHED 908.** Chemical analysis of metal contaminants in the freshwater of Wheeling. **N. King**, M.E. Railing
- CHED 909.** Synthesis of metal-impregnated xero- and aero-gel catalysts for carbon dioxide reduction. **C. Jackson**, M. Mansell
- CHED 910.** Quantification of heavy metals in freshwater fish in Wisconsin through atomic absorption spectrometry. **J. Nowak**, M.D. Schuder
- CHED 911.** Quantification of uranium in soil collected near Leupp, AZ on the Navajo reservation. **A. Koritzke**, A. Lister, J.C. Ingram
- CHED 912.** Contaminant transport and chromatography: Developing an experiment for the undergraduate laboratory. **C.J. Zimmerman**, J. Piatt
- CHED 913.** Quantifying calcite precipitation dynamics in a rivulet of a calcareous fen. **L.T. Yonke**, J. Piatt
- CHED 914.** Quantification of THC-COOH in wastewater: A tool to assess cannabis consumption in WA State. **D. Westerman**, R. Carpenter, D.A. Burgard
- CHED 915.** Exploring the mechanism for iron uptake by phytoplankton: A biomarker study. **A. Gatmaitan**, M. Christie, C.D. Hatch
- CHED 916.** Formic acid uptake on montmorillonite clay: An FTIR study. **J. Kim**, L.A. Hancock, A. Gloyna, C.D. Hatch
- CHED 917.** Evaluating the efficacy of TMDL implementation actions on fecal bacteria concentrations in Mill Neck Creek, NY. **T.J. Vogel**, R. Brinkmann, S. Garren, M. Hunter, K. Bisceglia
- CHED 918.** Kinetic studies of the reversible photodegradation of dienone and trienone steroids. **S.M. Berg**, J.E. O'Brien, K.C. Anderson, D.M. Cwiertrny, E. Kolodziej, K.H. Wammer
- CHED 919.** Aerosol growth through photosensitized VOC oxidation. **M. Ippolito**, K. Yordanova, M. Galloway
- CHED 920.** Investigation of molecular interactions between cationic Au nanoparticles and cell-wall defected *B. subtilis*. **H. Frew**, K.P. Johnson, A. Vartanian, C.J. Murphy, C.L. Haynes, V. Feng
- CHED 921.** Understanding the aqueous phase transformation of glyoxal. **F.P. Hyler**, C.M. Strollo
- CHED 922.** Using inverse model catalysts to investigate CO<sub>2</sub> chemistry. **W.J. Andahazy**, D.T. Boyle, C. Stopak, A. Baber
- CHED 923.** Arsenic, cadmium, copper, nickel, and mercury concentrations in liver, gills, and muscle of spotted seatrout (*Cynoscion nebulosus*) from the Ashley River in Charleston, South Carolina. **B. Molnar**, B. Adair
- CHED 924.** Quantification of trace elements in unregulated water sources on the Navajo and Hopi reservations. **M. Simmonds**, J. Credo, T. Rock, J.C. Ingram
- CHED 925.** Development of a portable nanoparticle sensor for the detection of aquatic toxins. **N. Mandeep**, J. Kim, B. Miranda, P. Hall
- CHED 926.** Comparison between winter and summer *E. coli* levels in the Saginaw River. **E. Short**, D.S. Karpovich
- CHED 927.** Investigation of possible contamination of surface water by fracking in northern WV. **W. Workman**, M.E. Railing
- CHED 928.** Withdrawn.
- CHED 929.** Toxicity assessment of nanoparticles in lithium-based battery materials to model bacterium. **O. Martinez**, H. Frew, M. Hang, I. Gunsolus, R.J. Hamers, C.L. Haynes, V. Feng
- CHED 930.** Comparative interactions of gold and silver nanoparticles and lead in the rates of germination and root elongation of radish plants. **R. Noriega Rivera**, A. Cruz Torres, E.J. Ferrer Torres, C. Osorio Cantillo, J.I. Ramirez Domenech

**CHED 931.** Correlation study between weather and PAH concentrations: Bio-monitoring of pine trees near the I-405 freeway in west Los Angeles. **S. Castillo, M. Ligot, A. Bautista, Y. Torres, S. Jimenez, S. Deprele**

**CHED 932.** Pd-Catalyzed hydrophosphinylation: The second step in the synthesis of phosphorus-based surfactants. **A. Castillo, A.C. De La Cruz, S. Deprele**

**CHED 933.** Determination of mercury levels in living and nonliving systems in historic cinnabar mining districts in southwest Arkansas. **M. Davis, A. Surf, R. Tumison, D. Bateman**

**CHED 934.** Incorporation of titania into porous PMMA for photocatalytic applications. **J. Glover, J.E. Boyd**

**CHED 935.** Leaching and transformation of trifluralin from herbicide-impregnated mulch. **F.A. Pavlovici, K.J. Bisceglia**

**CHED 936.** Comparison of experimental aerosol optical properties to Mie scattering theory of multi-component aerosols. **J.A. Land, A.N. Jarman, H.E. Kay, K.S. Dooley**

**CHED 937.** Glyphosate-induced phosphate desorption in the Maumee River watershed. **M.N. Bowling, C.E. Spiese**

**CHED 938.** Transesterification of hypophosphorous esters and the direct esterification of hypophosphorous acid. **N. Neris, D. Morales, A.V. Carmona, S. Deprele**

**CHED 939.** Analyzing reactions of MAE and atmospheric oxidants. **J. Dulla, A. Godoy, T. Zunguze, D. Pierce, L. Connor, R. Jauregui, K. Purvis, P. Van Rooy, D.J. Price, D. Cocker**

**CHED 940.** Analyzing reactions of MEA and DMA and atmospheric oxidants. **T. Zunguze, D. Pierce, J. Dulla, A. Godoy, L. Connor, R. Jauregui, K. Purvis, P. Van Rooy, D.J. Price, D. Cocker**

**CHED 941.** Declining seagrass meadow coverage and its correlation to bleach contamination in South Caicos. **A. Goranov, A. Murray**

**CHED 942.** Preliminary assessment of volatile organic compounds in indoor parking facilities in the greater Houston area. **R.B. Reed, S. Tarver, B. Wilson**

**CHED 943.** Fractionation of organic carbon through natural transfer processes between sea water and sea spray aerosols. **R.E. Hernandez, M.H. Thieme, D. Crockner**

**CHED 944.** Analytical evaluation between polycyclic aromatic hydrocarbons and particulate matter in Los Angeles via bio-monitoring of cypress trees. **Y. Torres, M. Ligot, A. Bautista, S. Deprele**

**CHED 945.** Oil contamination in the Salt Lake City watershed. **A. Jorgensen, R.M. Hyde**

**CHED 946.** Enhancement of phytoremediation through in situ metal chelation. **M.E. de Vries**

## Section H

San Diego Convention Center  
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### Undergraduate Research Posters Geochemistry

*Cosponsored by GEOC and SOCED*

N. Di Fabio, *Organizer*

#### 12:00 - 2:00

**CHED 947.** Oxalic acid influences kinetics of strong chelate exchange reactions. **A. Wildman, N.E. Boland**

**CHED 948.** Influence of calcium on rates of ligand exchange between strong chelating agents by capillary electrophoresis. **Y. Xu, N.E. Boland**

## Section H

San Diego Convention Center  
Halls D/E

### Undergraduate Research Posters

#### Green Chemistry & Sustainability

*Cosponsored by CEI, I&EC and SOCED  
Financially supported by ACS GCI*

N. Di Fabio, *Organizer*

#### 12:00 - 2:00

**CHED 949.** Synthesis of camphor using ionic liquids. **F.C. Mayville, N.R. Carpenter**

**CHED 950.** Solar soxhlet extraction of turmeric. **S. Murphy, D.J. Swartling**

**CHED 951.** Synthesis of sustainable materials – paints & biofuels – through the early career undergraduate research experience (eCURE) at Pasadena City College. **J. Blatti, J. Portillo, C. Sepulveda-Torres, A. Cuccinello, B. Juarez, W. Liang**

**CHED 952.** Homogeneous functionalization of biomass using ionic liquids. **E.D. Anderson, M. Bullard, W.M. Reichert**

**CHED 953.** Ionic liquids as green extractants of biofuels from microorganisms. **J. Melessa, C. Fordham, A. Young, D. Stapleton, J. Aklinski, C. Migliori, D. Warner, A.T. Koppisch, R.E. Del Sesto**

**CHED 954.** Natural sources used as light harvesters in dye-sensitized solar cells. **C. Gunther, C. Hastings, F. Kozareva, M. Nie, A. Ormond**

**CHED 955.** Development of green digestion methods of soils for recovery of cadmium, arsenic, and lead. **S. Patel, J.D. Leyba**

**CHED 956.** Determining green chemistry metrics for comparison of syntheses of tetraphenylporphyrin. **S. Kingston, T.D. Hamilton**

**CHED 957.** Entrainment sublimation as a green purification method for porphyrins. **V. Hoelscher, T.D. Hamilton**

**CHED 958.** Preparation of 6-nitro-2,3-di-phenylquinoxaline: Green multistep organic synthesis. **H.O. Miller, I.J. Levy**

**CHED 959.** Electrochemical polymerization of conductive PEDOT in neat monomer solution using organic electrolytes. **C. Byron, P.A. Mabrouk**

**CHED 960.** Continuing synthesis of meso-tetraphenylporphyrins using solar irradiation. **T. Pinto, D.J. Swartling**

**CHED 961.** Differences in light gas production from the gas-phase pyrolysis of guaiacol, 4-methylguaiacol, and 4-ethylguaiacol. **J.N. Hoang, A. Mullery, E.B. Ledesma**

**CHED 962.** Ebonization of wood: Tailoring and quantification of ferrous acetate solutions via spectroscopic analysis. **A. Gomez, S.C. Butler**

**CHED 963.** Tetraarylphosphonium salts as ionic liquids of unusually high long-term stability in air at high temperatures. **J.H. Davis, C. Cassidy**

**CHED 964.** Can Gutman acceptor number be used to determine the relative content of protic ionic liquids in mixtures of protic and aprotic ILs? **J.H. Davis, F. Edhegard**

**CHED 965.** Investigating reactions of coniferyl alcohol with aldehydes in acidic pyrolysis oils. **P. Speight, E.A. Stemmler**

**CHED 966.** Green Hantzsch reactions suitable for the teaching laboratory. **D. Andujar, V.J. Curfman, I.J. Levy, K. Van Kirk**

**CHED 967.** Microwave-assisted direct amidation: A green chemistry laboratory preparation. **J.L. Bilancieri, A.A. Lutz, S. Zuidema, I.J. Levy**

**CHED 968.** Evaluation of air quality sensors as a tool to educate middle school children on the environmental and social injustices resulting from exposure to diesel exhaust. **D.M. Cardoza, J. Hooper, E.J. Brush**

**CHED 969.** Bridging the educational divide between diesel use and social justice: A participatory action research approach. **J. Hooper, D.M. Cardoza, E.J. Brush**

**CHED 970.** Application of green chemistry principles to improve the efficiency of bio-diesel synthesis from waste vegetable oil: Optimizing methanol use and recovery. **P. Kurris, E.J. Brush**

**CHED 971.** Development of green chemistry metrics to assess improvements to the efficiency in the synthesis of biodiesel from waste vegetable oil. **K. Roebuck, E.J. Brush**

**CHED 972.** Applying <sup>1</sup>H NMR spectroscopy to develop a kinetic model for the transesterification of glycerol fatty acid triesters. **L. Sprague, E.J. Brush**

**CHED 973.** Surfactants with reversible linkers for micelle-facilitated organic synthesis. **K. Craig, R. Stauffer, D. Brownholland**

**CHED 974.** Green extraction of shikimic acid from star anise using solar irradiation. **D.J. Swartling, R. Chan**

**CHED 975.** Dehydration of alcohols by solar irradiation. **S.M. Amin, D.J. Swartling**

**CHED 976.** Withdrawn.

**CHED 977.** Further progress with solar Fisher esterification. **C.R. Buckner, D.J. Swartling**

**CHED 978.** Expanding imidazolium-iron ionic liquid catalysts for carbon-carbon bond formation. **J. Waddell, J. Moerdyk**

**CHED 979.** Coffee to biodiesel: A quest for green energy in the undergraduate lab. **R. Rupasinghe, A.E. Fischer**

**CHED 980.** Solar thermal decoupled electrolysis: Reaction mechanism of cobalt oxidation. **W. Prusinski, J. Grade, D. Kotter, C. Larson, R. Palumbo, J. Schoer, N. Leonard**

**CHED 981.** Towards a catalytic synthesis of substituted biphenyls. **C.E. Harris, P.L. Geisler, D.G. Burns, B. Estepa Bernabeu**

**CHED 982.** Experimental study on the vapor-phase cracking of 4-ethylguaiacol. **A. Mullery, J.N. Hoang, E.B. Ledesma**

**CHED 983.** Markovnikov hydration of alkenes using greener, alternative reagents. **I.R. Commins, E.A. Fjellstad, L.J. O'Donnell, A. Swartzel, M. Paul, I.J. Levy, K. Van Kirk**

**CHED 984.** Tagging alcohols onto polycarbonates derived from carbon dioxide and 3,4-epoxy-tert-butylbutanoate. **D. Rosenbaum, Y. Wang, D.J. Darenbourg**

**CHED 985.** Surface-active properties of bis-quaternary ammonium-sulfate Gemini surfactant-conventional ionic and nonionic surfactant mixtures. **S. Heacock, K.A. Daus**

**CHED 986.** Experimental and first principles prediction of UV-vis spectra of natural dye molecules as a function of solvent and pH. **E.A. Jarvis, S. Schuffels**

**CHED 987.** Kinetic study of a green Diels-Alder reaction between 2-furfural and maleimide. **J. Chu, M.S. Erickson**

**CHED 988.** *Endo to exo* thermal isomerization of a green Diels-Alder adduct. **M. Douglass, M.S. Erickson**

**CHED 989.** Solar thermal decoupled electrolysis: Developing a method for quantifying current efficiency. **W. Prusinski, D. Kotter, J. Grade, C. Larson, R. Palumbo, J. Schoer, N. Leonard**

## Section H

San Diego Convention Center  
Halls D/E

### Undergraduate Research Posters

#### Inorganic Chemistry

*Cosponsored by INOR and SOCED*

N. Di Fabio, *Organizer*

#### 12:00 - 2:00

**CHED 990.** Synthesis, characterization, and electrochemistry of acrylamide manganese porphyrin complexes. **A. Bevak, B. Armstrong, D.R. Powell, N. Xu**

**CHED 991.** Mesostructured surfaces for water/oil separation. **S. Martens, T.E. O'Loughlin, S. Banerjee**

**CHED 992.** Structural characterization of the reaction products of zinc chloride and phenylenediamines. **P.L. Zick, D.K. Geiger**

**CHED 993.** Toward efficient molecular catalysis: A proposed investigation into soft-donor biomimetic complexes with V, Mo and W. **C. Samaan, A. Montgomery, J. Brown-McDonald**

**CHED 994.** Direct 2D DOSY NMR evidence for oligomer formation by transition-metal substituted polyoxotungstates in nonpolar solvents. **W. Swanson, M.M. Kozik**

**CHED 995.** DNA-binding and cytotoxicity studies of some organorhenium flufenamate complexes. **S. Parnell, S. Pramanik, S.K. Mandal**

**CHED 996.** Synthesis and characterization of a bipyridine bridged trimetallic ferrocene-ruthenium-ferrocene photosensitizing complex. **S. Muhammad, D.G. Giarikos**

**CHED 997.** Synthesis of phosphine catalyst for potential bond activation. **J.H. Murray, S. McCarthy, A.T. Radosevich**

**CHED 998.** Mechanism of simple alcohol oxidation by quinone complexes of chromium (III) ion. **L.M. Whitt, R.F. Johnston**

**CHED 999.** Treatment of triple negative breast cancer cells with photodynamic therapy using a novel water-soluble porphyrin. **J. Compton, J.E. Bradshaw**

**CHED 1000.** Synthesis and characterization of dynamic porous coordination polymers (DPCPs) supported by pyridylamide ligands. **C. Mugenzi, E. MoMoran, L. Yang**

**CHED 1001.** Synthesis and characterization of novel fluoro-bridged copper(II) complexes. **B. Johnson, L. Yang**

**CHED 1002.** Synthesis and characterization of water-soluble dinitrosyl iron complexes with amino acid derived N-heterocyclic carbene ligands. **A. Hughes, J. Janowicz, J.L. Young**

**CHED 1003.** Toward mercapto-terminated linear azulenyl and biazulenyl linkers relevant to molecular electronics. **D.V. Boe, J.C. Applegate, N.R. Erickson, M.V. Barybin**

**CHED 1004.** Synthesis & characterization of novel heterocyclic cyclodiphosphor(III)azane tungsten complexes. **B.M. Cole, I. Schranz**

**CHED 1005.** Synthesis, characterization, and cytotoxicity of a series of novel water-soluble porphyrins. **A. Hegi, J.E. Bradshaw**

**CHED 1006.** Synthesis of novel phosphonium ligands. **K.M. Gass, Y. Wang, R. Sykora, J.H. Davis, B. Wicker**

- CHED 1007.** Ru(*p*-cymene) complexes featuring a redox non-innocent  $\alpha$ -iminopyridine and  $\alpha$ -aminopyridine ligand. **A. Lanquist, B. Wile, L. Wiener**
- CHED 1008.** Synthesis, characterization, and cytotoxicity of a novel water-soluble porphyrin. **J.M. Hargis, J.E. Bradshaw**
- CHED 1009.** Modular synthesis of a tetradentate HNaCNac ligand. **M.T. St. Lawrence, R. Sykora, B. Wicker**
- CHED 1010.** In search of new synthetic routes for the preparation of N-heterocyclic carbene complexes of first row transition metals. **D. Gilleland, R.M. Meier**
- CHED 1011.** Analysis of potential alcohol oxidation catalysis involving metal-quinone complexes. **B. Hubert, R.F. Johnston**
- CHED 1012.** Partial displacement of a triamine ligand from platinum (II) by guanosine 5'-monophosphate. **A.M. Wright, K. Williams**
- CHED 1013.** Coordination chemistry of divalent group 12 thiocyanate complexes containing 2,4'-bipyridine. **L.B. Walter, P.M. Secondo**
- CHED 1014.** Luminescent metal-organic frameworks containing metal complexes of ruthenium, osmium, or rhenium: Framework structure and photophysical properties. **L.A. Hemler, R.C. Castro, J.A. Lenkiewicz, K. Kneas, J.A. Rood**
- CHED 1015.** Coordination chemistry of group 12 thiocyanate complexes with 1,4-dicyanobenzene and 1,4-ditetracyanobenzene. **W. Irrek, P.M. Secondo**
- CHED 1016.** Boronic acid electrografting precursors for the covalent modification of glassy carbon surfaces. **S.N. Doden, S.E. Shaner**
- CHED 1017.** Withdrawn.
- CHED 1018.** Microwave-assisted synthesis of 1,3-bis(picoly)benzimidazolium bromide. **T. Pham, M. Guino-o**
- CHED 1019.** Synthesis and investigation of dinuclear rhodium pincer complexes as catalysts for alkyne dimerization. **B. Morse, M. Klimes, A.S. Larsen, O. Ozerov**
- CHED 1020.** Synthesis, modification, and experimentation of Tb-mesoMOF, HKUST-1, and MOF-5. **S. Montag, M. Nivison, M. Rodriguez, Z. Mensinger**
- CHED 1021.** New Cp\* vanadium nitride complexes. **G. Risica, L.E. Shepard, N. Tsamchoe, N. Onishi, J. Niklas, J.D. Gorden, C.D. Abernethy**
- CHED 1022.** Trifluoroborates as precursors for the covalent modification of conductive substrates. **F. Mujid, S.E. Shaner**
- CHED 1023.** Oxidation of a lignin model compound by iron, manganese, and cobalt complexes of a pentadentate ligand. **K. Aletty, L. Niu, K.J. Young**
- CHED 1024.** Synthesis and structural characterization of germanium coordination complexes incorporating multidentate Schiff base ligands. **J. Pigga, J.A. Rood, C.D. Schaeffer**
- CHED 1025.** Investigating the thermal stability of DNA in the presence of metal cations by measuring DNA melting temperatures. **K.A. Heinrichs, J. Price, A. Raley, M.J. Kendrick-Murphy**
- CHED 1026.** Synthesis, characterization, and reactivity of ruthenium(II) complexes involving tris(2,2,2-trifluoroethyl)phosphite and electron-rich arene ligands and extension to N-heterocyclic carbene ligand. **P. Zdlunek, J.P. Lee**
- CHED 1027.** Silica and gold nanoparticle matrices for eDNA detector. **T. Palof, J.S. Kirk**
- CHED 1028.** Preparation of novel ligands and their related metal-organic frameworks. **J. Chavez, N.H. Erfurth, E.A. Morley, J.J. Pak**
- CHED 1029.** Synthesis of a multi-electron transfer reagent using click chemistry. **D.M. Beagan, J. Ringo, H.D. Manamperi, J.A. Krause, W. Connick**
- CHED 1030.** Reversible storage of I<sub>2</sub> via CaSDB MOF: Potential use in nuclear waste management. **K. Daly, X. Chen, A. Plonka, J.B. Parise**
- CHED 1031.** Synthesis and catalytic properties of a novel triazole based N-heterocyclic Iridium carbene complex. **E. Dalbey, S.A. Roberts, E. Rajaseelan**
- CHED 1032.** Analysis of fresco pigments and substrates by powder x-ray diffraction. **S. Miller, A. Smalley**
- CHED 1033.** Synthesis and characterization of zinc oxide micro and nanomaterials. **B. Woolsey, R.G. Harrison**
- CHED 1034.** Initial investigation on structural mimicking of the photosynthetic catalysts. **B. Long, A. Saha**
- CHED 1035.** Synthesis, structure and physicochemical characterization of I<sub>2</sub>-II-IV-VI<sub>4</sub> sulfides with potential for infrared non-linear optical applications. **M.M. Cribbs, J.A. Aitken, J.R. Glenn**
- CHED 1036.** Synthesis and characterization of diruthenium complexes and the mode of death in Hep G2 cells. **Z. Rye, R.M. Chin, K. Dhanwada, K. Fay**
- CHED 1037.** Catalytically active copper-containing aerogels. **Z.M. Tobin, A. Bechu, L. Posada, M.K. Carroll, A.M. Anderson, B.A. Bruno**
- CHED 1038.** Effect of ligand binding location on luminescence of copper-based metal-organic smart materials. **J. Meyerhofer, J.K. Vohs**
- CHED 1039.** Anion-controlled synthesis, characterization and structure of copper(II) and zinc isonicotinamide metal complexes. **E. Cavazos-Escobar, R.A. Adrian**
- CHED 1040.** Ruthenium centered organometallic catalysts for benzimidazole synthesis. **A. Romano, K.D. Sienerth**
- CHED 1041.** Use of <sup>195</sup>Pt NMR to characterize Pt-Ru heterometallic complexes in undergraduate research. **Z.J. Manning, N.C. Dopke**
- CHED 1042.** Recyclability and stability of high surface area CaO for converting algae polar lipids to biodiesel. **A. Trainor, D.S. Heroux**
- CHED 1043.** Experimental and computational studies of zinc curcuminoid complexes with duplex and quadruplex DNA. **B. Helbert, F.A. Beckford**
- CHED 1044.** Synthesis, characterization, and DNA reactivity of half-sandwich ruthenium complexes containing ferrocene curcuminoid ligands. **K. Webb, F.A. Beckford**
- CHED 1045.** Withdrawn.
- CHED 1046.** Electronic properties of GaAs microstructures grown using CSVT. **L. Strange, A. Greenaway, S.W. Boettcher, J. Boucher, M. Sharps**
- CHED 1047.** Ternary transition metal nitrides through ammonolysis: Synthesis and physical properties. **J.T. Martin, J.L. Hunting**
- CHED 1048.** Synthesis and characterization of metal complexes from pyridylimine ligands derived from amino acids and 2-pyridinecarboxaldehyde. **E. Bain, E. Sylvester**
- CHED 1049.** Comparative synthesis between glytine-nitrate process and facile co-precipitation of La- and Ce-based perovskites. **J.M. Speer, J.L. Hunting**
- CHED 1050.** Ligand-exchange reactions in biomimetic model copper(II) Schiff-base complexes. **C. Williams, J.J. Stace**
- CHED 1051.** Magnetic properties of cobalt(II) containing metal-organic frameworks. **C. Higgins, C.L. Weeks, P.M. Shand**
- CHED 1052.** Synthesis and NMR characterization of a series of quinoline-2-carboxaldehyde thiosemicarbazones and their palladium(II) complexes. **E.C. Liscic, J.R. Chen**
- CHED 1053.** Silica templated zirconia catalysts for condensation reactions. **Z. Minor, D.S. Heroux**
- CHED 1054.** Synthesis, characterization, and catalytic screening reactions of N-heterocyclic carbene-containing iron carbonyl complexes. **J. Mann, S.C. Chmely**
- CHED 1055.** Synthesis and NMR characterization of a new series of 6-bromo-2-pyridinecarboxaldehyde thiosemicarbazones. **J.T. Kimrey, E.C. Liscic**
- CHED 1056.** Synthesis and characterization by NMR of 2-acetyl-5-methylthiazole thiosemicarbazone compounds: Pd (II) complexes show inhibitory activity against microbes. **S. Grossarth, T.B. Milligan, E.C. Liscic**
- CHED 1057.** Reactivity of water-soluble iridium(I) complexes with small molecules. **S.H. Schreiner, J. Knapp**
- CHED 1058.** Absorbance constant determination and kinetic study of copper (II) phenanthroline complexes. **M. Solomon, S.P. Watton**
- CHED 1059.** Investigation of the thermal decomposition of *cis*-dicarbonylbis(dioorganodithiocarbamato)iron(II) using TGA/FTIR and density functional theory. **E. Hodel, B. Szeligo, J. Fuller, J. Coffield**
- CHED 1060.** Soft donor thioamide ligands derived from 1,10-phenanthroline-2-carboxylic acid, and 1,3-dipicolinic acid and analogs for separation of actinides (An) from lanthanides (Ln). **I.F. Chapple, I. Lehman-Andino, J. Jhon, K. Kavallieratos**
- CHED 1061.** Development of aerogel-plateform oxygen sensors for optical measurement in flow-through applications. **N. Hawthorne, M.K. Carroll, A.M. Anderson**
- CHED 1062.** Synthesis and reactivity of covalent ruthenium complexes with 5'-guanosine monophosphate. **S.H. Schreiner, G. VanEck**
- CHED 1063.** Synthesis, characterization, and electrochemical studies of a ruthenium organometallic complex. **M. Fleming, K.D. Sienerth**
- CHED 1064.** Bis-thioamide ligand derived from *o*-phenylenediamine as an extraction-based optical sensor for toxic metals. **O.E. Fernandez, M.F. Alvarado, B. Venegas, Y. Chiu, K. Kavallieratos**
- CHED 1065.** Ligand exchange reactions of an enzyme-mimic Schiff-base copper(II) complex. **B. Rose, S. Colling, S. Williams, J.A. Krause, J.J. Stace**
- CHED 1066.** Synthesis and properties of carbide Bucky paper. **K.E. Madsen, B.M. Leonard**
- CHED 1067.** Reactions of 1,2-bis[(2,4,6-trimethylphenyl)imino]acenaphthene (mes-BIAN) with vanadium-containing compounds. **N. Tsamchoe, C.D. Abernethy, J.D. Gorden, J. Niklas, G. Risica, N. Onishi**
- CHED 1068.** Synthesis of cobalt-iron bimetallic nitric oxide complexes as potential water-soluble antibacterial agents. **B. Enzenauer, T. Lin, J.L. Young**
- CHED 1069.** Optimizing the synthesis of low-symmetry ABAB phthalocyanines. **R. English, P. Chrysostomidou, C. Mix, M. Schmelzer, T. Gardner**
- CHED 1070.** Polymer stabilized iron phosphine complexes for the selective removal of nitrogen from natural gas streams. **B. Doherty, R. Gustafson, B. Han, J.W. Gohdes**
- CHED 1071.** Optimizing the synthesis of luminescent lanthanide(III) complexes through microwave technique. **B.T. Bustrom, M. Guino-o, A. De Bettencourt Dias**
- CHED 1072.** Synthesis of a ligand scaffold for bimetallic catalytic hydroformylation. **M. Schoenberger, E. Llabani, R.J. Rosso**
- CHED 1073.** Synthesis of nickel and iron complexes with amino acid derived Schiff base ligands. **S. Caddies, E. Sylvester**
- CHED 1074.** Synthesis and characterization of MOF-supported NHC catalysts. **W. Schumacher, M. Mathews, S. Larson, C. Lemmon, K. Campbell, B. Crabb, B. Chicoine, L.G. Beauvais, M.C. Perry**
- CHED 1075.** Use of powder x-ray diffraction to identify trace amounts of cosmetics on textiles. **R. Hudson, A.L. Smalley**
- CHED 1076.** Synthesis and characterization of a N-heterocyclic carbene pincer type ligand with glycine side arms and the corresponding cobalt complex. **B. Kawamala, J.L. Young**
- CHED 1077.** Effects of the iron-zinc ratio on the formation of a phosphophyllite coating on steel. **R. Perdue, A.L. Smalley**
- CHED 1078.** Physical characterization of organically modified polyoxometalates through Langmuir-Blodgett deposition and fluorescence microscopy. **J. Perryman, E.J. Atkinson**
- CHED 1079.** Synthesis and characterization of [Rh(bopy)<sub>2</sub>(dppz)]<sup>3+</sup> (bopy = 2-benzoylpyridine): A new potential metal-organic intercalator possessing a mixture of nitrogen and oxygen donors. **M.R. Norton, S.C. Haefner**
- CHED 1080.** Synthesis and characterization of dipyrzinyloformamide and its reactions with d<sup>8</sup> M(II) halides (M = Pd and Pt). **B.L. Mash, S.C. Haefner**
- CHED 1081.** (Metal-ligand)-directed organic synthesis of drug molecules from natural sources. **J. Garcia, J.F. Eubank**
- CHED 1082.** Tuning excited state properties of Ru(II) complexes with a 4-substituted pyridine ligand. **J. Hale, A.T. Vu, D.A. Santos, R.N. Garner**
- CHED 1083.** Determination of catalytic activity of P<sup>in</sup>BIM and various boranes for CO<sub>2</sub> reduction. **F. Monzon, K. Mandla, B.R. Barnett, J.S. Figueroa**

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

CHED **1084**. Effect of a facial terminal ligand on a bimetallic asymmetric ruthenium(II) complexes' DNA interactions. **A. Abdulkarim, M. LaCorte, J. Osei-Fosu, K. Thomas, M.T. Mongelli**

CHED **1085**. Synthesis and characterization of Cp\*Ir(III) diphenyl complexes. **N. Wolford, E.A. Ison**

CHED **1086**. NMR studies of the dielectric effect of solvents on counterion association. **C. Jamshidi, A. Marts, D.L. Tierney**

## Section H

San Diego Convention Center  
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### Undergraduate Research Posters

#### International Research Experience for Undergraduates

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1087**. DNA origami as a scaffold for ordered protein assembly. **A. Osunsade, Y. Tokura, Y. Wu, T. Weil**

CHED **1088**. Bimetallic alloys: A theoretical study of hydrogen adsorption on Ag/Pt(111) alloys. **E. Bringley, J. Mueller, T. Jacob**

CHED **1089**. Understanding fungal metabolism using chemically modified substrates. **L. Qiao, R. Cox**

CHED **1090**. Synthesis of argyran B analogue for SAR studies. **L. Lotti Diaz, P. Engel Garcia, M. Kalesse**

CHED **1091**. Claisen rearrangement under supercritical conditions. **S. Dickinson**

CHED **1092**. Research towards the total organic synthesis of (+)- and (-)-parthenolide in Jena, Germany. **B. Snyder, R. Freund, H. Arndt**

CHED **1093**. Microfluidics and emulsion for sub-micron PLGA self-assembly. **C. Dobson, M. Leiske, S. Schubert, U.S. Schubert**

CHED **1094**. Molecular model for interactions between metal oxides and covalently-linked photosensitizers for hydrogen evolution systems. **W.C. Howland, S. Schönweiz, C. Streb**

CHED **1095**. Arsenic removal from water by treated cellulose fibers. **S. Padgaonkar, S. Vallyaveetil**

CHED **1096**. Modulated hydrothermal synthesis and optimization of Hf/Zr-fumarate metal-organic frameworks. **I. Castano, D. Zhao, Z. Hu**

CHED **1097**. Metal-organic framework-derived electrocatalyst for oxygen reduction. **J. Cavanaugh, Y. Qian, D. Zhao**

CHED **1098**. Investigation of surface enhanced Raman scattering activity in silver-coated magnetic nanoparticles. **M. Hayes, D. Graham, S. Mabbott**

CHED **1099**. Development of new materials for bulk heterojunction solar cells. **S. Chapman, N. Findlay, P. Skabara**

CHED **1100**. Heterogeneous palladium-catalyzed catellani reaction in a sustainable media. **A.M. Kahler-Quesada, L. Vaccaro, S. Santoro**

CHED **1101**. Effect of concentration, solvent, and nanoparticle concentration on the photophysical behavior of 9ACA. **A. Davis, G. Zampini, L. Latterini**

CHED **1102**. Expanding human perception of electromagnetic radiation to the ultraviolet region through fuzzy logic photochromic systems. **A.L. Rightler, P. Gentili**

CHED **1103**. Visible light-driven water oxidation by molecular iridium catalysts. **K.R. Ellingwood, I. Corbucci, A. Macchioni**

## Section H

San Diego Convention Center  
Halls D/E

### Undergraduate Research Posters

#### Medicinal Chemistry

*Cosponsored by MEDI and SOCED*

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1104**. Synthesis of hydroquinone derivatives as inhibitors of sarco/endoplasmic reticulum calcium ATPase (SERCA). **R. Kempton, T.A. Kidd, S. Laurenceau, S.F. Paula**

CHED **1105**. Investigation of the effect pH has on the release mechanism of naproxen from ethyl cellulose/microcrystalline cellulose beads. **F.C. Mayville, T.A. Cadmus**

CHED **1106**. Extraction, isolation, and antioxidant analysis of annonacin from fruit of the North American pawpaw. **Asimina triloba**. **F.C. Mayville, E.C. Charamut, C.R. Kovaleski**

CHED **1107**. Scaffold-hopping of multicationic amphiphiles yields new classes of antimicrobials. **M. Mitchell, A. Iannetta, M. Jennings, M. Fletcher, W.M. Wuest, K.P. Minbiole**

CHED **1108**. TNF- $\alpha$  is increased following bilateral cavernous nerve injury, leading to enhanced recruitment of neurotoxic M1 macrophages. **H. Matsui, N.A. Sopko, A.A. Reinhardt, M. Kates, D.M. Lough, X. Liu, M. Albersen, J.L. Hannan, T.J. Bivalacqua**

CHED **1109**. Synthesis of dimeric binders of the GRB2 SH2 domain. **J.J. Gladfelder, C. Arpin**

CHED **1110**. Solvolytic mechanisms of common  $\beta$ -keto carbonyl compounds. **A. Bilbrough, M.J. D'Souza**

CHED **1111**. Synthesis and characterization of three oleoyl-PEG orthoester micelles for drug delivery. **F.M. Ippoliti, L.E. Prevette**

CHED **1112**. Design of ionic liquids as topical antimicrobial materials. **C. Migliori, K. Merrett, A. Young, J. Melessa, C. Fordham, D. Stapleton, J. Aklinski, D. Warner, A.T. Koppisch, D. Fox, R.E. Del Sesto**

CHED **1113**. Synthesis of a dendritic scaffold with a dual functionality on the surface. **U.G. Huynh, J. Sharkey, C.Y. Lee**

CHED **1114**. Development of a novel synthesis for inhibitors of GRB7. **N. Holmberg-Douglas, C. Arpin**

CHED **1115**. Hydrophobic aspirin analogues for better delivery. **T.A. Ruiter, A. Kumar, B. Banik, A. Kalathil, S. Dhar**

CHED **1116**. Towards the synthesis of erythrin H and its analogs. **T. Berns-Moores, V. Chan, V. David, G. Jump, M. Carranza**

CHED **1117**. Animal models of visceral pain: Challenges and opportunities. **M.K. Murie, E. Mohammadi, B. Greenwood-Van Meerveld**

CHED **1118**. Synthesis and phototoxicity of a novel water-soluble porphyrin-chalcone complex. **R.E. Tucker, J.E. Bradshaw**

CHED **1119**. Progress towards structure-based *de novo* design and synthesis of small molecule inhibitors of protective antigen (PA): An anti-toxin approach for combating anthrax. **K.E. Jones, E. Watkins, A.E. Philip, A. Castleman**

CHED **1120**. Synthesis of APOBEC3 inhibitors based on high-throughput screening hits. **S. Breunig, M.E. Olson, D. Dana, M. Li, R.S. Harris, D.A. Harki**

CHED **1121**. Evaluation of the antioxidant properties of 4,7-disubstituted coumarin derivatives. **J.K. Murray, P. Ross**

CHED **1122**. Synthesis of indazolones and pthalimides as potential cyclin dependent kinase inhibitors. **V.C. Miles, F.M. Joseph, N. Pham, R. Schroeder, M. Iqbal, J. Sridhar**

CHED **1123**. Design and synthesis of novel 1,2-dihydroquinazolin-2-one derivatives for the treatment of human African trypanosomiasis. **T. Pham, M. Walden, E. Krakoff, B. Kopec, R. Gonzalez-Diaz, M. Navarro, M.P. Pollastri, A.B. Dounay**

CHED **1124**. Analysis of PPAR1 interactions with cannabinoids. **S. Heslep, J. Little, L. Hensley, M.D. Perry**

CHED **1125**. Expression, purification, and analysis of the biological activity of human low molecular weight protein tyrosine phosphatase. **S. Tinucci, H.V. Jakubowski, E.J. McIntee**

CHED **1126**. Withdrawn.

CHED **1127**. Protein networks in Alzheimer's disease. **T. McGee, L. Rattanavong, O. Alzate**

CHED **1128**. Synthesis and biological evaluation of a library of chalcones as cytotoxic agents. **Z. Tucker, A. Krzysiak**

CHED **1129**. Synthesis and biological testing of phosphonate inhibitors for human low molecular weight protein tyrosine phosphatase isoform B. **R. Flynn, H.V. Jakubowski, E.J. McIntee**

CHED **1130**. Enzymatic and bacterial activity of fungal strains isolated from *Alpinia zerumbet*. **J. Rosa-Vega, D. Pacheco, G.I. Orta, C.A. Robert, W. De Jesus-Bonilla**

CHED **1131**. *Alpinia zerumbet* as antibacterial and antifungal agent. **N. Millan-Serrano, A. Tomassini, E. Lopez, W. De Jesus-Bonilla**

CHED **1132**. Anti-hyaluronidase activity of various methanolic plant extracts and implications in neurodegenerative repair. **J. VanCampen, A. Hoffman**

CHED **1133**. Synthesis of aryl-guanidino spermidine conjugates as potential trypanothione reductase inhibitors. **J. Lesh, T. Utz, J. Fodero, M.C. O'Sullivan**

CHED **1134**. Structural studies of *Salmonella enterica* NAD kinase: An investigation of a novel antibiotic target. **M. Cyr, P.A. Sims**

CHED **1135**. Identification of epigenetic drugs that possess lung anticancer activity from a series of 13 analogues of JIB-04. **N. Phan, A. Tran, E.D. Martinez**

CHED **1136**. Structure activity relationship (SAR) studies of a selective reactive oxygen species (ROS) activated agent. **M.K. Sira, A. Kizhakkekara Vadukoot, E.J. Merino**

CHED **1137**. Synthesis and evaluation of aminomethylphenols as anti-malarial agents. **A. Abdullaeva, A. Tummala, M. Singh, S. Arnett, C. Eickhoff, F. Sverdrup, M.J. Meyers**

CHED **1138**. Prodrug approach to radionuclide decorporation. **J. Mosley, C. Niedeck, H. Charafeddine, G. Ramey, N. Kirkman, M. Ibrahim, B. Wilks, K.J. Friedrich**

CHED **1139**. Preparation of antimicrobial amphiphiles derived from polyamine dye scaffolds. **S. Duggan, M. Jennings, M. Fletcher, W.M. Wuest, K.P. Minbiole**

CHED **1140**. Synthesis and preliminary biological evaluation of analogues of a naturally occurring diarylheptanoid. **R. McLane, M. Boyle, J. Mester, A.J. Onorato**

CHED **1141**. Biased allosteric modulators for mGluR5. **C. Poparad-Stejar, B. Curtis, A. Abdallah, S. Koh, M. Hampton, K.J. Friedrich**

CHED **1142**. Intentional mistakes: Synthesis and evaluation of tautomericly ambiguous nucleosides as potential antiviral agents. **D.A. Ha, W.R. Fernandez, V.K. Dunlap**

CHED **1143**. Conjugation inhibitory activity of alkyonic fatty acids. **J. Mooney-Garozzo, C. Esquelin, N. Vazquez-Moreno, Y. Rivera-Torres, C. Morales-Guzman, J. Rodriguez, F. De La Cruz, N.M. Carbalreira, D.J. Sanabria Rios**

CHED **1144**. Chiral histone deacetylase inhibitors: Synthesis and biological evaluation. **A.J. Onate, J. Tucker, E. Hogle, T.D. Do, F.S. Thowfeik, E.J. Merino, L. Ma**

CHED **1145**. Extraction of antibacterial substance from *Cinchyra alloclada*. **B. Hipple, J.B. Easter**

CHED **1146**. Comparison of the anticancer effects of free vs. lyposome encapsulated bilberry extract. **S. Thibado, J. Thornthwaite, T. Ballard, B. Goodman**

CHED **1147**. Design, synthesis, and evaluation of N,N'-diarylurea complexes as next-generation inhibitors of the bacterial enzyme MTN. **J.H. Thurston, L. Wayment, N.M. Hunter, P. Erstad, D. Xu, K. Cornell**

CHED **1148**. Progress towards the synthesis of a novel trifluoromethyl substituted aurone as a promising inhibitor of cyclooxygenase-2 activity. **M. Polk, S. Forbes-Pentecost, C.J. Mills**

CHED **1149**. Degradation of non-natural amino acid containing peptides capping gold nanoparticles by non-specific proteases. **N. Porter, M.A. Fisher**

CHED **1150**. Determination of the decomposition kinetics of doxorubicin in aqueous solution. **E. Yeiser, E. Csuhai**

CHED **1151**. Synthesis of a potential inhibitor of type IV prelinin peptidase with a reduced amide functionality. **E.A. McGurk, P.W. Baures**

CHED **1152**. How HuR and CP1 are affected by KRas and stressors in pancreatic cancer cells. **M. Gurski, P. Campbell**

CHED **1153**. Improving activity of a fatty acid synthase inhibitor by structural mimicry. **E.M. Dunkley, L.E. Lupien, W.B. Kinlaw, P.W. Baures**

CHED **1154**. Analyzing the effects gestational exposure to trichloroethylene on the development of autoimmune disease. **H. Daniel, R. Lee, D. Barnette, K. Gilbert**

CHED **1155**. Acylphloroglucinols from an acetone leaf extract of *Hypericum densiflorum*. **J. Bixler, A. Smith, J. Kizina, G.E. Henry**

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- CHED **1156.** Chemistry of an hexane extract of *Hypericum densiflorum*. J. Kizina, J. Bixler, A. Smith, G.E. Henry
- CHED **1157.** Design and synthesis of metal-chelating peptoids for the treatment of Alzheimer's disease. J. Hamati, E. Gersz, Y. Kim, S.C. Young
- CHED **1158.** Synthesis of a new palladium 2-acetyl-6-methoxy-pyridine thiosemicarbazone (AMOPY-TSC) complex: NMR characterization and MIC studies. A.M. Barnes, M.K. Monroe, E.C. Lisic
- CHED **1159.** Comparison of a series of 2-acetyl-6-methoxypyridine (AMOPY) thiosemicarbazone ligands and their Cu(II) complexes. M.K. Monroe, A.M. Barnes, E.C. Lisic
- CHED **1160.**  $\beta$ -Cyclodextrin mediated controlled release of naproxen from hydroxypropyl methacrylamide/poly(vinylpyridine) hydrogels for targeted delivery. J. Athelstone, D. Fish
- CHED **1161.** Synthesis and NMR characterization of the complete series of 2-acetyl-6-bromopyridine thiosemicarbazone ligands: The [Cu(ABrPy-TCS)Cl] complexes inhibit growth of gram positive bacteria. T.B. Milligan, J.T. Kimrey, E.C. Lisic
- CHED **1162.** Probing the molecular mechanism of pancreatic antiproliferative agents derived from natural product templates. Y.Y. Wang, E.E. Goodman, A. Webb, D. Carrico-Moniz
- CHED **1163.** Natural produce discovery through bioassay methods in *Ilex decidua*. K. Gaiser, M.J. Campbell
- CHED **1164.** Synthesis of novel flavonoid derivatives as acetylcholinesterase inhibitors for the treatment of Alzheimer's disease. J. Minnick, J. DePhillips, S. Martin, C.J. Mills
- CHED **1165.** Examination of bioactivity in *Croton capitatus*. M. Bell, M.J. Campbell
- CHED **1166.** Synthesis and testing of novel compounds to fight the parasitic disease leishmaniasis. E. Zywot, A.A. Farahat, A. Abdelhameed, D.W. Boykin, K. Werbovetz
- CHED **1167.** Polyphenolic compounds from cabernet franc (*Vitis vinifera*) fall leaves. J. Heneks, R. Force, J. Kizina, M. Bruer, G.E. Henry
- CHED **1168.** Synthesis of novel heterocyclic chromone analog libraries and evaluation of their biological activity. A. Delawder, E. Segrist, Y. Wang
- CHED **1169.** Probing local environments in co-solubilized solutions of vancomycin and piperacillin/tazobactam. A.A. Rivera Hernandez, R.N. Mason
- CHED **1170.** Development of a selective inhibitor for human  $3\beta$ -hydroxysteroid dehydrogenase 1 ( $3\beta$ HSD1). C.M. Will, V.L. Mack, J.L. Thomas, K.M. Bucholtz
- CHED **1171.** Synthesis of  $C_4$ -substituted aminopyrrolidines. H.E. Peredo, A.T. Bayasi, C. Santee, Z. Woydziaik
- CHED **1172.** Synthesis and cytotoxic evaluation of ethyl amino and heteroaromatic ether analogues of naphthoquinone. K.P. Liles, A. Delawder, E. Segrist, M. Manpadi
- CHED **1173.** Synthesis and evaluation of libraries of metalloenzyme inhibitors. P. Glatt, C. Perez, S. Cohen
- CHED **1174.** Synthetic paths towards selected analogues: Assembling anti-viral 2,3-bis-aryl-3-chloropropenal skeleton and further transformations. R.C. Joseph, T.L. Perry
- CHED **1175.** Design, synthesis and biological evaluation of sulfonamidobenzimidazole derivatives as potential inhibitors of IspF. C. Voss, M.J. Rouffet
- CHED **1176.** Towards the synthesis of MTX-phenylalanine derivatives for the treatment of glioblastoma in antibody directed enzyme prodrug therapy. G. Abass, M.J. Rouffet

## Section H

San Diego Convention Center  
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### Undergraduate Research Posters

#### Nanochemistry

Cosponsored by SOCED

N. Di Fabio, Organizer

12:00 - 2:00

- CHED **1177.** Developing a sustainable catalyst: Synthesis, characterization, and catalytic application of palladium nanoparticles in carbon microsphere composites. C. Livingston, K.M. Metz
- CHED **1178.** Synthesis of metal heterostructure nanocrystals. J.R. Miller, J. Martin, B. Roman, M. Sheldon
- CHED **1179.** Surface enhanced Raman spectroscopy using silver and gold nanoparticles. I. Iradukunda, L.H. Rickard
- CHED **1180.** Molecular interactions of aryl thiols and  $C_{60}$  fullerenes in multi-component self-assembled monolayers as probed by scanning tunneling microscopy. G. Avila-Bront, K. Blanco, B. Dougherty
- CHED **1181.** Characterization of lipooligosaccharide binding to polystyrene nanoparticles. M. Timm, B. King, J. Fiegel
- CHED **1182.** Graphene oxide: A controlled reduction using ascorbic acid. D.C. Alvarez, A.H. Trusty, G.J. Mancini-Samuelson
- CHED **1183.** Directed assembly of porphyrin Coulomb islands by nanografting and click chemistry. E. Avery, A. Pawlicki, M.J. Jurow, C.M. Drain, J.D. Batteas
- CHED **1184.** Novel bridging ligands based on sugar acids for stabilizing inorganic nanoparticles. L. Allison, V.L. Kolesnichenko, G. Goloverda
- CHED **1185.** Synthesis and characterization of nickel nanoparticles in ionic liquid. O.A. Hull, E.J. Roberts, L. Wang, C.J. Kunze, N. Malmstadt, R.L. Brutchey
- CHED **1186.** Colloidal dispersions of  $C_{60}$  fullerene in mixed solvent solutions. L.D. Bienski, C. Aronson, C. Doby, C. Holt, J. Ballard, K. Morris
- CHED **1187.** Enhancement of monodispersity during the synthesis of gold nanoparticles with cyclodextrin derivatives. T. Nguyen, J. Hollingsworth, B. Mellis
- CHED **1188.** Investigation on the local environment of functionalized mesoporous silica nanoparticles using fluorescence instrumentation. D. Singappuli-Arachchige, L. Sherman, S. Manzano, I.I. Slowing
- CHED **1189.** Surface enhanced infrared absorption on optimized copper nanostructures. B. Wilde, D.A. Perry
- CHED **1190.** Stability and ordering of alkane-thiol monolayers on nanoporous gold surfaces. R.B. Chevalier, A.M. Weller, D. Patel, E.C. Landis
- CHED **1191.** Photothermal effects of biotinylated gold nanoparticles on cell viability. A. VanderWal, M. Urbaningsih, S.L. Grisales, B. Mellis, M.A. Steiger
- CHED **1192.** Antimony doped organo-lead halide perovskite nanocrystals. F. Zhu, L. Men, N.E. Gentry, A.A. White, J. Vela-Becerra
- CHED **1193.** Ligand-copper silver nanoparticles for the detection of heavy metal ions. A. Thompson, J. Zemke
- CHED **1194.** Probing the structure of new membrane-mimetic lipid nano-rings using continuous-wave EPR spectroscopy. A. Bali, A. Craig, I.D. Sahu, D. Konkolewicz, C.D. Smith, G.A. Lorigan
- CHED **1195.** Adsorption of BSA protein on  $SiO_2$  nanoparticles in aqueous solution: Impact of pH on size and zeta potential at the nanoparticle-protein interface. N.D. Diklich, B.E. Givens, V.H. Grassian
- CHED **1196.** Synthesis of layered polyoxometalate/organic polymer-coated metal nanoparticles. K. Chen, N.T. Flynn, E. McLoughlin
- CHED **1197.** Development of Pd nanostructures on infrared transparent salt plates. M. Sweere, T. Huntington, J. Chen, D.A. Perry
- CHED **1198.** Single-crystal lead halide perovskites nanomaterials: Iridazolum lead iodide and methylammonium lead trihalide alloys. A. Schrader, Y. Fu, S. Jin
- CHED **1199.** Optimization of low molecular weight organogelators for drug delivery. C. Otteson, D. Arnabilino
- CHED **1200.** Catalytic activity of Au, Ni and Au/Ni nanostructures in the reduction of p-nitrophenol. L. Bankert, J.K. Mbindyo
- CHED **1201.** Improved synthesis of diazonium gold(III) salts and their applications in gold-carbon nanoparticles. J. Ford, C.E. Mullen, A.L. Hernandez, Y. Pajouhafsar, J.J. Borski, C.R. Witkowski, A. Mohamed, H. Abdou
- CHED **1202.** Scientific study determining variables affecting metal oxide oxidation states coloring high fire ceramic art glazes. V. Willard, W.E. Schatzberg
- CHED **1203.** Use of graphene quantum dots to assist in photocatalysis. C. Dokler, S.J. Gravelle
- CHED **1204.** Generating hydrated electrons from Mn doped quantum dots. J. Estwick, D.H. Son, D. Rossi
- CHED **1205.** Encapsulation of CdSe quantum dots with silica to increase biocompatibility. A.D. Flores, J.G. Medina, J. López, O. Primera-Pedrozo
- CHED **1206.** Direct growth of MnO nanoparticles on stainless steel and their electrochemical properties. L. LeBan, C.L. Arnold, L. Meda
- CHED **1207.** Dependable and reproducible procedure for the production of atomically sharp and electrically isolated STM tips. H.R. Morgan, A. Carr, C. Cleveland, E.V. Iski
- CHED **1208.** Nanoscale investigation of thermally-stable silver halide films on Au(111). L. Jackson, J.A. Phillips, E. Lopez Quiroz, E.V. Iski
- CHED **1209.** Withdrawn.
- CHED **1210.** Surface enhanced Raman spectroscopy on optimized AgAu nanoparticles. T.E. Huntington, D.A. Perry, J. Chen
- CHED **1211.** Investigation of fabrication methods for atomically-thin 2D tungsten dichalcogenides film, heterojunctions and devices. Y. Zhang, M. Shearer, S. Jin
- CHED **1212.** Antibiotic delivery in resistant *Escherichia coli* using PEG-modified nano-graphene oxide. K. Fiocca, N. Normil, M.D. Ellison, A. Lobo
- CHED **1213.** STM studies of functionalized functionalized polyamidoamine (PAMAM) dendrimers. P. Kress, A.F. Raigoza, T.N. Jones
- CHED **1214.** Motion of methanol through single-walled carbon nanotube nanopores. S. Menges, L.M. Nebel, M.D. Ellison, M. Strano
- CHED **1215.** Use of tetracycline-functionalized single-walled carbon nanotubes to overcome tetracycline resistance in *Escherichia coli*. M. Force, M.D. Ellison, A. Lobo
- CHED **1216.** Selective growth of ZnO nanorods with applications in photovoltaics through the development of 3D printed structures. R.A. Kuntz, E. Adcock Smith, K. Roberts
- CHED **1217.** Synthesis of thermoresponsive magnetic nanoparticles by coprecipitation to improve diagnostic assays. R. Jauregui, J. Lai
- CHED **1218.** Optimization of silica encapsulation process of CdSe QD's capped with different thiol-ligands. J.G. Medina-Feliciano, A.D. Flores, M. Rodriguez-Torres, O.D. Rivera, O.M. Primera, J. Lopez-Colon
- CHED **1219.** Applications of ZnO nanorods for PV solar cells. M. Herl, E. Adcock Smith, K.P. Roberts
- CHED **1220.** Stability of solutions and colloidal suspensions of  $C_{60}$  fullerene. C. Aronson, L.D. Bienski, C. Doby, C. Holt, J. Ballard, K. Morris
- CHED **1221.** Effect of silver nanoparticles and ethyl alcohol in specimens of *Daphnia Magna*. K. Santiago Orengo, S. Vazquez Velazquez, J.J. Ramirez Domenech, L. Figueroa, M. Santiago Mercado, K. Rodriguez, E.J. Ferrer Torres
- CHED **1222.** Effects of adrenaline and silver nanoparticles exposure on *Daphnia magna*. J.J. Colon Rodriguez, M. Negron Garcia, K. Cintron Silva, G. Montanez Barreto, E.J. Ferrer Torres, J.J. Ramirez Domenech
- CHED **1223.** Influence of surface functionalization on the photothermal properties of gold nanorods. E. Cruz, A.L. Smalley
- CHED **1224.** Exploration of metal-oxide surface structure and stoichiometry in oxygen depleted nanoparticles. E.A. Jarvis, A. Garcia Taormina
- CHED **1225.** Electrochemical behavior of nanostructured nickel oxide as pseudocapacitor and battery. J. Adkins, C.L. Arnold, L. Meda
- CHED **1226.** Design and synthesis of copper oxide on stainless steel as an anode for lithium-ion batteries. J. Williams, C.L. Arnold, L. Meda
- CHED **1227.** Low pressure chemical vapor deposition of nanosized iron oxide for the anode in lithium-ion batteries. D. Phan, A. Dangerfield, C.L. Arnold, L. Meda
- CHED **1228.** Theory and modeling of metallic nanoparticles for the detection and photobleaching of cancer cells. A. Branch, J.M. Montgomery
- CHED **1229.** Doping complex oxides: Consequences for electronic structure. J.W. Jude, S. Banerjee, G. Horrocks, G.R. Waeltzig
- CHED **1230.** Hydrothermal synthesis and characterization of cobalt oxide nanoparticles. M. Duszynski, A. Simpson, A. Wanekaya
- CHED **1231.** Investigation of nanoscale oligomerization amyloid beta peptide at the gold metal and ice interface. D. Hartnett, M. Bladis, K. Yokoyama

## Section H

San Diego Convention Center  
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## Undergraduate Research Posters

## Organic Chemistry

Cosponsored by SOCED

N. Di Fabio, Organizer

12:00 - 2:00

- CHED **1232**. Total synthesis of pyropheen. H.E. Burdige, K.P. Reber
- CHED **1233**. Liquid-liquid extraction and analysis of the antioxidant, resveratrol, from various red and white wines. F.C. Mayville, E.N. Sauschuck, A.M. Myers
- CHED **1234**. Asymmetric catalysis with chiral at metal copper complexes. M. Zafferani, C. Streu
- CHED **1235**. Synthesis of key intermediates for the generation of benzoporphyrins. W.T. Darrow, T.D. Lash
- CHED **1236**. Finding the sweet spot for ternary cocrystal formation. J. Reardon, D. Adsmoind
- CHED **1237**. Synthesis of indolyl/indazolyl (N1 substituted) quinolones (C6 substituted) for study as possible anticancer/antibiotic/antimicrobial agents. M.M. Msaki, J.N. Thomforde, T.M. Trygstad
- CHED **1238**. Preparation of anticancer analogs that target metastatic breast cancer. L. Hosek, T. Soderling, K. Tawara, C.L. Jorczyk, D.L. Warner
- CHED **1239**. Synthesis of new alkyne-containing geranylgeranyl diphosphate analogues. M.A. Bruening, S. Chava, K. Suazo, M.D. Distefano
- CHED **1240**. Novel synthesis of cyclooctanoids via tandem 6-exo dig cyclization/Claisen rearrangement sequence. E. Stone, T.V. Ovaska
- CHED **1241**. Synthesis of novel biphenyl-ester gelators: The role of cholesteryl vs. methyl and ethyl esters on aggregation and gelation behavior. D. Morell, W. Roberts, C. Geiger
- CHED **1242**. Fresh Centnerzwer: Accessing inaccessible quasaracetates. J.M. Spaniol, K.A. Wheeler
- CHED **1243**. Dimerization of apocynin and its derivatives. B. Coffaro, L. Rosales, J. David
- CHED **1244**. Diastereoselectivity of the nucleophilic addition of ( $\pm$ )-menthyl-magnesium chloride with sp hybridized electrophiles. R. Maedgen, K. Tomlinson, N.S. Werner
- CHED **1245**. Substituent effects on the antioxidant potential of anthocyanidins: A computational study. T.L. Seto, B.W. Gung
- CHED **1246**. Preparation of *trans*-stilbene derivatives by palladium-catalyzed cross-coupling reaction. H. Holt, N.S. Werner
- CHED **1247**. Triggered hydrogen sulfide donors. K. Eckhart, M.D. Pluth, A. Steiger
- CHED **1248**. Reaction development of Pd-catalyzed synthesis of substituted 2-pyridones. B. McLernon, S.R. Waetzig
- CHED **1249**. Synthesis and evaluation of a tetradentate chiral cobalt (II) complex as a Lewis acid catalyst. T. Hall, C. Streu
- CHED **1250**. Technology assisted synthesis of fluoropharmaceuticals and PET ligands. H. Koota, G. Jones
- CHED **1251**. Exploration of triazole synthesis from propargylamine-derived Ugi-Smiles products. A. Hancock, S. Luesse
- CHED **1252**. Synthesis of novel 1,2,3-triazole chemosensors for detection of anions and heavy metals cations. S. Njemo, K.S. Aiken, D. Ghosh, S.M. Landge, N. Shuber
- CHED **1253**. Palladium-catalyzed synthesis of esters using a novel CO generator. B.J. Gerold, S.N. Gockel, A.J. Rago, J.E. Rossen, J. Wang, K.L. Hull
- CHED **1254**. Investigation of [5+2] cycloadditions. S. Pohani, C. Law, H.N. Gelfund, S. Willens, T. Mitchell
- CHED **1255**. DFT study of cruciform benzobisoxazole derivatives for use in OPVs. A.L. Tomlinson, D. Wheeler
- CHED **1256**. Mechanism of chlorocarbene additions to diarylcyclooctynes. V. Estes, A. Scorese, A. Nadeem, A. Urquilla, E. Dalchand, S. Tsuno, D.C. Merrer
- CHED **1257**. Role of proline in the folding of conotoxins. C.M. Fry, H.J. Harteis, M.R. Hargittai, B. Hargittai
- CHED **1258**. Synthesis of three bis(trifluoroalkyl) putrescine analogs using 95% and 100% ethanol. F.C. Mayville, E.P. Brown
- CHED **1259**. Synthesis of three bis(trifluoroalkyl) spermidine analogs using 95% and 100% ethanol. F.C. Mayville, T.A. Salim, J.G. Almocherki
- CHED **1260**. Soxhlet extraction and analysis of capsaicin from various pepper seeds and flesh. F.C. Mayville, S.J. Cavosi, J.L. Cawley, J.A. Julien
- CHED **1261**. [Cp\*<sup>+</sup>Ru]<sup>+</sup>-complexed phenol derivatives in the context of hyperpolarized <sup>129</sup>Xe NMR sensing. E. LaFrance, A.N. Ley, K.T. Holman
- CHED **1262**. Total synthesis of a serine-based analog of avenic acid. T.M. Binder, M.G. Stocksedale
- CHED **1263**. Investigation of the shape of atropisomers using dipolar couplings. E.E. Schiller, W. Carroll
- CHED **1264**. Halogen bonding arylene ethynyls in host-guest chemistry. R. Plahuta, L. Neyer, N.P. Bowling
- CHED **1265**. Room temperature, non-metal promoted formation of *N*-sulfonyl imines using iminodinanines. K.A. Scott, H.R. Morgan, J.A. Macgruder, A.A. Lamar
- CHED **1266**. Investigations into gold catalyzed amination reactions. K. Jesse, A.G. Wenzel
- CHED **1267**. Alternative methods of reductive amination in the synthesis of T-0632 analogs. E. Ambrogio
- CHED **1268**. Lithium-mediated reaction of *N*-acylimides with aldehydes: Expanding the scope to include electron-rich aldehydes. M.S. Paeth, Y.T. Sankari, J.L. Grinde, T.R. Wittman, L.I. Wurtz, P. Willoughby
- CHED **1269**. Phthalimide-catalyzed reaction of aldehydes with *N*-acylphthalimides. J.L. Grinde, L.I. Wurtz, C. Tan, M.S. Paeth, T.R. Wittman, Y.T. Sankari, J. Scanlon, P. Willoughby
- CHED **1270**. Cyclization of alkyne containing amines to aromatic heterocycles. G. McCormick, J.A. Jaye, E.H. Fort
- CHED **1271**. Curious case of Bader's bond paths: A computational study of congested hydrogen-hydrogen interactions through the calculation of experimentally measurable parameters. C. Berti, A.J. Shusterman, K. Martin
- CHED **1272**. Synthesis of *S* -(+/-)-lycoperdic acid. J. Singh, R.W. Denton
- CHED **1273**. Synthesis of flavonoids in room temperature ionic liquids. C. Johnson, R.N. Manchanayakage
- CHED **1274**. Synthesis and characterization of novel chiral ionic liquids and ionic liquid polymers. J. Perry, R.N. Manchanayakage
- CHED **1275**. GC-MS determination of phytosterol concentrations in dried mushrooms. S. Quint, T.W. Nalli, A. Overgard
- CHED **1276**. Synthetic methodology studies on the synthesis and reactions pyrazolidone-derived azomethine imines. T. Bader, W. Pugh, C. Jasperse
- CHED **1277**. Testing the limits of intramolecular halogen bonding. A.B. Perez, E.R. Robinson, D. Widner, E. Bosch, N.P. Bowling
- CHED **1278**. Synthetic studies on squamostanin C. M. Caporello, R. Walsh, K.J. Quinn
- CHED **1279**. Progress towards a catalytic method for generating imine nucleophiles. S.M. Mitchell, A.E. Hoffman, C.E. Taylor
- CHED **1280**. Ferrocenyl chalcones based scaffolds containing heterocyclic moieties as potential antimalarial agents. A.M. Alsina-Sanchez, S.M. Delgado-Rivera, I. Montes-González, A.R. Guadalupe-Quiñones, E. Colón-Lorenzo, A. Serrano
- CHED **1281**. Transition metal complexes of 4,4'-bipyridine/1,2-bis(2'-pyridineethynyl) benzene hybrids. C. Branham, N.P. Bowling
- CHED **1282**. Generation and study of trap-zeoidal arylene ethynylene complexes. H. Vang, Z. Driscoll, E.R. Robinson, E. Bosch, N.P. Bowling
- CHED **1283**. Synthesis of diamino multiphenol ligands using the Mannich condensation. J.R. Farrell, N.J. Maniatis, M.A. Wallace
- CHED **1284**. Organocatalytic debenzoylation of secondary amines. B. McLernon, M.A. Leon, M.D. Clift
- CHED **1285**. Synthesis of aza-Diels-Alder products. J. Wolfgang, D.P. Predecki
- CHED **1286**. Fluorescent cucurbituril. A. Grice, W. Mobley, A.R. Urbach
- CHED **1287**. Solvent reactions of lauryl chloroformate. M. Toseef, M.J. D'Souza
- CHED **1288**. Synthesis of disubstituted pyrazoles by I<sub>2</sub>- and Br<sub>2</sub>-mediated oxidative C-N bond formation from  $\alpha,\beta$ -aldehydes and arylhydrazines. G. Thomas, D. Fish
- CHED **1289**. Towards water soluble BODIPY dyes. A.L. Cantu, S. Abeywardana, M.P. Schramm
- CHED **1290**. Facile synthesis of chiral 5-substituted 1,3-oxathiolanes. T. Ryan, F. Robertson
- CHED **1291**. Preparation of tripyrrane intermediates for the synthesis of *N*-methylbenzocarbaporphyrins. A. Latham, T.D. Lash
- CHED **1292**. Crystal structure comparison of sulfisomidine and sulfamethazine cocrystals with various benzoic acids. S.H. Douglas, D. Adsmoind, K.A. Wheeler
- CHED **1293**. Antimicrobial properties of lavender and cinnamon derivatives. K.L. Scrudders, C. Chandler, N. Beres
- CHED **1294**. Rapid access to 2-substituted tetrahydrothiophenes. I. Nag, F. Robertson
- CHED **1295**. Synthesis of transition state analogs for application in Baeyer-Villiger enzyme mimics. I. Murray, F. Robertson
- CHED **1296**. Novel surface catalyzed cyclopropagation in mechanochemical synthesis. D. Leslie, L. Chen, M.G. Coleman, J. Mack
- CHED **1297**. It's just a phase: Visibly-switchable liquid crystals. S. Cordero, A. Kinge, K. Grabias, L. Lam, P. Cohn
- CHED **1298**. Efforts towards the formal synthesis of laureatin. A. Chamberland, D. Chennamadhavuni, A.R. Howell
- CHED **1299**. One-pot sequential conversion of aldehydes to *N*-alkyl hindered amides. R.C. Mebane, R. Cecil
- CHED **1300**. Synthesis of the suspected biologically active portion of teixobactin. M. Audi, J. Smyth, J.T. Ippoliti
- CHED **1301**. Matrix isolation investigation of a benzothiazolyl carbene. S. Lucas, R.S. Sheridan, R. Ghimire
- CHED **1302**. Synthesis and characterization of monosubstituted ferrocenyl chalcones salts derivatives: Study of their electrochemistry and antibacterial properties. G.E. Pérez Ortiz, S.M. Delgado-Rivera, Y. Rivera-Torres, R. Gutierrez, D.J. Sanabria-Ríos, A.R. Guadalupe-Quiñones, I. Montes-González
- CHED **1303**. Halogenation of pyrazoles with NaX and Oxone® and progress toward the total synthesis of withasomnine. M.R. Jensen, J.A. MacKay
- CHED **1304**. Synthesis of a 1-aza-9-crown-3-substituted coumarin for fluorescence living cell sensing of metal ions. C.J. Forsythe, X. Zhang, D. Nutbrown, R. Mgonigal, K. Schwinghamer, S. Claridge
- CHED **1305**. Core-substituted naphthalene diimide derivatives in donor-acceptor columnar liquid crystals. L. Abocado, J.J. Rezek
- CHED **1306**. Synthesis of analogs of the proteasome inhibitor belactosin A. N.K. Dunlap, Z. Fitzsimonds, A. Stephenson
- CHED **1307**. Effects of heating on the molecular structure of amber. T.V. Nguyen, A.J. Levy, N.R. Rueb, J.B. Lambert
- CHED **1308**. Synthesis of 4-acyl-5-thiopyrazolones: A comparison of synthesis methods. A. Ashburn, J.C. Easdon
- CHED **1309**. Synthesis and characterization of a new selenocysteine derivative. A. Schroll, A. Sasuclark
- CHED **1310**. Accelerated Eschenmoser coupling reaction using mechanical force. S. Huang, S.R. Hussaini
- CHED **1311**. Kinetic examination of the impact of cyclopentadienone substitution in a series of iron catalysts. K.P. Fodale, A.R. Mahoney, T.W. Funk
- CHED **1312**. Convergent synthesis of a photocleavable linker for the purification of GlcNAcylated proteins. T.M. Sadka, K.R. Mrugalski, T.W. Funk
- CHED **1313**. Comparative investigation of "student-friendly" synthetic routes to prepare 2,2'-bipyridines as precursors for Ru-complexes. B. Aukshi, C.M. Burns
- CHED **1314**. Exploring oxidative cyclizations of diols to lactones using iron catalysts. R.I. Meador, T.W. Funk
- CHED **1315**. Development of synthetically available functional groups on 3D printed objects. M.B. Bolter, N.P. Mulready, C.E. Stilts
- CHED **1316**. Differentiating Brazilian cachaças using peptidic-based sensors. E. LeBovidge, M. Winkler, D. Rago, B. Schumm, M. Telles, K. Maknejiia, D. Portillo, M. Ramirez, E. Ghanem, E.V. Anslyn
- CHED **1317**. Chiral ketone and iminium ion catalysts for alkene epoxidation. K.R. Overly, S. Goralski
- CHED **1318**. Synthesis of pyridone ligands and iron precursors for the development of iron-based hydrogenation catalysts. B. Hanscam, L. Boisvert
- CHED **1319**. Synthesis and characterization of novel dithiocarbamates. V.L. Hall, S. Hansknecht, M.E. Railing

- CHED 1320.** Strategies towards the total synthesis of froidsin D via 5-*exo dig* cyclization/Claisen-rearrangement sequence. C.L. Robinson, T.V. Ovaska
- CHED 1321.** Synthesis of peptide-linked metal chelators: Molecular disruptors for amyloid- $\beta$  aggregation. M.D. Cundiff, L.T. Rodgers, K. Pickin
- CHED 1322.** Novel library synthesis of xanthogluos. J.I. Garcia, Z. Woydziak
- CHED 1323.** Syntheses and kinetic studies on the Bergman cyclization of diethynylquinoxaline isomers. Z.J. Tippins, B.F. Gherman, J.D. Spence
- CHED 1324.** Synthesis and evaluation of phenylglycine-derived heterocycles as anti-oxidants. B. Maki, M. Perea
- CHED 1325.** Utilization of nucleobase interactions to develop guanosine hydrogels and supramolecular polymer hybrids. G. Gilyot, M. Porter, C.M. Lawrence
- CHED 1326.** Biomimetic synthesis of pyrrole-based natural products. B. Maki, D. Pino
- CHED 1327.** Utilization of nucleobase hydrogen bonding interactions in supramolecular polymers: Synthesis of cytidine components. M. Porter, G. Gilyot, C.M. Lawrence
- CHED 1328.** Antioxidant heterocycles derived from alanine. B. Maki, K. Molinar
- CHED 1329.** Structural elucidation of novel pyrrolizidine alkaloids from cacaoid Asteraceae. D.A. Morales, C.R. Barton, A.C. Shreve, M.E. Hillman, R.B. Kelley
- CHED 1330.** Aiming for ferrocenyl epoxide derivatives to explore their biological potential as anticancer compounds. J. Davila, J.C. Aponle-Santini, I. Montes
- CHED 1331.** Palladium-catalyzed decarboxylative dearomatization. J.S. Compton, S.N. Mendis, J.A. Tunge
- CHED 1332.** Development of a novel undergraduate experiment: Using decomposition of DMF to facilitate an  $S_NAr$  reaction. D. Chapman, J. Sorrentino, J.I. Garcia, E. Diller, Z. Woydziak
- CHED 1333.** Synthesis of degradation products of clothianidin, imazosulfuron and benzobicyclon in the evaluation of their use in California rice fields. L.N. Rubottom, T. Schempp, D.B. Ball
- CHED 1334.** Synthesis of tricyclic compounds with a cantharidin-like pharmacophore via Diels-Alder addition in aqueous solution. A.O. Spengler, G.D. Bennett
- CHED 1335.**  $\beta$ -Proline-derived chiral auxiliaries. M. Rashed, C. Hariskos, T. Vattadi, K.J. Friedrich
- CHED 1336.** Investigation on palladium-catalyzed  $\alpha$ -heteroarylation of ketones. N. Johnson, T.D. Do, L. Ma
- CHED 1337.** Synthesis of G-quadruplex macrocycles. J. McCallum, L. Thurlow, S. Lardy
- CHED 1338.** Thiophene rings as semiconductor building blocks. K.S. Yamaguchi, K. Namjuyuan
- CHED 1339.** Exploring methodologies for the synthesis and characterization of 1,1'-symmetric ferrocenyl chalcones from 1,1'-diacetylferrocene. N.E. Caldero-Rodríguez, I. Lehman-Andino, I. Montes-González
- CHED 1340.** Synthesis, characterization, and toxicity studies of chlorinated paraben derivatives. K. Pate, C. Janson, A. Schaeffer
- CHED 1341.** Rapid synthesis of *N*-(4-*t*-butylbenzyl)-*N*-methylformamide. S. Park, L.I. Bobyleva, M.M. Bobylev
- CHED 1342.** Pd<sub>2</sub>L<sub>4</sub> supramolecular cages as drug delivery agents. L. Diga, M.P. Schramm
- CHED 1343.** Effects of extraction methods and concentrations on the different ratios of neral to geranial in lemongrass essential oils. S. Mize, M.C. Koether
- CHED 1344.** Selective neurotransmitter transport using calixarenes. J.L. Collins, S. Roshandel, A. To, A. Fujii, M.P. Schramm
- CHED 1345.** Rapid synthesis of *N*-methyl-*N*-(1-naphthylmethyl)formamide. H. Lee, L.I. Bobyleva, M.M. Bobylev
- CHED 1346.** Reaction of dihydroxyacetone and glycolaldehyde with prebiotically relevant minerals under aqueous conditions. K. Watson, C. Crake, V.P. McCaffrey, N. Zellner
- CHED 1347.** Synthesis of fluorinated rhodamine analogs. J. Sorrentino, Z. Woydziak
- CHED 1348.** Evidence for the generation of *p*-diphenylquinodimethane: A Biphenyl-based reactive *p*-quinodimethanes. C. Hayes, S.P. Lorimer
- CHED 1349.** Rapid synthesis of *N*-(2,4-dichlorobenzyl)-*N*-methylformamide. J.A. Collins, L.I. Bobyleva, M.M. Bobylev
- CHED 1350.** Rapid synthesis of *N*-(3-indolylmethyl)-*N*-methylformamide. J. Torgunrud, L.I. Bobyleva, M.M. Bobylev
- CHED 1351.** Comparison of synthetic methods for copper(II)-catalyzed fluorinated triazoles. L.F. George, B.M. Tracey, A. Duensing, A.M. Schoffstall
- CHED 1352.** Rapid synthesis of *N*-(3-indolylmethyl)acetamide. B.M. Hatfield, L.I. Bobyleva, M.M. Bobylev
- CHED 1353.** Solvent effect on the regioselective synthesis of 3,4- versus 3,5-disubstituted isoxazoles. P. Rahman, R.W. Denton, J. Singh
- CHED 1354.** Synthesis of spiropyrrolizidines and 3-substituted quinoline-4-carboxylic acids from 7-bromoisatin. A. Imanishimwe, L. Desrochers, T.E. Goodwin
- CHED 1355.** Rapid synthesis of *N*-(4-chlorobenzyl)-*N*-ethylformamide. K. O'Keefe, M.M. Bobylev
- CHED 1356.** Green synthesis of spiro-pyrrolizidines via a three component condensation in a variety of solvents. P. Ravikumar, J. Murdock, L. Desrochers, T.E. Goodwin
- CHED 1357.** Synthesis of spiro-pyrrolizidines from aryl-isatins, proline, and methyl cinnamate. K. Sintigo, L. Desrochers, T.E. Goodwin
- CHED 1358.** Synthesis of 3-substituted quinoline-4-carboxylic acids from 5-fluoroisatin via the Pfitzinger reaction. M. Abdulrahim, L. Desrochers, T.E. Goodwin
- CHED 1359.** Expanding the scope of the silica sulfuric acid catalyzed synthesis of diarylacetic acids. D. Moore, W.E. Brenzovich
- CHED 1360.** Synthesis of 5- and 6-(4-fluorophenyl)-*N*-acetylglucosylamides. S. Lee, N. Ngo, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin
- CHED 1361.** Synthesis of spiro-pyrrolizidines and 3-substituted quinoline-4-carboxylic acids from 6-(4-trifluoromethylphenyl)-isatin. F. Musari, L. Desrochers, T.E. Goodwin
- CHED 1362.** Progress towards total synthesis of janulosimide A & B. A.R. Demeritte, K.J. Graham, T.N. Jones
- CHED 1363.** Development of an enantioselective allenolate Claisen rearrangement. R. Hamilton, A.G. Wenzel
- CHED 1364.** Synthesis, structure, and stability of *trans*-1,2-cyclohexanediol. K. Jenkins, W. Bryant, L. Lovings, K. Morgan
- CHED 1365.** Preparation and isolation of a reactive intermediate produced during electrophilic aromatic substitution of dichlororesorcinol. A.J. Beffa, B.H. Frohock, B.P. Marcoux, G.H. Purser
- CHED 1366.** Microwave-assisted synthesis of highly substituted anthraquinones. L. Holokai, J.J. Reczek
- CHED 1367.** Photolysis of polystyrene. J. Howard, D. Fish
- CHED 1368.** Investigation of silver and gold catalysis for cyclopropanation of allenylsilanes. J. Iannuzzelli, K.P. Vu, T.M. Gregg
- CHED 1369.** Synthesis and characterization of electron donating components of donor-acceptor columnar liquid crystals (DACLCs). K. Aagesa, J.J. Reczek
- CHED 1370.** Synthesis and biological activity of new fluorescent ABQ-48 (NSC D-763307) derivatives: 7-(2,3,4-trimethoxybenzyl)- and 3,4,5-trimethoxybenzyl)-3-aminobenzimidazo[3,2-*a*]quinolinium chloride. J.M. Nina Ruperto, I. Acevedo, E. Correa, S. Ocasio, O. Cox
- CHED 1371.** Co-crystallization experiments for the topochemical polymerization of 1,4-bis(4-bromophenyl)buta-1,3-diyne. A.E. Burgos-Aviles, N.S. Goroff, M. Kim
- CHED 1372.** Dimerization of the pyramidalized alkene pentacyclo[4.3.0.0<sup>2,4</sup>.0<sup>3,8</sup>.0<sup>5,7</sup>]non-4-ene. M.A. Forman, R. Troxell, S. Schallenger, D.J. Walz
- CHED 1373.** Synthesis of fluorescent sensors for the detection of organophosphate pesticides. D.T. Wolf, S.P. McClintock
- CHED 1374.** Amino-acid diversification of thiol phosphonamides. M.A. Hardy, J.L. Fulton, S.R. Sieck
- CHED 1375.** Development of a practical Sonogashira experiment for implementation in an undergraduate organic chemistry lab. J.M. Massicot, S.P. McClintock
- CHED 1376.** Synthesis of the mycalolide A polypropionate chain using an epoxide-based approach. N.M. Robles Matos, G. Torres, K. Morales, A. Cruz-Montanez, J.A. Prieto
- CHED 1377.** Catalyzed interesterification of short and medium chain fatty acid triacylglycerols: Synthesis & characterization. S. Gargis, R.P. D'Amelia, W.F. Nirode
- CHED 1378.** Exploring regioselective oxazole formation through a transition metal complex catalyzed [3+2] cycloaddition reaction. S.H. Brooks, J.A. MacKay
- CHED 1379.** Stereospecificity of chlorosulfonyl isocyanate reactions with alkenes. M.S. Bucardo, D.F. Shellhamer
- CHED 1380.** Quantitative kinetic study of S<sub>N</sub>1 and S<sub>N</sub>2 reactions - undergraduate organic lab. J.K. Roth, C. Nicholson
- CHED 1381.** Synthesis of a series of multi-dentate podand ligands and initial complexation trials with transition metal cations. J. Payne, J. Roehl, M.A. Benvenuto
- CHED 1382.** Synthesis and characterization of 4,4'-bis(*p*-methoxyphenylethynyl)-*p*-phenoxy) diphenylacetylene (1) and related derivatives. B. Montz, T.W. Nalli
- CHED 1383.** Progress toward the synthesis of cyclopropene and allyloxy containing substrates for protein farnesyltransferase. K. Her, J. Wollack
- CHED 1384.** Synthesis of a series of novel molecules utilizing 2,6-diaminotoluene, 1,3-diaminobenzene, or 2,6-diaminopyridine. S. Tinawi, M.A. Benvenuto
- CHED 1385.** Solvent effects in hydrogen bonding catalyzed hydride migration in alpha-hydroxycarbonyls. Q. Solano, T. Bazzi, S. Marincean
- CHED 1386.** NBS bromination of 3-bromocyclohexene. E. Willcox, T.W. Nalli
- CHED 1387.** Syntheses and reactivity of phenylethynyl-substituted quinoxalenediynes isomers. S.A. Valenzuela, M.H. Daly, B.F. Gherman, J.D. Spence
- CHED 1388.** NMR transverse relaxation measurements are utilized to detect the di-radical intermediate for reaction of chlorosulfonyl isocyanate with alkene. S.L. Elwin, D.F. Shellhamer
- CHED 1389.** BB<sub>3</sub>-Initiated cyclization of *O*-alkynylanisoles to form benzofurans. T.M. Kosak, M.E. Barylski, R.L. Lord, A.L. Korich
- CHED 1390.** Development and synthesis of supramolecular polymers utilizing nucleobase interactions: Synthesis of cytidine polymer precursors. B. Simms, J. Hunter, C.M. Lawrence
- CHED 1391.** Recent progress towards the synthesis of *trans*-avicennol. K.J. Bennett, H. Lant, S.R. Sieck
- CHED 1392.** Synthesis of triazole containing  $\beta$ -lactam antibiotics using 'click' chemistry. J.J. Bellill, J. Zula, N. Swope, S.A. Brouet
- CHED 1393.** Incorporation of TEMPO and PEG functionalities into ROMP polymers via click reaction. S. Roessler, H.J. Schanz
- CHED 1394.** Development and synthesis of supramolecular polymers utilizing nucleobase interactions: Synthesis of guanosine polymer precursors. J. Hunter, B. Simms, C.M. Lawrence
- CHED 1395.** Gold-catalyzed intermolecular nucleophilic interception chemistry. R. Chado, T.A. Knoerzer
- CHED 1396.** Synthesis and evaluation of the solvatochromic properties of various 2,6-diaryl-3*H*-imidazo[4,5-*b*]pyridines. J.K. Murray, M.J. Castaldi, M.N. Bauman, S. Ragheb
- CHED 1397.** Efforts toward dihydroveratrol dimers. B.R. Bricker, M.W. Fultz
- CHED 1398.** Synthesis and NMR characterization of a new series of 2-propionylthiazole compounds. V.G. Rand, E.C. Liscic
- CHED 1399.** Molecular recognition profiles of oxazolidinone crystalline quasaracemates. A.M. Meyer, K.A. Wheeler
- CHED 1400.** Microwave Knoevenagel condensation of  $\alpha$ -cyano and ester substituted chalcones. H.M. Colliton, M.J. Pesch, S.R. Sieck
- CHED 1401.** Revisiting a classic chemical reaction: Exploring the effect of Lewis acids and ionic liquids on the Diels-Alder reaction. E. Slate, S.A. Waratuke, D. DeSousa
- CHED 1402.** Counter-ions tune the fluorescent properties of a 2,6-bis(2-anilinoethynyl)pyridine bis(amide) anion receptor. A. Emig, B.W. Tresca, M.M. Haley, D.W. Johnson
- CHED 1403.** Computational and experimental study of the final ring closure of BN-pyrene. J.A. Jaye, G. McCormick, E.H. Fort
- CHED 1404.** Environmentally benign synthesis of potential antimalarial 1,2,4-dioxazinanes. R. Marfatia, H. Sharma, M. Abdel, D.M. Rubush
- CHED 1405.** Synthesis and characterization of dapoxy sulfonic acid analogues for use in aqueous phase luminescence-based sensing. H.A. Sofka, J.A. MacKay
- CHED 1406.** Unexpected route to imidazolones. G.W. Larson, J.T. Ippoliti



- CHED 1407.** Synthesis of novel blood sugar lowering compounds. L.J. Crippes, J.T. Ippoliti
- CHED 1408.** Novel synthesis of tetrasubstituted furan molecules. T. Tuohy, J.T. Ippoliti
- CHED 1409.** NMR comparison of two series of thiosemicarbazone ligands based on 2-formylpyridine and 2-acetylpyridine. L.T. Parrish, E.C. Lisic, J.T. Kimrey
- CHED 1410.** Synthesis of an organic dye-sensitizer for solar cells bearing triphenylamine end-capped with pyrene. A. Dahl, V.A. Sichula
- CHED 1411.** Synthesis of carotenoid-based dye via Doebner modification: Research approach for undergraduate organic chemistry students. R.P. Farwell, A.J. Cruz, L. Dorn, F. Edwardson, S. Markham
- CHED 1412.** Attempted synthesis of cyclobutanone by intramolecular Barbier reaction. D. Olson, G.L. Milligan
- CHED 1413.** Attempted peptide synthesis in water using detergent. A. Soto, G.L. Milligan
- CHED 1414.** Studies toward the total synthesis of humanamycin A. S.M. Kennedy, J.W. Dreer, M. Carta
- CHED 1415.** Optimizing an organic chemistry elimination experiment. N.J. Beyer, M.M. Bruns
- CHED 1416.** Synthesis of 2-((4-aminophenyl) diazenyl)anthracene-9,10-dione and derivatives for purification of lactate dehydrogenase. Q.T. Wauters, J.A. Mueller
- CHED 1417.** Attempted synthesis of resveratrol by McMurry reaction. B.T. Brunner, G.L. Milligan
- CHED 1418.** Green and microscale synthesis of flavones and UV-Vis fluorescence spectroscopy. J. Pemerton, N. Rowland, A. Hinton, P. Powers
- CHED 1419.** Studies aimed at lowering the catalyst loading in cobalt-catalyzed Kumada coupling reactions. J.C. Perez, M.C. Perry
- CHED 1420.** Decarboxylative protein functionalization via photoredox catalysis. M. Daemo, D.W. MacMillan
- CHED 1421.** Redox-responsive supramolecular hazy sacks. D. Dieppa Matos, L. Negron, M. Acosta Santiago, J.M. Rivera
- CHED 1422.** Synthesis of asymmetric viologens with electron rich aromatic rings. A.S. Koch, T.C. Donahue, P.A. Whitesell
- CHED 1423.** Assessing the feasibility of a one-pot, tandem olefin metathesis and isomerization sequence to synthesize conjugated aromatic olefins. A. Makwana, K.S. Knight
- CHED 1424.** Synthetic investigations towards polypeptide natural products and xenotide analogues. M. Wickman, J. Beecher, E.K. Leggans
- CHED 1425.** Novel synthetic tools for phosphoramidite regioselectivity in the synthesis of RNA monomers. S.D. Holt, J.E. Brockett, V.K. Dunlap
- CHED 1426.** New electron rich aryl viologens. A.S. Koch, P.A. Whitesell, T.C. Donahue
- CHED 1427.** Synthesis and diels-alder reactivity of 1-(furanmethoxy)nonafluorobiphenyl and 4,4'-bis(furanmethoxy)octafluorobiphenyl. T. Jones, W. Hollis, P.A. Deck
- CHED 1428.** Synthesis and characterization of curcumin analogues to improve its bioavailability. X. Santiago Maldonado, J. Rivera Hernandez, M.R. Otaño Vega, Y. Rivera-Torres, R. Gutiérrez, D.J. Sanabria-Ríos, A.R. Guadalupe-Quiñones, I. Montes-González
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- CHED 1430.** Modified Sonogashira-style coupling reaction with incorporation of carbon monoxide. M.J. Mio, Y.M. Brikhio, A.G. Fei, W.K. Fuchs, N.H. Hussein, K.M. Sultier
- CHED 1431.** Development and characterization of an immobilized ruthenium chloride surface for synthetic applications. J.A. Harris, C.M. Jones
- CHED 1432.** Synthesis and testing of GLP-1 stimulants. J.D. Goodwin, J.T. Ippoliti
- CHED 1433.** Five-membered ring closure via intramolecular nucleophilic attack by nitrogen ylides on C=C bond of cyclopropenes. C. Barrett, M.A. Rubin
- CHED 1434.** Silylacetylene protecting group sterics allow for synthetic orthogonality in a modified Sonogashira coupling reaction. M.J. Mio, K.M. Barbour, T.M. Dierker, R. Beltman, M.J. Ponkowski, J. Samona, R. Wong
- CHED 1435.** Extraction of alkaloids from blue cohosh root. S. Musch, M.P. Maddox
- CHED 1436.** Symmetrically substituted building blocks for the preparation of hybrid organic-polyoxometalate-based frameworks. K. Pearson, W.A. Neiwert
- CHED 1437.** Progress towards the synthesis and chemistry of (2-alkyl-3-(4-substitutedphenyl)diaziridin-1-yl)(4-nitrophenyl) methanones. S.M. Bonser, N. VanLeuven
- CHED 1438.** Microwave synthesis of benzimidazole anticancer agents. K. McCullough, F.L. Payton, K. Dodson
- CHED 1439.** Anti-mycobacterial metabolites from a Gram-positive marine bacterium. J.A. Trischman, D. Yee
- CHED 1440.** Synthesis of 2-alkylidene-calcixarenes from 2-oxo-*p-tert*-butyltetra-methoxycalcix[4]arene. I.M. Delahunty, J.L. Fantini
- CHED 1441.** Continued progress towards the synthesis and chemistry of some benzene-1,2-disulfonyl-, and 2-sulfonyldiaziridines. S.M. Bonser, R.D. Bechtel, O.J. Misner
- CHED 1442.** Synthesis and characterization of calix[4]arenes with a triaryl- or tetraaryllalkene group incorporated at the 2-position. N. Tran, J.L. Fantini
- CHED 1443.** Synthesis of a far-red carbazine-based fluorophore for protein tagging. S. Janisse, S.R. Levine, K.E. Beatty
- CHED 1444.** Synthesis of di-cyano NDIs and its applications in donor-acceptor columnar liquid crystals. D. Allen, J.J. Reczek
- CHED 1445.** Anions sensing studies of isoniazid-derived ligands and their rhodium (I) complexes. J.P. Warner, M.O. Odago
- CHED 1446.** Synthesis of sulfonated dicalixarenes for supramolecular assemblies via non-covalent host-guest interactions. M.E. Lance, J.L. Fantini
- CHED 1447.** Progress towards gram-scale catalytic diazoalkane-carbonyl homologation reactions. B. Smolarski, J.S. Burman
- CHED 1448.** Synthesis of organic linker molecules to coordinate nanomaterials. E. Juette, N. Kiassat, J. Zhang
- CHED 1449.** Synthesis of a modular traceless Staudinger reagent. B. Mehari, C. McDevitt, J.C. Jewett
- CHED 1450.** Survey of commercially available dried mushrooms for the presence of lovastatin and citrinin. B.A. Clement, I. Eason, N. Wilson, M. Frazier, E. Jeong, K. Cunningham, M. Hooper
- CHED 1451.** Oyster mushrooms: The fate of lovastatin and citrinin during cooking. B.A. Clement, R.S. McKinley, M. Hooper, R. Solano, K. Cunningham, A. Symons, S. Ponce, S. Campbell, K. Talcott, R. Hostak, A. Elder, E. Anciso
- CHED 1452.** Synthetic investigations towards biologically active derivatives of polypeptide macrolactones. M. Montgomery, E.K. Leggans
- CHED 1453.** Efforts to lower phase transition temperatures in asymmetrically substituted oxadiazole containing liquid crystals. S. Lewis, E. Scharer
- CHED 1454.** Structural elucidation of pyrrolizidine alkaloids in *Omphalodes aliena*. J.I. Burklund, L.P. Guerin, C.J. Burghard, R.B. Kelley
- CHED 1455.** Kinetic colorimetric determination of sugar identities in copper (II) chloride solutions (variations on the Benedict test and Fehling's test for sugars). D. Gable, T. Ready
- CHED 1456.** Synthesis and characterization of chalcones. M.L. Rivera-Claudio, J. Castillo-Ramirez, M. Sepúlveda
- CHED 1457.** Extraction of morphine from poppy seeds. L. Harbaugh, D. Fish
- CHED 1458.** Surfactant production via organic chemistry synthesis. H.L. Fasiang, R.M. Hyde, C. Boxley
- CHED 1459.** Synthesis and evaluation of novel G-quadruplex-stabilizing molecules. J. McCallum, C. Coyle, N. Baghdasaryan, V. Ovalle
- CHED 1460.** Selective lithiation of 2,6-dichloropyridine and nonselective iodination thereof. Z. Parksey, R.W. Fitch
- CHED 1461.** Progress towards the synthesis of aziridinomitosene analogs with varying quinone substitution patterns. S. Irving, R. Olsen, J. Huber
- CHED 1462.** Adsorption and characterization of fibrinogen using thin films. A. Shepherd, S. Barnett, K.A. Pacheco, S. Mackessy
- CHED 1463.** Isolation of a natural product from a marine bacterial culture challenged with *Mycobacterium marinum*. J.A. Trischman, A. Bulthuis
- CHED 1464.** Synthesis of glycopeptide analogs of a glycosylated VEGF peptide. M. Fanucchi, S.W. Suljak, M.R. Carrasco
- CHED 1465.** Synthesis and screening of novel polyphenol compounds targeted to inhibit IAPP amyloid aggregation. J. McCallum, D.A. Moffet, O. Valle, S. Gigli, N. Pihl
- CHED 1466.** Synthesis and characterization of thiophosphoramidates. L. Hagel, L. Portilla, T. Grohovsky, J. Cook, S.M. Schellbe
- CHED 1467.** Synthesis and characterization of novel paraben compounds. K. Pate, S. Merrill, I. Hildebrandt, M. Bache, C. Dalrymple, D. Carlsen, C. Alderman
- CHED 1468.** Measuring an intramolecular force of hydrogen bond in 2-fluorophenol. E. Jung, R.E. Rosenberg
- CHED 1469.** How effective is an oxidizing agent? L. Farber, J. Fierro
- CHED 1470.** Analysis of e-cigarette composition and toxicity. J. Pemerton, C. Jackson, A. Hinton, P. Powers
- CHED 1471.** Binding of environment pollutants to host molecules using fluorescence spectroscopy. O. Michels, D. Itanze
- CHED 1472.** Multi-step fluorination reaction of 2-hydroxybenzyl alcohol. C. Green, R.E. Rosenberg
- CHED 1473.** Oxidation of water catalyzed via natural and synthetic organic species. E.A. Jarvis, J. McCallum, C. Ortiz, D. Cohrs, A. Horvath, E. Radomyshevsky
- CHED 1474.** Preparation of A-factor analogue 2-heptan-1'-oyl-3-hydroxymethyl-gamma-butyrolactone. J.P. Woods, J.C. Henrikson, T.K. Ellis
- CHED 1475.** Regio-selective fluorination of azaarenes. M.A. Lnu, S. Spurlin, M.H. Blocker
- CHED 1476.** Synthesis of bis-azo dyes using 2,6-diaminopyridine and the analysis of its metal chelation properties and their characterization. E. Crull, J.R. Berk
- CHED 1477.** Decarboxylative nucleophilic addition of keto acids to imines and ketones; Synthesis of unusual fluorine-containing amino acids. M.A. Lnu, D. Van Leuven
- CHED 1478.** Synthesis of cyclodextrin derivatives and the investigation of their liquid crystalline properties. I. Graves, S. Ward
- CHED 1479.** Toward the total synthesis of analogues of cucurbit[7]uril with varying solubility in water and organic solvents. S. Ellis, L. Figueroa
- CHED 1480.** Release of provitamin D and other substituted 1,3-cyclohexadienes by a retro-nitroso-Diels-Alder reaction: A diene structure-kinetics study. B.E. Lynde, N.A. Yakelis
- CHED 1481.** Anti-mycobacterial drug discovery from bacterial strain UA 774 from the surface of *Ulva californica*. J.A. Trischman, J. Guzman, C. Saucedo
- CHED 1482.** Synthesis and biological investigation of promysalin analogs. S. Williams, A. Steele, K. Knouse, C. Keohane, W. Wuest
- CHED 1483.** Ceramide derivatives produced by a marine bacterial strain and active against *Mycobacterium marinum*. J.A. Trischman, G. Allognon, C. Oh
- CHED 1484.** Extraction and characteristics of flavonoids from prickly pear cactus. A.M. Gallegos, B.A. Clement, G.L. Kinchloe, C.W. Travis, K.K. Sedillo
- CHED 1485.** Diene structure and the retro-nitroso-Diels-Alder reaction: Kinetic parameters and structural effects. D.A. Nehrenberg, B.E. Lynde, N.A. Yakelis
- CHED 1486.** Identification of anti-mycobacterial compounds from the extract of a marine bacterial isolate (UA446) taken from the surface of *Ulva californica*. J.A. Trischman, T. Fallert, L. Cubar
- CHED 1487.** Extraction and characteristics of fructans from nopal cactus. A.M. Gallegos, B.A. Clement, H. Teel, T. Spohrer
- CHED 1488.** Synthesis of indolyl/indazolyl (C3 substituted) quinolones (C8 substituted) for study as possible anticancer/antibiotic/antimicrobial agents. E.M. Rogers, B.N. Schafer, T.M. Trygstad
- CHED 1489.** Modification of anthracyclines to reduce cardiotoxicity and improve potency against cancer cell lines. A. Petty, P.L. Barnes, J. Holdaway, D.L. Warner
- CHED 1490.** Synthesis, design & reactivity of bismuth(III)-chiral anion complexes. A. Harrison, N. Till, K. Halloran, H. Kim, L. Kupper, J. Mendoza, L. Morick, C. Young, R. LaLonde
- CHED 1491.** Toward isomorphous bridge-flipped isomers: Crystal structure of a hydrated phenylhydrazone. K. Kassekert, W.H. Ojala
- CHED 1492.** Withdrawn.

- CHED 1493.** Crystal structures of reactive nitrile oxides: 2,6-Dichlorobenzonitrile oxide. **K. Idzorek, W.H. Ojala**
- CHED 1494.** Solid-state nitrile oxide dimerization: Crystal structure of bis(4-methylphenyl)furoxan. **S.R. Whitcomb, W.H. Ojala**
- CHED 1495.** Energies and conformational preferences of perfluorinated  $\alpha$ -furanoses. **A.A. Hunt, J.S. Rhoad**
- CHED 1496.** Natural product-derived quaternary ammonium compounds with potent antibacterial activity. **M. Joyce, M. Jennings, C. Santiago, M. Fletcher, W.M. Wuest, K.P. Minibiole**
- CHED 1497.** Using singlet oxygen to synthesize natural products and drugs. **A. Ghogare, A. Greer**
- Section H**  
San Diego Convention Center  
Halls D/E
- Undergraduate Research Posters**  
**Physical Chemistry**  
*Cosponsored by SOCED*  
**N. Di Fabio, Organizer**
- 12:00 - 2:00**
- CHED 1498.** Study of the structural rearrangement and electrocyclozation pathway of a diarylethene derivative. **C. Jones, V.A. Spata, S. Matsika**
- CHED 1499.** Spectroscopic characteristics of lumazine. **A.A. Crook, C. Cole, L. Mier**
- CHED 1500.** Effect of solvent on the equilibrium constant of the H- $\pi$  complexation of phenol and benzene. **B.B. Bowers, K.J. Feierabend**
- CHED 1501.** Density functional study of the association reaction of iron with nitric oxide. **A. Gamarra, R.E. McClean**
- CHED 1502.** Peptoid interactions with artificial lipid membranes. **A.L. Calkins, A.A. Fuller, G.Y. Stokes**
- CHED 1503.** Spectroscopic and electrochemical properties of a series of anthraquinone and its derivatives: A combined experimental and computational study in an undergraduate research setting. **N.A. Donis, M.M. Allard**
- CHED 1504.** Examining the air-water interface during carbon dioxide uptake to aqueous monoethanolamine surfaces. **N.M. Vincent, L. McWilliams, G.L. Richmond**
- CHED 1505.** Exploration of the surface properties of naphthalene diimides (NDI) at the air-water interface. **J.D. Dillenburger, A. Muentner Edwards, J.J. Reczek**
- CHED 1506.** Barbituric acid: A polymorph and tautomer chameleon. **M. Marshall, B.S. Hudson, V. Lopez**
- CHED 1507.** Energetic stability of endo- and exohedral metallofullerene derivatives of C<sub>24</sub>. **C.A. Haynes, K.A. Beran**
- CHED 1508.** Empirical analysis of "reverse chemical garden" precipitation behaviors. **H. Basinger, C.M. Jensen, S. Partovi, G. Miter, M.A. Horn**
- CHED 1509.** Apparent molar volumes and isentropic compressions of cyclic ethers in aqueous solutions from 288.15 K to 313.15 K at atmospheric pressure. **P. Bernal, K.R. Tucker, J. Walsh, L. Brown**
- CHED 1510.** Comparison of stability and solubility of creatine gluconate to creatine ascorbate. **M.A. Henneberry, A.S. Wallner**
- CHED 1511.** Withdrawn.
- CHED 1512.** Adsorption and reactivity of ethanol on Au(111)-based inverse model catalysts. **D.T. Boyle, W. Andahazy, C. Stopak, V. Lam, D. Schlosser, D. Boeckmann, A. Baber**
- CHED 1513.** Difficulties with diastereomers: The effect of a chiral phosphorothioate on the backbone conformations and dynamics of DNA: A preliminary study of the Cre Sequence. **S. Werby, M. Hatcher-Skeers, M. Kyinn**
- CHED 1514.** Separation of single-walled carbon nanotubes by size-exclusion gel chromatography. **E. Cooney, J.J. Peterson, E. Naioti, A. Amori, T. Krauss**
- CHED 1515.** Enantiomeric interactions of amino acids adsorbed in zeolites: An investigation using solid-state NMR and molecular modelling. **D. Cizmeciyan, L. Topchyan, A. Papazyan**
- CHED 1516.** Deuterium line shape simulation of D<sub>2</sub>O in gypsum. **D. Cizmeciyan, J. Helston, G. Olivares, K. Palombo**
- CHED 1517.** Photophysical and spectroelectrochemical characterization and solvent effect on the tautomerism of free-base corrole. **F.R. Kohl, G.N. Calvillo, S. Lupercio, A. Loogman, S. Klein, E.A. Alemán**
- CHED 1518.** Single molecule approach to study the repair mechanism of T4 endo V. **J. Lee, M. Vander-Schuur, E.A. Alemán**
- CHED 1519.** Synthesis and characterization of lipid coated gold nanoparticle cores. **V. Wood, C. Munjar, B.D. Gilbert**
- CHED 1520.** Study of a series of photochromic salicylidene imines using kinetics and molecular modeling. **S.L. Gillingham, J.B. Dudek**
- CHED 1521.** Study of the buffer compound POPSO-sesquisodium salt for pH Measurements from 5 to 55°C. **Y. Kang, T. Wehmeyer, K. Hundley, L.S. Tebbe, C. Smith, L. Roy, R.N. Roy**
- CHED 1522.** Analysis of the impact of pH upon solution phase degradation of carminic acid. **A. Carmichael, S.J. Sobek**
- CHED 1523.** Analysis of <sup>29</sup>Si chemical shift anisotropy and <sup>1</sup>H T<sub>1</sub> spin-lattice relaxation of triphenylsilylanol via variable temperature solid-state NMR spectroscopy. **C. Plavchak, S. Mesinere, R. Iuliucci**
- CHED 1524.** Synthesis, degradation, and solubility analysis of creatine folate. **J. MacDonald, A.S. Wallner**
- CHED 1525.** Comparative study of tin-doped germanium sulfide dielectric layers in conductive-bridging random access memory devices. **B. Poulter, M.G. Gonzalez, R. Rodriguez, L. Lau, M. Mangun**
- CHED 1526.** Fluorescence studies on a series of carboxylic acid dyes. **H. Ashberry, M.S. Eloff**
- CHED 1527.** Characterization of the mechanical stability of chemically functionalized carbon nanotubes by scanning probe microscopy. **J.A. Armas, M.J. De Silva, K.A. Houchen, G.E. Scott**
- CHED 1528.** Metastable fragmentation of photoionized furan clusters. **F.A. Khan, W.T. Embry, C.J. Hoffman, D.A. Hales**
- CHED 1529.** Photofragmentation of photoionized furan clusters. **W.T. Embry, C.J. Hoffman, F.A. Khan, D.A. Hales**
- CHED 1530.** Metastable fragmentation and photofragmentation of photoionized tetrahydrothiophene clusters. **C.J. Hoffman, W.T. Embry, D.A. Hales**
- CHED 1531.** Computational study of cluster ion fragmentation: Furan and tetrahydrothiophene. **B.E. Patterson, D.A. Hales**
- CHED 1532.** Density functional study of the association reaction of manganese with nitric oxide. **P. Bess, R.E. McClean**
- CHED 1533.** Why does the acetaldehyde enolate favor reaction at the oxygen atom during gas-phase nucleophilic substitution? Contributions by resonance and inductive effects. **C. Seitz, J.M. Karty**
- CHED 1534.** Mapping the internal energy flow of molecules by studying thermal diffusion mechanisms. **B.S. Clem, H.J. Castejon**
- CHED 1535.** Temperature dependence of dipolar couplings in amides. **A.D. Wilson, W. Carroll**
- CHED 1536.** Effect of char creation process on methane storage capacities of carbon. **N. Hill, Y.C. Soo, C.A. Miderski**
- CHED 1537.** New flow conductivity cell for high concentration aqueous solutions and elevated pressures. **T. Behrent, G.H. Zimmerman**
- CHED 1538.** Investigation of NMR relaxation mechanisms of aqueous solutions of physiologically important ions. **J.M. Thornton, C. Breaux**
- CHED 1539.** Determination of the limiting equivalent conductivity and ion-pairing constants in aqueous rare earth solutions. **F.E. Rodemer, G.H. Zimmerman**
- CHED 1540.** Photodegradation of p-amino-benzoic acid in different ambient and pH environments, and impact of antioxidants on stability. **B. Marlatt, S.J. Sobek**
- CHED 1541.** Solvent effects on the quantum efficiencies and UV-induced photodegradation of PABA and padimate-O. **P. Borah, S.J. Sobek**
- CHED 1542.** Synthesis and photochemistry of dimethylaminobenzoic acid derivatives. **H. Rossiter, S.J. Sobek**
- CHED 1543.** Ammonia radiolysis: An interstellar source of nitrogen. **M.S. Gebre, H. Schneider, C. Arumainayagam**
- CHED 1544.** Exploring differences between condensed phase photolysis and radiolysis. **J. Campbell, A. Zhou, C. Arumainayagam**
- CHED 1545.** Role of low-energy (< 20 eV) electrons in astrochemistry. **L. Gates, K. Cui, C. Arumainayagam**
- CHED 1546.** Electron stimulated desorption and post-irradiation analysis in a single ultrahigh vacuum chamber. **J. Zhu, J. Huang, C. Arumainayagam**
- CHED 1547.** Syntheses and characterization of single-walled carbon nanotube – porphyrin complexes. **D.E. Skiba, R. Selzer**
- CHED 1548.** Critical conditions for droplet coalescence in common microfluidic environments. **D. Pluhar, D. Horvath, P. Abbyad**
- CHED 1549.** Withdrawn.
- CHED 1550.** Photochemical reduction mechanism of SiW<sub>11</sub>Co<sup>6-</sup> in nonpolar solvents. **N. Fusco, T. Tumiel, S.H. Szczepankiewicz**
- CHED 1551.** Kinetic studies of the photodegradation of bisphenol derivatives with gold-doped titanium oxide nanoparticles. **M. McCausland, D. Brown**
- CHED 1552.** Identification of universal cytochrome P450 binding modes using continuous wave electron paramagnetic resonance spectroscopy. **S. Blankenship, M.M. Lockart, A. Cruce, M.K. Bowman**
- CHED 1553.** Chromatographic investigation of the interaction between the polymorphic compound mCyPU and tailored surface. **B. Smiddy, R.E. Sours**
- CHED 1554.** Histidine-modified polypropylene-13 explores the nature of two-state cooperativity. **D.B. Rogers, T.J. El-Baba, L. Shi, F.A. Khan, D. Kim, D.A. Hales, D.H. Russell, D.E. Ciemmer**
- CHED 1555.** Photoreduction of carbon dioxide using a novel quantum dot. **K. Bay, M. Li, I. Parchamzad**
- CHED 1556.** Correlating characteristic frequencies of the CF<sub>3</sub> stretching band of lithium triflate in polyamine and polyether systems. **C. Bradley, N.G. Harji, R.N. Mason**
- CHED 1557.** Pulsed Nd:YAG laser Raman and infrared spectroscopic investigation of bismuth(III) chiral anion complexes. **J. Bang, R. LaLonde, D. Gerrity**
- CHED 1558.** Spectroscopic characterization of the molecular aggregation of N-alkylated perylene diimides. **A. Austin, J.M. Szarko**
- CHED 1559.** Application of Pitzer ion-interaction treatment for thermodynamics of HBr + KBr + H<sub>2</sub>O, HBr + NiBr<sub>2</sub> + H<sub>2</sub>O and HBr + GdBr<sub>3</sub> + H<sub>2</sub>O systems at 25°C. **L. Roy, R.N. Roy**
- Section H**  
San Diego Convention Center  
Halls D/E
- Undergraduate Research Posters**  
**Polymer Chemistry**  
*Cosponsored by PMSE, POLY and SOCED*  
**N. Di Fabio, Organizer**
- 12:00 - 2:00**
- CHED 1560.** Optimization of first generation poly(amidoamine) starburst dendrimer synthesis. **J. Feldhaus, D.J. Oostendorp, D.L. Johnston**
- CHED 1561.** Fuel cell membrane polymer degradation mechanisms by density functional theory. **K. Utterbeck, J.E. Stevens**
- CHED 1562.** Improving PLA processability and recycling through branching. **S.J. Ortiz, L. Gu, C.W. Macosko**
- CHED 1563.** Sustainable pressure-sensitive adhesives. **M. Coughlin, T.R. Panthani, A.M. Mannion, C.W. Macosko, F.S. Bates**
- CHED 1564.** Monitoring polymerization kinetics with IR and Raman spectroscopy in undergraduate laboratory. **N. Vu, S. Kadar, Y. Lin**
- CHED 1565.** NMR binding studies of glycosaminoglycans and cell-penetrating compounds. **H. Drazenovich, L. Prevette**
- CHED 1566.** Carbon Nanotube: Self-immolative polymer composites as dosimeters. **P.T. Chazovachii, M.B. Herbert, T.M. Swager**
- CHED 1567.** Endgroup functionalization of radiopaque polyesters. **M. Topping, L. Allison, K.R. Houston, V. Sheares Ashby**
- CHED 1568.** Effects of nitric oxide on the rate of wound healing in rats. **V.L. Johnson, N. Beres, D. Blum**
- CHED 1569.** Catalyst hemilabile group variation and lactide ring-expansion polymerization. **S.E. Wright, Y.D. Getzler**
- CHED 1570.** Conjugate number effects on nanoparticle activity and stimuli response. **O. Browne, J. Manono, S.C. Dimaggio**
- CHED 1571.** Mesogenic oligomer with alternating electron acceptor and donor units for organic electronic applications. **S.T. Mensah, L. Sosa-Vargas, D. Kreher, F. Mathevet, A. Attias**

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

- CHED 1572.** Synthesis of click-chemistry ligands for dendrimer functionalization. **J. Shropshire, J. Manono, S.C. Dimaggio**
- CHED 1573.** Click ligands for stimuli response polymer-dendrimer conjugation. **K.D. Watson, J. Manono, S.C. Dimaggio**
- CHED 1574.** Adapting an undergraduate physical chemistry experiment to add polymers to the curriculum. **I.J. Tatosian, D.M. Miller**
- CHED 1575.** Electropolymerization and characterization of polyaniline-TiO<sub>2</sub> nanocomposites for sensing applications. **J.S. Novobilsky, A.O. Sezer**
- CHED 1576.** Design and synthesis of potential small molecule hydrogelators. **A.N. Downing, J.L. Crane**
- CHED 1577.** Destruction of chemical warfare agents at interfaces. **T. Thompson, H.N. Gray**
- CHED 1578.** Improvement of mechanical properties of polylactones through pi stacking. **A. Lehr, K. Allen**
- CHED 1579.** Synthesis of a hydrogel via grafting of polystyrene onto an isobutylene-maleic anhydride alternating copolymer. **T. Freeman, L. Jia, Y. Zhao**
- CHED 1580.** Macromonomer synthesis towards improving the healing efficiency of a self-healing epoxy matrix. **M.M. Schmauch, D. Chang, S.R. Hussaini, M.W. Keller**
- CHED 1581.** Solvent and base effects in the synthesis of poly(3-hexylthiophene) via direct arylation polymerizations. **E.R. King, N.D. Ferrey, T.M. Pappenfus**
- CHED 1582.** Analysis of polymers through direct detect spectroscopy. **S. Sloane, D. Konkolewicz, S. Averick**
- CHED 1583.** RAFT polymerization for preparation of MAM-LAM block copolymers. **B. Tate, S. Harrison, M. Destarac**
- CHED 1584.** Synthesis and characterization of a perfluorocyclic tripod polymer. **Z. Perry, T.A. Knoerzer, S.T. Iacono**
- CHED 1585.** Modification of poly-valerolactone through hydrogen bonding. **M. Thompson, K. Allen**
- CHED 1586.** Controlled polymerization of D,L-lactide with titanium(IV) tartrates. **E. Mueller, C. Seitzinger, B.M. Chamberlain**
- CHED 1587.** Synthesis and polymerization of lactone monomers derived from fatty acids. **I. Prichett, C. Seitzinger, C. Hemstad, B.M. Chamberlain**
- CHED 1588.** Poly(ionic) liquids: Imidazoles with ester linkages. **E.R. Reynebeau, M.J. Campbell**
- CHED 1589.** Polymeric sulfonation. **M. Bright, E. Nellhaus, M.W. Fultz**
- CHED 1590.** Stabilization of battery electrode/electrolyte interfaces by hybrid polymer films. **T. Makkapati, N.S. Brown, D.C. Teeters**
- CHED 1591.** Processing and characterization of polycarbonate-polyurethane/nanosilver composites. **R. Colon Morillo, T. Julien, J. Harmon**
- CHED 1592.** Facile synthesis of biodegradable hydrogels for drug delivery applications. **E. Foster, A. Morrell, J. Hao**
- CHED 1593.** Chain length analysis of polyacrylamide. **T. Murphy, L. Goss, J.J. Pak, C. Brisco, D. Roberts**
- CHED 1594.** Facile synthesis of thermo-responsive biodegradable polymers for drug delivery applications. **A. Morrell, E. Foster, J. Hao**
- CHED 1595.** Investigating polymer-based immobilized radicals using dynamic nuclear polarization-enhanced MRI. **E. Makhoul, N. Salameh, M. Saracanie, M. Rosen, M.D. Lingwood**
- Undergraduate Teaching at the Frontiers of Inorganic Chemistry**
- Innovations in the Classroom**  
*Sponsored by INOR, Cosponsored by CHED*
- Diversity-Quantification-Success?**  
*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CIN, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*
- Preparing for the Real World: Challenges Faced by Young Investigators**
- Research at PUI's**  
*Sponsored by MPPG, Cosponsored by CHED, CIN, COMP, PHYS and YCC*
- MONDAY EVENING**
- Section A**  
Manchester Grand Hyatt San Diego  
Coronado D
- Potpourri of Polymer Projects: Take a Byte out of the NGSS**  
*Cosponsored by PMSE, POLY and RUBB*
- S. C. Rukes, Organizer, Presiding**
- 4:30** Introductory Remarks.
- 4:35** **CHED 1596.** Basic polymer science for the science classroom. **S.C. Rukes, A. Nydam**
- 5:25** **CHED 1597.** How to change an old lab to do new tricks! **S.C. Rukes, A. Nydam**
- 5:45** **CHED 1598.** Polymers: New twists on old favorites. **S.C. Rukes, A. Nydam**
- 6:35** Intermission.
- 6:40** **CHED 1599.** BioPlastic: Going from synthetic to natural polymers. **S.C. Rukes, E.J. Escudero**
- 7:20** **CHED 1600.** Polymer food chemistry: Have fun with Polymer Chemistry by making mountain dew'viar. **S.C. Rukes, E.J. Escudero**
- 7:40** **CHED 1601.** Using nanotechnology and polymer science to connect to a real life scenario. **S.C. Rukes**
- 8:00** Discussion.
- 8:05** **CHED 1602.** Mimicking natural surfaces using polymer coatings: A lesson about wetting. **K.A. Cavicchi, D. Moore**
- 8:25** Concluding Remarks.
- Section B**  
San Diego Convention Center  
Halls D/E
- Successful Student Chapters**  
*Cosponsored by SOCED*
- N. Di Fabio, Organizer**
- 8:00 - 10:00**
- CHED 1603.** Northeastern University Student Affiliates of the American Chemical Society: Efforts in embracing and emphasizing the importance of green chemistry. **J. Conway, B. Laramée**
- CHED 1604.** Chapter activities for the Henderson State University Student Affiliate Chapter. **B.A. Rowland, W. Garrett, P.C. Bayliss**
- CHED 1605.** Wesley College brings the chemistry of color to Delaware's family science adventure. **A. Jones, A. Luna, D. Wentzien, M.J. D'Souza**
- CHED 1606.** Sonoma State Chemistry Club community outreach to the youth of the Sonoma County. **C. Leveille, T. Deleva, A. Staidle, C.F. Works**
- CHED 1607.** Promoting science literacy and communication. **E. Castracane, N. Marcella, A. Corrao, K. Daly, K. Aubrecht**
- CHED 1608.** We Are KU chem club: The ACS Student Affiliate Chapter at the University of Kansas. **T.A. Kerr, M. Holtz, C. Barrett, R.A. Latimer, E.R. Lorenzo, P.R. Hanson, R.S. Black**
- CHED 1609.** Great journey towards achieving the Outstanding Chapter Award: The ACS Student Chapter from the University of Puerto Rico at Cayey. **A.M. Gonzalez-Sanchez, E. Rivera-Tirado**
- CHED 1610.** Collaboration is key: The pros and cons of working with the local section on chemistry outreach. **A. Shepard, J. Callus, M. Smoker, M. Shook, J.L. Farley, A.T. McDonald, D. Kesterson**
- CHED 1611.** Lock Haven University of Pennsylvania Chemistry Club. **S. Shreiber, K. Range**
- CHED 1612.** Building a successful ACS student affiliate through professional development, community outreach & community service. **S. Quintero, A. Doong, S. Hood, E. Hayes, S. Denton, R.V. Valcarce, P.J. Iles, S. Richards, L.D. Giddings, N.R. Bastian, M. Alvarez**
- CHED 1613.** #MIGoggleFace: Stayin' fab in the lab. **T.M. Dierker, G. Nguyen, J. Pothoof, S. Kurtovic, M.Y. Wu, J. Samona, S. Maurice, K.R. Evans, M.J. Mio**
- CHED 1614.** When history and chemistry collide: Dedication of Thomas Edison's Menlo Park laboratory. **T.M. Dierker, G. Nguyen, J. Pothoof, S. Kurtovic, M.Y. Wu, J. Samona, S. Maurice, K.R. Evans, M.J. Mio**
- CHED 1615.** University of Texas at Tyler ACS Student Chapter. **M. Terra, L. Calvo, L. Leamer, L.E. Boyd**
- CHED 1616.** Step for success: Interaction at chemistry shows. **P. Silvestry-Padilla, M. Martinez-Mercado, A. Rodriguez-Perez, A. Acosta, N. Irizarry, C. Perez-Rodriguez, G. Diaz, A. Santiago, N. Caraballo, A.M. Gonzalez**
- CHED 1617.** UTPB chemistry club: Promoting chemistry in west Texas. **J.M. Snitker, C. Taylor, C. Hammon, G. Munoz-Portillo, S. David**
- CHED 1618.** Warriors Chemistry Club at Stanislaus State: Building chemistry awareness by serving the community. **J.J. Lee, J. Yang, L. Vossekuil, G.N. Calvillo, J. Stillford, E.A. Alemán**
- CHED 1619.** Wayne State University ACS Student Affiliates. **A.R. Breckenridge, N. Hardin, Y.K. Elghoul, R. Dixon, A. Dao, N. Chouaib**
- CHED 1620.** University of Central Arkansas ACS Student Chapter: Integral component of our department. **T. Huntington, R. Mayo, J. DeYoung, D. Welter, J. Moore, F.M. Yarberry, K.S. Dooley, K.L. Steelman**
- CHED 1621.** NCW 2015 at UPB Humacao: A colorful celebration. **J. Suarez, R.I. Quinones-Lopez, N.M. Lopez**
- CHED 1622.** Activities and accomplishments of Midland College ACS Student Chapter, 2015. **P. Nandakumar, J. Anderson, R. Ramos, M. Ennis, G. Riggs, D. Gable**
- CHED 1623.** College chemistry outreach and programs for K-8 Schools, high schools and the community. **G. Coronado, J.S. Bloodsworth, A. Cortinas, T. Keele, M. Brown, P.E. Flores Gallardo**
- CHED 1624.** Western Washington University Student Chapter of the American Chemical Society. **T.R. Clinkingbeard, D. Myers, S.R. Emory, E. Raymond**
- CHED 1625.** Small liberal arts college perspective. **M. Poulsen, S. Tahan, R.M. Hyde, J. Tobin**
- CHED 1626.** Actions to publicize the green chemistry culture. **G.W. Arocho-Caban, N. Rios-Cardona, R. Jiménez-Hernández, B.J. Ramos-Santana, C.R. Ruiz-Martinez**
- CHED 1627.** Chemistry's energy catalyzes our shine. **R. Jiménez-Hernández, R. Pitre-Yulfo, B.J. Ramos-Santana, C.R. Ruiz-Martinez**
- CHED 1628.** Waynesburg University ACS Student Chapter: A year of exploration and adventure. **J.J. Kyle, J. McKinley, K. Wilson, B. Bosley, C. Gates, E.A. Baldauff**
- CHED 1629.** Importance of demo shows. **A. Prokay, E.P. Kippenhan, K.E. Kohler, Z.T. Wilhelm**
- CHED 1630.** Promoting chemistry through Carroll University Chemistry Club. **S. Khan, M. Hetzel, T. Bowser, J. Rountree, V. Wartenwiler, N. Biewer, C. Garcia**
- CHED 1631.** Diene to know what chemistry is like at Xavier? **K. Crosby, V.C. Miles**
- CHED 1632.** Learning to use the force to have a successful ACS student member chapter. **M.A. Ochoa, A. Gonzalez, A.Y. Navarro, L. Avila**
- CHED 1633.** Leading a successful ACS Student Chapter. **A. Fick, M. Heidarimeybodi, V. Narby, M.P. Snyder, A.J. Sanders**
- CHED 1634.** Motivating chemistry club in Santa Barbara. **A. Dawson, T. Kohlgruber, L. Laverman**
- CHED 1635.** Belmont student members show the community that science is awesome. **R. Agh, A.B. Moore**
- CHED 1636.** SMACS attacks chemistry! **S. Lowery, B.M. Day, C.B. Lodder**
- CHED 1637.** TCU Chemistry Club: Effective organization and communication methods for outreach. **A. Vu, K. Vu, K. Hermanson, M. McGarity, M. Ortiz, R. Abdeljalil, M. Bowers, C. Simmons, R. Itoh, M. Barnett, S. VanCuren, K. Upton, E. Akhimien, B.G. Janesko, J. Fry, K.N. Green**
- CHED 1638.** American Chemical Society Student Chapter at the University of St. Thomas, Houston, TX. **A.I. Rivera, P. Zaibaq, C. Chidi, H. Nguyen, A. Hernandez, A. Mullery, B. Mellis, E.B. Ledesma**
- CHED 1639.** Chemistry club at University of California Riverside. **J.M. Jenkins, M.N. Smith, D. Barragan, C. Endozo, A. Abello, L. Velez**
- CHED 1640.** ACS UPB-RP Student Chapter: Guiding the science leaders of tomorrow. **I. Montes, K.M. Collazo Maldonado, A.E. Burgos, E. Santiago Aponte, P. Urbistondo Jiménez, J. Cosme Silva, E. Pagán Colón, N.E. Caldero-Rodríguez, A.M. Alsina-Sanchez, S.M. Soto Kortright, G. Rodríguez Díaz, F.N. Serrano Martínez, J.E. Muñoz Padilla, B. Vega Collazo, J.A. Méndez Román, J.J. Soto Pérez, R. Colon Morillo**
- CHED 1641.** Reinvention of the modern day ACS Student Chapter through the use of novel and conventional ideas. **R. Wood, M. Zamora, V. Linero, U. Swamy, C. Garcia, A. Almauger**

- CHED 1642.** Pasadena City College Chemistry Club: Bringing science to students and the community in an excited state. V.I. Jaramillo, J. Portillo, A. Varelas, V. Aquirre, Y. Tiemsanjai, A. Pang
- CHED 1643.** [A]: Adams atoms ACS activities. S. Sargent, D.M. Karlin, R.P. Beeton
- CHED 1644.** Aquinas Chemistry Society. N.D. Diklich, N. Dunn, J. McAfee, C. Jensen, A. Wagner, T.L. Phillips, E.A. Jensen
- CHED 1645.** Invigorating and innovating: Breathing new life into an old chapter. A. Lolinco, P.M. Luna, B. Mason, B. Rodriguez, B. Fagan, S.D. Kendrick, M.L. Golden, D. Golden
- CHED 1646.** Universidad del Sagrado Corazon ACS Student Chapter: A new engine for chemistry in our society. J. Rosado, J. Olmo, A. Rodriguez Velazquez, J. Vega, A. Hernández, C. Aviles
- CHED 1647.** Increased communication and collaboration promoting growth of Nittany Chemical Society. C. Poirer, G. Leone
- CHED 1648.** North Dakota State University's Chemistry and Biochemistry Club. B. Benz, W. Sharkey, R. Hessman, S.C. Rasmussen
- CHED 1649.** Saint Edward's University ACS Student Chapter. C. Jackson, P. Torres, M. Kopecki Fjelland
- CHED 1650.** GGC10 getting their game on: Georgia Gwinnett College chemistry outreach. G.E. Rudd, R. Kalman, P. Robertson, E. Valenzuela, Z. Goldstein, F. Will, K. Coscia, W. Schutte
- CHED 1651.** Create gold with Missouri Western State University Alchemist Club. N. Chapman, M. Sway, A.J. Luke, A.A. Hunt, S.P. Lorimer
- CHED 1652.** Catalysts: Changing reactions through professionalism, community, and outreach. D. Andujar, V.J. Curfman, E. Fjellstad, D. Gray, M. Nauman, L.T. Walsh, I.J. Levy
- CHED 1653.** Working on the future of the Puerto Rico local section: The student chapters. A.G. Colon, O.J. Morales Martinez, H. Ocasio Rodriguez, S. Chaparro, E.J. Ferrer Torres, E. Gordian Martinez
- CHED 1654.** Student chapter of the American Chemical Society: Minot State University. S. Park, J. Choi, J.A. Collins, B.M. Hatfield, H. Lee, J. Torgunrud, M.M. Bobylev
- CHED 1655.** PUCPR celebrates 60 years of success! N. Rivera, J. Vale, C. Aviles, L. Santos
- CHED 1656.** University of Kentucky students of the American Chemical Society. D. Wallace, J.M. Mattingly, A.N. Heighton
- CHED 1657.** Programming our youth through chemistry. A.R. Chappell, K. Weeber
- CHED 1658.** ACS Student Chapter at the University of Central Florida. B.L. Mourant, S.M. Kuebler, L. Gandy, O.A. Tarano, Y. Yee Li-Sip, E. Simpson, P.M. Cole
- CHED 1659.** College of New Jersey Student Chemists Association: Connecting our members, the local community, and science. S. Knox, K.M. Fomchenko, D.H. Nguyen, B.C. Chan, A.R. O'Connor
- CHED 1660.** Southeastern Oklahoma State University ACS Student Members Chapter: Chemistry from the savage storm. S.A. Eaves, E. Landers, K. Gaskill, M. Madewell, A. Heath, J.M. Lewis, N.L. Paiva
- CHED 1661.** Student chapter of Suffolk University expands with chemistry. J. Bautista, K.A. McCarthy, T. Nguyen, S. Aguiar, E. DeFrank, M. Rojas, S. Thomas
- CHED 1662.** Events and outreach of the University of Colorado Denver SAACS Chemistry Club. A. Mattson, C. Garza, M.K. Maron
- CHED 1663.** Successful ACS student chapter at Wilkes University: Community outreach events that apply green chemistry principles and science education. M. McCleaf, J. Colvin, B.S. Clem, K.M. Rehrig, R. Hohol, C. Henkels, T. Donnelly
- CHED 1664.** ChEmory: Emory University's undergraduate chapter of the American Chemical Society. J. Fu, S. Gupta, A. Kim, K. Woolard, M.F. McCormick, D.R. Mulford
- CHED 1665.** Colorfully vibrant activity of the ACS student chapter at Inter American University of Puerto Rico Metropolitan Campus. I. Rosado, G. Almeyda, K. Salas, A. Gonzalez
- CHED 1666.** We all scream for more than LN<sub>2</sub> ice cream: Creative outreach and involvement of the Chemistry and Biochemistry Club at Union College. A. Bechu, Z.M. Tobin, S. Kleinberg, K.M. Fox, A.J. Huisman
- CHED 1667.** Bridging the gap: Developing relationships among the university and the local communities. J.D. Diaz, M. Scanlan, B.J. Bellott
- CHED 1668.** DeSales University's ACS student chapter activities during the Fall 2014 and Spring 2015. F.C. Mayville, A.M. Myers, E.N. Sauschuck, N.R. Carpenter
- CHED 1669.** Chemistry with the cru: Successful outreach to the children's hospital. K. McGahey, D. Mckinze, J. Ahlgren-Beckendorf, L. Gao
- CHED 1670.** Saint Louis University's successful student chapter. N. Schlarman, P. Sweeney, E. Mai, A. Chatrath, L. Green, D. Sepe, N. Gandhi, A. Yoon, M. Cheneler, P. Trivedi, B. Znosko
- CHED 1671.** Cooking at the speed of light: Microwave chemistry for the collegiate environment. B. Sheetz, M. Yurkevicius, C. Murphy, S.K. O'Shea
- CHED 1672.** Student members of the American Chemical Society at Morehead State University. A.N. Hunter, B. Knicely, M.T. Blankenbuehler
- CHED 1673.** ACS student chapter: Millersville University. J.E. Thames, J.W. Dreer, E.E. Dalbey, P. Bekere, L.H. Rickard
- CHED 1674.** Hygeine education. A. Smith, A. Smith, M.W. Fultz
- CHED 1675.** Barry University Chemistry Club: Service, seminars, and socials! H. Silverstein, Q. Su, V. Hoelscher, D. Cordero, T.D. Hamilton, G.H. Fisher
- CHED 1676.** Priory of biology and chemistry at ELAC: Bonding the community around us. D. Serradell, V. Corona, L. Portillo-Hernandez, A.M. Rivera Figueroa
- CHED 1677.** Chemistry is central: Inspiring students at UCO. C.B. Frech, D.R. Rundle, R. Evans, A. Arnold, D. Fleming, H. Park
- CHED 1678.** Color of chemistry at Tarleton State University. B.A. Martinez Ortega, C.E. Earp, T.B. Roberson, L.D. Schultz
- CHED 1679.** Be a chemist: St. Ambrose University Chemistry Club. A.R. Daniel, I.R. Schwantes, K.M. Giddens
- CHED 1680.** ACS Inter Ponce: Making a difference in our community. L. Ramirez Santiago, J. Irizarry Piliarte, C. Osorio Cantillo, J.I. Ramirez Domenech, E.J. Ferrer Torres
- CHED 1681.** Saint Michael's College Student Affiliates Chapter. Z. Minior, C. Ricciardi, D.S. Heroux
- CHED 1682.** Eastern Oregon University ACS Student Member Chapter: Promoting community outreach and professional networking. J. Bard, D.A. Morales, K. Hamann, P. Deenik, A.G. Cavinato
- CHED 1683.** Inspiring scientific inquiry at Ouachita Baptist University and beyond. T. Meece, J.C. Bradshaw, M.D. Perry, S. Hubbard
- CHED 1684.** SMSU Chemistry Club: For the love of chemistry. N.J. Beyer, M.M. Bruns, R. Sears
- CHED 1685.** Last of us chemists: MTSU SMAACS activities in 2015-2016. T. Chitpanya, X. Aguilar, J.M. Plant, C. Moore, C. Cacchioli, K. Ding, G.D. White
- CHED 1686.** Student chapter events and activities done at Tennessee Tech University. K. Richards, S.M. Amin, A.M. Barnes, A.D. Wilson, M. Mifflin, M.K. Monroe, S. Murphy, J.G. Coonce, A.J. Crook, D.J. Swartling
- CHED 1687.** Santa Monica College Chemistry Club provides a supportive community environment for science students. S. Purucker, N. Kristie, H. Kim, T. Peccorelli, J.M. Hsieh
- CHED 1688.** Centenary College of Louisiana chemistry club is moving on up! H. Deschautelle, K.M. Senagbe, L.B. Grafton, T.M. Ticich
- CHED 1689.** Miami University Student Affiliate Chapter of the American Chemical Society widely increases community outreach for 2016. B.D. Center, C.N. Worley, C. Williams, D. DeGenova, A. Simoni, D. Tierney
- CHED 1690.** Enhancing community engagement in chemistry at Kennesaw State University. S. Mize, K. Haim
- CHED 1691.** Colorado School of Mines American Chemical Society Student Chapter: Inspiring the next generation of chemists. J. Starks, L. Gay, A. Caster
- CHED 1692.** Loras College Chemistry Club carnival and Olympics. D.J. Oostendorp, C. Paulson, B. Burchardt, P. McClimon, Z. Schroeder
- CHED 1693.** Chemistry is a rainbow of reactions: IVCC is broadening the spectrum. A. Skoff, A.A. Molln, R. Pointer, K. Murphy, J. Roessler, S. Nelson, T. Perry, P.K. Yong, M. Johl
- CHED 1694.** Withdrawn.
- CHED 1695.** Georgia College's outstanding student chapter is tickled pinker than a pink pig in a purple prom dress to be here. J.L. Minnick, J. Minnick, T.L. Self, I. Filer, K. Miller, S. Stephenson, S. Stephenson, C.H. Lisse
- CHED 1696.** Park University Chemistry Club: Colorful chemistry. A. Davis, A. Nicholson, C. Nelson, A. Ermak, R. Tait, A. McMullen
- CHED 1697.** Student members of the American Chemical Society: University of Arizona Chapter. J. Lopez, M. Delaney, S. Arvetan, N. Oliver, K. Durham, M. Chung, J.R. Pollard
- CHED 1698.** Finding success through ChaoS: Chemistry and Other Sciences Club at The Evergreen State College. L.K. Harding, P. Lin, R. Sunderman
- CHED 1699.** Florida Southern College's ACS student chapter activities in 2015-2016. B. Crosby, M. Hewett, K. Martinet, R. Petit-Homme, S. Wilson, J.M. Montgomery
- CHED 1700.** Catawba College Chemistry: Periodically dyeing to do chemistry. J. Burroughs, R.V. Macri, C.A. Miderski, C.K. Saner
- CHED 1701.** ACS UPRM: 60 Years in the making. T.L. Massas Le Cleres, J. Feng Baez, R. Zamora, I. Casiano, P.J. Velez Vega, I.C. Rios Cruz, O.D. Álvarez Lorenzo, G. Álvarez Martínez, N.D. Massas Le Cleres, L.C. Calderón, N. Echevarría, N.V. Tristani Silvestrini, M. Barreto Pérez, J. Torres Candelaria
- CHED 1702.** NKU SAACS: Where sometimes H<sub>2</sub>C-CH<sub>2</sub>OH<sub>aq</sub> is the solution. K. McElheney, H. Hearn, E. Hogle, J. Callihan, B. Cecil, C.A. Morris, A.J. Onorato
- CHED 1703.** Sustainable science service: Building partnerships with the UM-Flint Chem Club. C. Wilhelm, A.N. Rizo, A. Shah, D. Duzdar, A. Hernandez, G. Martin, J.L. Tischler, M.R. Wilhelm, S.S. Grathoff
- CHED 1704.** Gruen Chemistry Society: Student affiliate activities at Olivet College. Z. Kitzmiller, C. Lamp, A. Partlo, K. Langer, M. Carr, S.M. Lewis
- CHED 1705.** Chemistry in action: The Heidelberg University perspective. L. White, C. Chandler, N. Beres, A.F. Bauer, A.K. Perry, E.N. Riffle, D. Blum
- CHED 1706.** The sacred heart of chemistry. J. Fierro, S. Aanonsen, M. Stewart, C. Ruvalo, K.M. Campos, S.C. Jareb, A. Anderson, S. Baer, C. Infrerra, C. Domville, A. Boering, L. Farber
- CHED 1707.** Southwestern Oklahoma State University ACS Student Chapter. Y. Hernandez, M. Tran, L. Ngo, D. Ramirez, M. Hays, A. Thomas, T.K. Ellis, L. Gwyn, J.C. Hennikson
- CHED 1708.** South Dakota School of Mines and Technology: A successful student chapter of the American Chemical Society using outreach to promote the chemical sciences. Z. Crandall, T. Rytter, J. Meyer, T. Clemmons, T. Johnson, M. Braasch-Turi
- CHED 1709.** SMACS network with Northwest Tennessee STEM hub to help with science education. S. Oliva, B.M. Ide, L.R. Gargus, S.K. Airee
- CHED 1710.** Erskine College ACS Student Chapter: Serving with science. R. Barham, C. Formby, A. Houston, C.G. Holbrooks, T.R. Hayden, J.E. Boyd
- CHED 1711.** Continuing a tradition: Missouri State University Student Affiliates of the American Chemical Society. J. Blankenship, K. Travlos, M. Fender, A. Hunsel
- CHED 1712.** ACS Inter Ponce: Promoting green chemistry to develop a quality world. A. Almodovar Ortiz, C. Perez Ramirez, L. Ramirez Santiago, E.J. Ferrer Torres, J.I. Ramirez Domenech
- CHED 1713.** Sustainable learning and outreach by members of the University of Minnesota-Morris ACS Chapter. M. Nivison, G. Komaniecki, H. Goemann, B.J. Gerold, T. Sheehan, M. Smith, C. Cicha, W. Adrian, J.D. Alia
- CHED 1714.** ACS-Inter Ponce Forensic Division. J.J. Colon Rodriguez, S. Vazquez Velazquez, J.I. Ramirez Domenech, E.J. Ferrer Torres

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

CHED **1715.** Newberry College Student Chapter of the American Chemical Society. **B.E. Lacy, O. Valentin**

CHED **1716.** University of Utah American Chemical Society Student Chapter. **C. Jennings, M.R. Kiley, G. Christensen, C. Jennings, K. Brown, N. Pratt, L. du Preez, T.G. Richmond, H.L. Sebahar**

CHED **1717.** Broadening participation. **I. Christensen, C. Flanery, A. Henderson, D. Rekemeyer, A.M. Munro, N.A. Yakelis**

CHED **1718.** Advancements and contributions of the ACS-Student Affiliates of UC San Diego. **L. Pilapil, C. Carter, H. Weizman, S. Brydges**

CHED **1719.** Optimization of the structure and function of an ACS student chapter. **A.L. Cantu, J. Kyees, H.N. Dinh, P.V. Pardo, H. Nguyen, A. Aki, L. Digal, J.L. Collins, J. Ramirez, V. Chen, P.T. Buonora, M.P. Schramm**

CHED **1720.** Tiffin University: New ACS chapter. **L. Parsons, K.R. Estright, J. Frizman, M. Sabo**

CHED **1721.** Trifecta night: Elementary, middle, high and college students' hands and minds on science. **S. Ike, E. Volovich, S. Rolle, J. Giraldo, J.A. Adam, M. Exposito, M. Delgado**

CHED **1722.** Enlightenment on ocean acidification. **E. Volovich, K.F. Sanchez, N.N. Pierre, S. Ike, M. Exposito, M. Delgado**

CHED **1723.** Society of Chemistry Students at North Georgia. **W. King, K. Todd, A. Allred, M. Whitfield, R.M. Meier**

CHED **1724.** Recruitment of minority students in science in the Los Angeles, California region. **R. Fernandez, J.L. Maradiaga, C. Cusack, K. Ku, M. Estrada, E. Navas, M. Sanchez, J. Sanchez, R. Madyun**

CHED **1725.** Chemistry as a community: Stonehill College Chemistry and Biochemistry Club. **A. Harney, E. Zyguel, M.D. Crawford, M. Golding, C.S. Schnitzer**

CHED **1726.** Successful student chapter: University of New Mexico Chapter of the American Chemical Society. **A.K. Fernandez Oropeza, D.A. Garcia, E. Milarch, D.H. Puccetti, V. Barlas, J. Larson, L.J. Whalan**

CHED **1727.** Effective community outreach and fundraising for ACS student chapters. **J.P. Howland, G. Smith, A. Kiezulas**

CHED **1728.** Illinois State University Student Affiliate Chapter of the Heartland Section of the American Chemical Society year in review. **W.T. Darrow, E. Jugovic, T. Arledge, L.M. Stateman, D. Emery, G. Van Den Driessche**

## Section C

San Diego Convention Center  
Halls D/E

### Sci-Mix

I. Black, I. J. Levy, D. K. Wicht, *Organizers*

### 8:00 - 10:00

118, 123, 129-130, 133, 140, 147, 149, 151, 154, 165, 170, 173, 178, 183, 189, 196, 254, 259, 265, 1497. See previous listings.

1743, 1745-1748, 1752, 1755, 1762-1763, 1773, 1779, 1786-1787, 1791, 1794, 1810, 1814, 1879, 1893, 1897, 1931, 1943, 1945, 1953-1954, 1960-1962, 1964-1966, 1979, 1982. See subsequent listings.

## TUESDAY MORNING

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom A

**George C. Pimentel Award in Chemical Education: Symposium in honor of Richard S. Moog**

D. Bunce, *Organizer*

J. E. Lewis, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35** CHED **1729.** Cyber Peer-Led Team Learning (cPLTL) in organic chemistry. **P. Varma-Nelson, S.B. Wilson**

**8:55** CHED **1730.** Does POGIL make a difference in student achievement and process skills compared to traditional approaches? **D.M. Bunce, K. Neiles, E.A. Flens**

**9:15** CHED **1731.** Facilitating and assessing process skills in the classroom. **R.S. Cole**

**9:35** CHED **1732.** Concept-building approaches, student performance, and the effectiveness of active learning. **R. Frey, M.A. McDaniel, M.J. Cahill, J. Zhao**

**9:55** Intermission.

**10:10** CHED **1733.** Combining the science writing Heuristic, Process Oriented Guided-Inquiry Learning and green chemistry in large enrollment general chemistry courses. **T.J. Greenbowe, D.H. Exton**

**10:30** CHED **1734.** POGIL laboratory: Flipping your chemistry course. **F.J. Creegan**

**10:50** CHED **1735.** Creation of a POGIL lab collection for the new advanced placement chemistry curriculum. **S.G. Prilliman**

**11:10** CHED **1736.** How POGIL laboratory experiments can help students and faculty. **A. Grushow, S.S. Hunnicutt, R.M. Whitnell**

**11:30** Concluding Remarks.

### Section B

Manchester Grand Hyatt San Diego  
Mission Beach C

**Green Chemistry: Theory & Practice**

*Cosponsored by CEI, I&EC and SOCED  
Financially supported by NSF-CCLI  
Center for Sustainable Polymers at the  
University of Minnesota; ACS GCI*

E. J. Brush, *Organizer*

J. E. Wissinger, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35** CHED **1737.** Green chemistry education: Techniques and resources for adopting green chemistry theory and practice in K-12 through higher education programs. **A.S. Cannon, J.C. Warner, K. Anderson, M. Enright**

**8:55** CHED **1738.** Developing a participatory action research program with middle school students to explore the social (in) justice of chemical exposure: Diesel exhaust and childhood asthma. **E.J. Brush, J. Hooper, D.M. Cardoza**

**9:15** CHED **1739.** Integrating sustainability and authentic practice into the undergraduate curriculum at UC Berkeley. **M.C. Douskey, M. Robak, L.B. Armstrong, G.A. Kerstiens, P. Pande, A.M. Baranger**

**9:35** Intermission.

**9:50** CHED **1740.** Comparing the performance of a linear and convergent synthesis of bortezomib using an integrated approach to green chemistry metrics at a gate-gate level of analysis. **J. Andraos, A. Hent**

**10:10** CHED **1741.** International perspective on green chemistry and sustainability education. **G.M. Bodner**

**10:30** CHED **1742.** Green chemistry road map project: Charting a path forward for green chemistry education. **E.J. Brush, J.E. Wissinger, M. Sabahi, J. MacKellar**

**10:50** Panel Discussion.

### Section C

Manchester Grand Hyatt San Diego  
Solana Beach A/B

**General Papers**

S. A. Fleming, *Organizer*

J. J. Stankus, *Presiding*

**8:30** Introductory Remarks.

**8:35** CHED **1743.** Got standards? Using standards based grading in the general chemistry classroom and beyond. **S.A. Toledo, J.M. Dubas**

**8:55** CHED **1744.** Do-it-yourself: 3D models of atomic orbitals through 3D printing. **K.H. Fogarty, K. Griffith, R. De Cataldo**

**9:15** CHED **1745.** Implementing concept mapping for teaching general chemistry course. **T.A. Saleh**

**9:35** Intermission.

**9:45** CHED **1746.** CHEM-Start summer preparation for general chemistry at a Hispanic serving institution. **J.J. Stankus, R.N. Garner, S. Tallarovic, A. Guadian-Mendez**

**10:05** CHED **1747.** Using multiple components of the synthesis of biodiesel to connect labs across the chemistry curriculum. **A.S. Koch, L.R. Eller, K. Neiles, E.H. Bresslour-Rashap**

**10:25** CHED **1748.** Using a new 'Periodic Table of Shapes' to aid in bonding geometry and stoichiometry. **R.J. Schroeder**

**10:45** CHED **1749.** It's not over until they graduate: Interactive classes keep students engaged even after the final exam. **K.A. Sandberg**

**11:05** Concluding Remarks.

### Section D

Manchester Grand Hyatt San Diego  
Promenade A

**Advances in E-Learning**

*Cosponsored by MPPG*

C. J. Foley, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35** CHED **1750.** Flipping the organic chemistry classroom, a comparison study with a non-flipped section. **J.C. Shattuck**

**8:55** CHED **1751.** Visualizing molecular quantum properties: The Pitt quantum repository. **D. Lambrecht, G. Hutchison**

**9:15** CHED **1752.** Flipping organic! With iPads using iTunesU and the ChemWiki. **L.A. Morsch**

**9:35** CHED **1753.** 21st century innovation in chemistry: A comprehensive software program, interactively covering a full year of 'general chemistry'. **K. Trivedi**

**9:55** Intermission.

**10:05** CHED **1754.** Using mobile technology to make student thinking visible and promote active learning in organic chemistry. **S. Feuerwerker, R. Povolotsky, M. Chatterjee**

**10:25** CHED **1755.** Using iSpartan as a hands-on teaching approach for students learning IR spectroscopy. **L.A. Morsch, A.M. Balija**

**10:45** CHED **1756.** Design and implementation of an online and hybrid research methods course for freshman undergraduate students. **S. Sambasivan, T. Callender, C.J. Foley, N. Leonhardt**

**11:05** CHED **1757.** In-classroom use of *Valence*, a mobile app to support understanding of molecular structure. **L.B. Lewis, C. Kondor, M. Schira Hagerman, A. Clark**

**11:25** CHED **1758.** Online approaches in chemical education: Oral. **B. Gilman, L.A. Morsch**

**11:45** Concluding Remarks.

### Section E

Manchester Grand Hyatt San Diego  
Mission Beach A/B

**ACS-CEI Award for Incorporating Sustainability into Chemistry Education**

*Cosponsored by CEI*

S. O. Obare, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35** CHED **1759.** Investigating vitamin toxicity: A beginner's guide to chemical toxicology. **D.P. Carrette, D.E. Rainie**

**9:10** CHED **1760.** Connecting chemistry to issues of sustainability: Preparing students for transdisciplinary challenges. **K. Aubrecht**

**9:45** CHED **1761.** Incorporating sustainability in undergraduate chemistry education: A multi-faceted approach. **J.K. Mbindyo**

**10:20** Intermission.

**10:30** CHED **1762.** Sustainability education by the midland MI section kids and chemistry group. **R. Malczewski, M.L. Rivard**

**11:05** CHED **1763.** Teaching chemistry through feedstocks, process and products: A green chemistry framework accessible to K12 students, undergraduates and the general public. **R. Hudson, J.L. Katz, K.N. Esdale, S. Glasier, A. Bishop, K. Kawamura, D. Leaman**

**11:40** Concluding Remarks.

### Section F

Manchester Grand Hyatt San Diego  
Promenade B

**Strategies Promoting Success of Two-Year College Students**

L. J. Anna, T. B. Higgins, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35** CHED **1764.** Strategies for overcoming significant challenges faced by the two-year college student. **A.J. Sanders, J. Ewing, A. Fick, V. Narby**

**8:55** CHED **1765.** STEM: A look back at ten years of teaching general chemistry at Wayne Community College: How am I doing? **A.T. Griffin**

**9:15** CHED **1766.** Building attachment to support persistence in STEM majors. **B.M. Fetterly**

**9:35** Intermission.

**9:45** CHED **1767.** How change and customization became the definition of chemistry success for this two year college. **A.J. Calhoun, E. Zabcik**

**10:05** CHED **1768.** Improving student outcomes with supplemental instruction. **V. Flaris, K. Bailey**

**10:25 CHED 1769.** Opening doors to STEM teaching with a learning assistant program at the community college. C.P. Schick

**10:45** Intermission.

**10:55 CHED 1770.** NSF programs for community colleges. B. Driscoll, T.B. Higgins, D. Rickey

**11:15 CHED 1771.** Resources, hints, and tips for writing NSF proposals. B. Driscoll, T.B. Higgins, D. Rickey

**11:35** Concluding Remarks.

## Section G

Manchester Grand Hyatt San Diego  
Ocean Beach

### Chemistry Education Research

#### Learning in the Instructional Laboratory & Conceptual Understanding

K. J. Linenberger, S. Pazicni, J. R. Raker, *Organizers*

C. J. Luxford, *Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 1772.** Assessment of a hybrid laboratory course. S.J. Hansen

**8:55 CHED 1773.** How undergraduates conceptualize the purpose of general chemistry laboratory courses. S.M. Lo, T.R. Page, A. Haynes, S. Hatch

**9:15 CHED 1774.** Assessment of student attitudes about experimentation: Implementation of a laboratory module in analytical chemistry. S. Plummer Oxley

**9:35 CHED 1775.** Longitudinal study to measure students' meaningful learning in the undergraduate chemistry laboratory. K.R. Galloway, S. Bretz

**9:55** Intermission.

**10:10 CHED 1776.** Bridging students' conceptual understanding and problem solving abilities through a writing to learn activity in a general chemistry course. M.T. Dianovsky

**10:30 CHED 1777.** Emphasizing the significance of electrostatic interactions in chemical bonding and behavior. B. Venkataraman

**10:50 CHED 1778.** Transferring knowledge between the chemistry lecture and laboratory: Where are students having problems and what intervention material assists them? W.E. Schatzberg

**11:10 CHED 1779.** Concept maps for chemistry instruction: A meta-analysis. A. Leontyev, S. Pulos

**11:30** Discussion.

### Successful REU Programs

*Sponsored by PROF, Cosponsored by CHED and CMA*

### Developing, Implementing & Teaching Hazard Assessment Tools

*Sponsored by CHAS, Cosponsored by CCS and CHED*

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## TUESDAY AFTERNOON

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom A

#### George C. Pimentel Award in Chemical Education: Symposium in honor of Richard S. Moog

J. E. Lewis, *Organizer*

D. Bunce, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1780.** Developing a network of trained POGIL workshop facilitators. S.M. Ruder, A.R. Bressette

**1:55 CHED 1781.** POGIL in the land of the kiwi. L. Trout

**2:15 CHED 1782.** Building a community of transformation: A social network analysis of POGIL project change agents. S.E. Shadle, J.E. Lewis, V.M. Thorsell

**2:35** Intermission.

**2:50 CHED 1783.** Promoting faculty development: Coaching use of threshold concepts and active learning. V.M. Thorsell, J.A. Loertscher, J.E. Lewis

**3:10 CHED 1784.** In celebration of Rick Moog's influence. J.E. Lewis

**3:30 CHED 1785. Award Address** (George C. Pimentel Award in Chemical Education sponsored by Cengage Learning and the ACS Division of Chemical Education). POGIL: Participating in ongoing growth and interactions with lots (of people). R.S. Moog

**4:10** Concluding Remarks.

### Section B

Manchester Grand Hyatt San Diego  
Mission Beach A/B

#### Green Chemistry: Theory & Practice

*Cosponsored by CEI, I&EC and SOCED. Financially supported by NSF-CCLI Center for Sustainable Polymers at the University of Minnesota; ACS GCI*

J. E. Wissinger, *Organizer*

E. J. Brush, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1786.** Need for green chemistry at the undergraduate level. I. Sidhwani, R.K. Sharma

**1:55 CHED 1787.** Educational innovation in design-related STEM through interdisciplinary sustainable science education. K.R. Pearson, E. Maldonado

**2:15 CHED 1788.** Greener synthesis of thiosemicarbazones and a qualitative tyrosinase inhibition assay for organic chemistry laboratory. E. Stopler, J. Bennett

**2:35** Intermission.

**2:50 CHED 1789.** Green "Click" and olefin metathesis chemistry in water at room temperature enabled by biodegradable, micellar nanoparticles. B.H. Lipshutz, A.G. Wenzel, D.A. Vosburg

**3:10 CHED 1790.** Identification and greener synthesis of electroluminescent imines. N. Rosenfeld, M. Seidel, N. Capra, J. Bennett

**3:30 CHED 1791.** Role of psychology in combating stress through green chemistry in the undergraduate chemistry laboratory. V. Tucker, I. Sidhwani, S. Chowdhary

**3:50 CHED 1792.** Halogenation of vanillin using Oxone® and halide salts for a greener electrophilic aromatic substitution reaction in the organic chemistry laboratory. J.E. Wissinger, J. Palesch

**4:10** Panel Discussion.

### Section C

Manchester Grand Hyatt San Diego  
Solana Beach A/B

#### Teaching & Implementing Effective Data Analysis & Computational Approaches Across the Undergraduate Chemistry Program

*Cosponsored by MPPG*

C. T. Cox, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1793.** Going beyond add trend-line: Least squares and error analysis throughout the curriculum. K. Range

**1:55 CHED 1794.** Low- or no-cost online tools for student laboratory data submission and interactive verification. A. Le

**2:15 CHED 1795.** Building nonlinear fitting of student data into an undergraduate biochemistry lab-based course. T.J. Gries

**2:35** Intermission.

**2:50 CHED 1796.** Development of a kinetic Monte Carlo master equation simulation using object-oriented Python: An undergraduate project. R. Kenney, H. Jeon, A. Hill

**3:10 CHED 1797.** Modeling of contaminant transport and fate using MATLAB in an environmental chemistry course. A. Rihana

**3:30** Concluding Remarks.

### Section D

Manchester Grand Hyatt San Diego  
Promenade A

#### Advances in E-Learning

*Cosponsored by MPPG*

C. J. Foley, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1798.** Implementation of the serious solids chemistry game in the undergraduate chemistry classroom. J.G. Coonce, E. Vasilyev

**1:55 CHED 1799.** Assessment of student learning outcomes after implementation of a response-adaptive online homework system. B. McBurnett, J.J. Stankus, S. Tallarovic, A. Guadian-Mendez

**2:15 CHED 1800.** Flipped and Open: Exploring the dynamics around learner experiences in a flipped technology-enhanced classroom with open-educational resources. B. McCollum

**2:35** Intermission.

**2:45 CHED 1801.** Mobile devices in organic chemistry: Apps for visualization, documentation, and collaboration. J. Bennett

**3:05 CHED 1802.** Teaching organic chemistry: Challenges for creating an engaging, effective online learning community. T.R. Long

**3:25 CHED 1803.** Computer-based pedagogical strategies in large general chemistry classes to increase STEM undergraduate retention. M. Ilies

**3:45** Concluding Remarks.

### Section E

Manchester Grand Hyatt San Diego  
Mission Beach C

#### International & Multicultural Perspective

*Cosponsored by IAC*

C. H. Atwood, S. J. Hansen, S. Rajee, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1804.** DivCHED-IAC outreach opportunities. R.M. Kelly

**1:55 CHED 1805.** Best practices in international chemistry education. V.A. Jouraeva

**2:15 CHED 1806.** Fulbright scholar programs for academics and professionals in chemistry. C. Riess

**2:35 CHED 1807.** Crossing the border: Should ACS approve international undergraduate chemistry programs? E.A. Arriaga, T.J. Wenzel

**2:55 CHED 1808.** Experiences in chemical and crystallographic education and research in the developing world. J. Pradon, Z. Yav, S. Dereese, E. Changamu, P. Gitari, C. Groom, L. Whitehead

**3:15** Intermission.

**3:25 CHED 1809.** International educational experiences for science undergraduates: Study abroad during the academic year. M.Z. Hoffman

**3:45 CHED 1810.** Summer undergraduate research in the United Kingdom. T.A. Nile, A.G. Glenn, M. Crowe

**4:05 CHED 1811.** Comparison between achieving a Chemistry B.S in the USA and the B.Sc. the UK. S. Bibby, A. Bradford, M. Fowler, J. Lindley, K.H. Pannell

**4:25 CHED 1812.** From undergraduates exchange to research collaborations and vice-versa: A French-American experience. A. Milet, E. Saint-Aman, R. Duran

**4:45** Concluding Remarks.

### Section F

Manchester Grand Hyatt San Diego  
Promenade B

#### General Papers

S. A. Fleming, *Organizer*

R. Indralingam, *Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1813.** UV-visible absorption spectrophotometric determination of caffeine contents in soda, tea, and energy drinks and FAAS analysis of Fe content of selected fruits and vegetables: Professional development workshop for K12 science educators. S.O. Fakayode, V.T. Snipes, M. Kanipes-Spinks

**1:55 CHED 1814.** Drug-likeness and molecular property prediction by computational methods: A computational experiment for introductory and general chemistry students. R.L. Napoleon

**2:15 CHED 1815.** Perovskite solar panels: A multidisciplinary experiment in solar energy. S. Patwardhan, D.H. Cao, S. Hatch, G.C. Schatz

**2:35** Intermission.

**2:45 CHED 1816.** Taking on responsibility: A student-designed instrumental analysis experiment. R. Indralingam, C.T. Michael, E. Lomberg, E.C. Tiffany

**3:05 CHED 1817.** Enhancing introductory chemistry laboratory learning through collaborative teaching innovation. L. Wang

**3:25 CHED 1818.** Living lab manuals: An interactive platform for communication between students and instructors. **S. Burchett**, J.L. Hayes, K.H. Woelk

**3:45 CHED 1819.** Active learning classes: More challenges for deaf/hard of hearing students. **S.D. Kendrick**, M.L. Golden, M. Montelongo

**4:05** Concluding Remarks.

## Section G

Manchester Grand Hyatt San Diego  
Ocean Beach

### Chemistry Education Research

#### Affective Learning & Model-Based Reasoning

K. J. Linenberger, S. Pazicni, J. R. Raker, *Organizers*

S. Villafane-Garcia, *Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1820.** Development and preliminary testing of a STEM persistence model: Using a subset instrument to generate affective profiles. **S. Srinivasan**, K. Murphy

**1:55 CHED 1821.** Faculty beliefs and efficacy about pedagogy and content in chemistry education: Results from a national survey of postsecondary chemistry faculty. **S. Villafane-Garcia**, K.L. Murphy, J.R. Raker

**2:15 CHED 1822.** Revalidation of the Colorado learning attitudes about science survey for chemistry after redefining its categories. **G. Allen**, A. Guzman-Alvarez, C. Uvarov, M. Molinaro

**2:35 CHED 1823.** Exploring self-concept based groupings and item responses in high school chemistry students with cluster analysis and self-organizing maps. **S.E. Nielsen**, E.J. Yeziarski

**2:55** Intermission.

**3:10 CHED 1824.** Development and validation of a construct map to assess undergraduate chemistry students' reasoning about rate laws based on rate and concentration data. **A. Brandriet**, C. Rupp, N.M. Becker

**3:30 CHED 1825.** Characterizing undergraduate quantum chemistry students' modeling practices and understanding of scientific modeling. **M.N. Muniz**, J. Beck

**3:50 CHED 1826.** Characterizing students' reasoning about graphical models of reaction rate. **J. Harshman**, A. Harrison, N.M. Becker

**4:10 CHED 1827.** Exploring the role of meta-knowledge of modeling in students' reasoning with mathematical models in the introductory chemistry course. **N.M. Becker**

**4:30** Discussion.

#### Approaches for Engaging Students in Analytical Chemistry Courses

*Sponsored by ANYL, Cosponsored by CHED*

#### Developing, Implementing & Teaching Hazard Assessment Tools

*Sponsored by CHAS, Cosponsored by CCS and CHED*

#### James Bryant Conant Award in High School Chemistry Teaching: Symposium in honor of Julia Winter

*Sponsored by ORGN, Cosponsored by CHED*

## WEDNESDAY MORNING

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom A

#### Computer-Aided Data Analysis in Chemical Education Research (CADACER)

*Cosponsored by MPPG  
Financially supported by IBM (SPSS),  
ATLAS.ti, SAS, EyeWorks Inc.*

D. P. Cartrette, A. Mehta, *Organizers*

T. Gupta, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 1828.** New approach to data mining and visual communication of data via R. **J. Harshman**, S.E. Nielsen, E.J. Yeziarski, N.M. Becker

**9:10 CHED 1829.** Distillation of survey items with R: Instrument refinement using structural equation modeling. **R. Komperda**

**9:45** Intermission.

**9:50 CHED 1830.** "Good Chemistry" in chemistry laboratories: Network perspective of cooperative learning. **M. Huang**

**10:25 CHED 1831.** Use of non-inferiority testing in chemical education research. **G. Allen**, A. Guzman-Alvarez, A.F. Smith, M. Molinaro, D.S. Larsen

**11:00** Intermission.

**11:05 CHED 1832.** Assessing quality of concept inventory items with jMetrik. **A. Leontyev**, R.M. Hyslop, S. Pulos

**11:40** Concluding Remarks.

### Section B

Manchester Grand Hyatt San Diego  
Mission Beach A/B

#### Process Oriented Guided Inquiry Learning (POGIL)

R. S. Moog, *Organizer*

M. A. Yeager, *Presiding*

**9:00** Introductory Remarks.

**9:05 CHED 1833.** Implementing POGIL in the large lecture: Lessons learned. **G.P. Shusterman**, D. Atkinson, E. Skinner

**9:25 CHED 1834.** Exploration of student writing about POGIL a large physical chemistry courses. **S.S. Hunnicutt**

**9:45 CHED 1835.** Round-robins and the POGIL physical chemistry laboratory. **R.H. Paradise**

**10:05** Intermission.

**10:15 CHED 1836.** Developing materials to assess process skills in active learning classrooms. **S.M. Ruder**, R.S. Cole, J. Lantz

**10:35 CHED 1837.** Integrating lab experiments and guided inquiry activities to teach electrochemistry in general chemistry. **T.L. Longin**, D.B. Wacks

**10:55 CHED 1838.** Using Process Oriented Guided Inquiry Learning (POGIL) activities for STEM degree student recruitment and retention. **M.C. Roslonowski**

**11:15 CHED 1839.** Developing visualization and modeling skills using digital resources in POGIL activities. **J.B. Easter**

**11:35** Panel Discussion.

### Section C

Manchester Grand Hyatt San Diego  
Solana Beach A/B

#### Online Approaches in Chemical Education

*Cosponsored by MPPG*

D. A. Canelas, *Organizer*

A. L. Marsh, P. Sorensen, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 1840.** Insights into learner experiences in massive open online courses. **D.A. Canelas**

**8:55 CHED 1841.** Online methods in chemical education: The revolution is here. **R. Bates**

**9:15 CHED 1842.** Beneficial connections between an online and residential course in medicinal chemistry. **E.P. Stevens**

**9:35** Intermission.

**9:45 CHED 1843.** Flipped & blended organic chemistry and spectroscopy courses: Structure and evaluation. **A. Flynn**

**10:05 CHED 1844.** Blurring the lines between virtual and "bricks & mortar" classrooms: Using voicethread to foster collaborative learning in organic chemistry. **R.B. Finzel**, N.M. Wachter

**10:25 CHED 1845.** Blended organic chemistry: Is it sp<sup>3</sup>, sp<sup>2</sup> or sp instruction? **D. Baker**

**10:45 CHED 1846.** Computer-based learning to support understanding of structure and spectroscopy in organic chemistry. **S. Stokes**, **D. Misna**

**11:05** Intermission.

**11:15 CHED 1847.** Student-centered language and metaphor in a student-created online chemistry textbook. **B.C. Goess**, A. Tartaro, J. Miller

**11:35 CHED 1848.** Anyone can do it...the creation and distribution of educational tools. **M.A. Bishop**

**11:55 CHED 1849.** Using OER to drive innovation in chemistry education. **D. Harris**

**12:15** Concluding Remarks.

### Section D

Manchester Grand Hyatt San Diego  
Promenade A

#### Homework: Past, Present & Future

*Cosponsored by MPPG*

E. M. Epp, M. Richards-Babb, *Organizers*

J. H. Penn, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 1850.** Role of homework in the "grade game". **T. Holme**

**8:55 CHED 1851.** Have you done your homework? **C.M. Bump**, G.C. Nwokogu, E.N. Ndip, M.K. Waddell

**9:15 CHED 1852.** Creating "quasi-flipped" classrooms using online homework tools for general chemistry in the transformation of an undergraduate chemistry department. **B.H. Augustine**

**9:35** Intermission.

**9:55 CHED 1853.** Online homework in chemistry coursework: A ten year perspective. **M. Richards-Babb**, J.H. Penn

**10:15 CHED 1854.** Focusing on the preview component of the study cycle: Creation of an independent, interactive general chemistry text to direct and assess student reading prior to class. **S. Matchett**

**10:35 CHED 1855.** Methodological analysis while answering visual spatial problems in organic chemistry. **A. Garcia**, P.A. Janowicz

**10:55** Concluding Remarks.

### Section E

Manchester Grand Hyatt San Diego  
Mission Beach C

#### Implementing Discovery-Based Research Experiences in Undergraduate Chemistry Courses

C. H. Middlecamp, G. C. Weaver, *Organizers*

J. Labov, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 1856.** Discovery-based research experiences in physical chemistry: Hallucination or reality? **S. Nellutia**

**8:55 CHED 1857.** From structure to function: Using project-based learning to promote hypothesis-driven thinking in the undergraduate curriculum. **A. Goodman**, A. Ringer McDonald, P.A. Craig

**9:15 CHED 1858.** Research-based introductory organic chemistry laboratory experiment based on combinatorial synthesis of aromatic oligoamides. **A.A. Fuller**

**9:35** Intermission.

**9:45 CHED 1859.** Distributed research projects in the general chemistry curriculum. **D. O'Donnell**

**10:05 CHED 1860.** Experimenting with student-fabricated microfluidic devices in undergraduate curriculum. **V. Feng**, K. Edelman, B. Swanson

**10:25 CHED 1861.** Discovery of chemical concepts from 3D chemical information searches of crystal structure databases. **H.S. Rzepa**

**10:45** Intermission.

**10:55 CHED 1862.** Development, pilot testing, and full implementation of an authentic research experience in undergraduate analytical chemistry: Quantitative analysis of caffeine in coffee. **R.E. Sours**, S.E. Stitzel, J.D. Sivey, K.E. Kautzman

**11:15 CHED 1863.** Sustainable nanomaterials laboratory (SMAL): A research-based laboratory module for undergraduates. **K. Wheeler**, C. Nameth

**11:35** Discussion.

### Section F

Manchester Grand Hyatt San Diego  
Promenade B

#### Curricular Innovations in Undergraduate Chemical Education Impacted by NSF

R. K. Boggess, *Organizer*

C. A. Burkhardt, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 1864.** CLASS project: Community of learners achieving science success, an NSF S-STEM grant. **T.J. Clark**

**8:55 CHED 1865.** Impact of the NSF-S-STEM program on student retention in the sciences at Knox College. **M.A. Crawford**

**9:15 CHED 1866.** Impact of the NSF S-STEM Chemistry Scholars program on transforming the chemistry major and increasing the number of chemistry graduates at UNC Asheville. **S.A. Wasileski**, A.L. Wolfe, J.M. Schmelzter, B.E. Holmes, H. Holt

**9:35** Intermission.

**9:45 CHED 1867.** Creation of Academic Social Networks (ASNs) for effective online eLearning in general chemistry. **D.M. York, J. Brennan, E. Buginsky, F. Guerra, K. Chun**

**10:05 CHED 1868.** Expanding instrument access through collaborative sharing of portable instrumentation. **C.J. Stromberg, K.H. Bennett, D.J. Ellis, P. Wood, W. Nellis, C.A. Bradley**

**10:25 CHED 1869.** Chemistry collaborations, workshops and communities of scholars (cCWCS): Developing scholarly communities to transform undergraduate STEM education. **L.J. Kaplan, D.M. Collard, P.S. Hill, J.C. Smith**

**10:45 Intermission.**

**10:55 CHED 1870.** Measuring misconceptions: Student understanding of multiple representations in chemistry. **S. Bretz**

**11:15 CHED 1871.** Learning collaboration skills: Interdisciplinary project-based instruction for biochemistry and computer science majors. **A. Goodman, A. Dekhtyar**

**11:35 CHED 1872.** Participation of a professional advisory panel in a biochemistry laboratory course. **N. Goodey, C. Talgar**

**11:55 Concluding Remarks.**

## Section G

Manchester Grand Hyatt San Diego  
Ocean Beach

### Chemistry Education Research

#### Organic Chemistry Education Research & Physical Chemistry Education Research

K. J. Linenberger, S. Pazicni, *Organizers*  
J. R. Raker, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CHED 1873.** Symbolism before reactions: What is the effect of a stepwise approach to the mechanistic organic chemistry curriculum? **A. Flynn**

**8:55 CHED 1874.** Effort, interest, and self-efficacy: An exploratory investigation in organic chemistry. **S. Villafane-Garcia, J.R. Raker**

**9:15 CHED 1875.** Analysis of first- and second-semester organic chemistry students' examples of nucleophiles and electrophiles. **M. Anzovino, S. Bretz**

**9:35 CHED 1876.** Stereochemical relationships: A correlational study of performance on stereochemistry items, visual rotation ability, and field dependence. **J.R. Raker, S. Villafane-Garcia, A. Keith**

**9:55 Intermission.**

**10:10 CHED 1877.** Influences of instructors and course materials on student's conceptualization of thermodynamics. **C.L. Stanford, R.S. Cole, A.C. Moon, M.H. Towns**

**10:30 CHED 1878.** Analysis of the POGIL-PCL network. **S.S. Hunnicutt, A. Grushow, R.M. Whitnell**

**10:50 CHED 1879.** Multiple dimensions of "Wrong": Using student generated explanations of quantum chemistry concepts to explore student conceptual understanding. **H.P. Hendrickson, J. Feldblyum, K. Chen, M. Gysin, D. Porat, S. Choi, B.P. Coppola**

**11:10 CHED 1880.** Elucidating the relationship between the POGIL physical chemistry curriculum and classroom discourse. **A.C. Moon, C.L. Stanford, R.S. Cole, M.H. Towns**

**11:30** Discussion.

## WEDNESDAY AFTERNOON

### Section A

Manchester Grand Hyatt San Diego  
Harbor Ballroom A

#### Computer-Aided Data Analysis in Chemical Education Research (CADACER)

*Cosponsored by MPPG  
Financially supported by IBM (SPSS),  
ATLAS.ti, SAS, EyeWorks Inc.*

D. P. Cartrette, A. Mehta, *Organizers*

T. Gupta, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1881.** Large-scale analysis of open-ended student responses in questions involving randomly-generated combinations of values. **E.M. Epp**

**2:10 CHED 1882.** Eye tracking technology and methodology in chemistry and biochemistry education research. **W. Wong, J. Gough**

**2:45 Intermission.**

**2:50 CHED 1883.** Dedoose: Innovative web-based tools for qualitative and mixed method social science research. **E. Lieber**

**3:25 CHED 1884.** Study of problem solving behavior using ATLAS.ti qualitative software. **T. Gupta, A. Mehta**

**4:00 Intermission.**

**4:05** Panel Discussion.

**4:35** Concluding Remarks.

### Section B

Manchester Grand Hyatt San Diego  
Mission Beach A/B

#### Process Oriented Guided Inquiry Learning (POGIL)

R. S. Moog, *Organizer*

M. A. Yeager, *Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1885.** Developing invested learners: How POGIL strategies support high school chemistry students with learning disabilities. **M. Sullivan**

**1:55 CHED 1886.** Adapting the science writing heuristic for high school chemistry students (POGIL). **C. Lehman**

**2:15 CHED 1887.** Managing emotions: The key to success in a POGIL high school chemistry course. **M. Sullivan**

**2:35 Intermission.**

**2:45 CHED 1888.** Recipe for success: Mixing peer instructors into a POGIL classroom. **M.D. Perry**

**3:05 CHED 1889.** Using POGILs and blended learning to retain physical science students: A preparation to chemistry approach. **P.A. Boda**

**3:25 CHED 1890.** Transforming a second-semester organic chemistry course from traditional lecture to active-learning, challenges and successes. **M.N. Garrett**

**3:45** Panel Discussion.

### Section C

Manchester Grand Hyatt San Diego  
Solana Beach A/B

#### Online Approaches in Chemical Education

*Cosponsored by MPPG*

P. Sorensen, *Organizer*

D. A. Canelas, A. L. Marsh, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1891.** Teaching science in unconventional ways: Analysis of student learning in Science & Cooking. **P. Sorensen**

**1:55 CHED 1892.** Computer simulations, animations, and guided-inquiry tutorials: Stoichiometry, thermochemistry, and the kinetic molecular theory. **T.J. Greenbowe, J.J. Gelder, M.R. Abraham**

**2:15 CHED 1893.** Rethinking remedial chemistry: Preparing and motivating incoming undergraduate students for success in introductory chemistry using an adaptive-responsive online chemistry preparation course. **C. Uvarov, D. Dockter, A. Guzman-Alvarez, M. Molinaro**

**2:35 Intermission.**

**2:45 CHED 1894.** Incorporation of online learning tools and technology in a general chemistry setting. **S.A. Kennedy, E.E. Wilson**

**3:05 CHED 1895.** Successes and challenges in developing general chemistry II online at a traditional liberal arts and sciences college. **A.R. Noble**

**3:25 CHED 1896.** Impact of online video lectures on learning in undergraduate chemistry courses. **P.L. Mosley, D.A. Canelas**

**3:45 Intermission.**

**3:55 CHED 1897.** Chemistry online in the Montana frontier. **J.E. Alexander, J. Wenz**

**4:15 CHED 1898.** Online chemistry: The development and use of a custom in-house laboratory kit. **J.L. Hayes, S. Burchett**

**4:35 CHED 1899.** Withdrawn.

**4:55 CHED 1900.** Resources to enhance academics and learning in chemistry at Lebanon Valley College. **W.A. Patton, A.L. Marsh**

**5:15** Concluding Remarks.

### Section D

Manchester Grand Hyatt San Diego  
Promenade A

#### Citizens First!

*Cosponsored by CEI*

M. A. Fisher, *Organizer*

B. A. Davis, A. Hoffman, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1901.** Chemical weapons and how they can provide examples when teaching various topics in beginning chemistry courses. **M.A. Bishop**

**1:55 CHED 1902.** Paradox of water. **B. Venkataraman**

**2:15 CHED 1903.** Educating undergraduates on lead exposure as a civic issue. **S.J. Bachofer**

**2:35 CHED 1904.** Environmental justice: Chemical hazards and helpers. **E. Metzger, S. Glazier**

**2:55 Intermission.**

**3:05 CHED 1905.** Addiction: A forum for exploring real world issues and the relevance and principles of chemistry. **T.E. Hagan, C. Schweibenz**

**3:25 CHED 1906.** MythBusters and chemistry instruction for non-science majors. **K. Kostecka**

**3:45 CHED 1907.** Bringing cultural relevance to chemistry with chocolate. **J.A. Trischman**

**4:05 Intermission.**

**4:15 CHED 1908.** Introduction to science and technology in society: A class designed for high school students/undergraduates to relate scientific controversies and advancements with societal perceptions. **K. Finzel**

**4:35 CHED 1909.** iSubstance: Walking a semester in a substance's shoes. **W.H. Steel, J.M. Fautch, J.B. Foresman**

**4:55 CHED 1910.** Impact of incorporation of a "Pseudoscience Fair" in the STEM curriculum. **F.M. Yarbber**

**5:15** Concluding Remarks.

### Section E

Manchester Grand Hyatt San Diego  
Mission Beach C

#### Implementing Discovery-Based Research Experiences in Undergraduate Chemistry Courses

J. Labov, C. H. Middlecamp, *Organizers*  
G. C. Weaver, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CHED 1911.** Incorporation undergraduate research elements in some upper-level laboratory classes at a predominantly undergraduate institution. **M.M. Allard**

**1:55 CHED 1912.** Exposing undergraduate students to physical methods of chemical analysis in instrumental analysis laboratory. **A.J. Cruz**

**2:15 CHED 1913.** Template for the development of an upper division biochemistry laboratory course within an independent research structure while still teaching basic biochemical techniques. **R.L. McCann, T. Frielle**

**2:35 Intermission.**

**2:45 CHED 1914.** Using the violacein pathway for discovery-based biotechnology laboratory exercises on gene regulation and pathway optimization. **J.A. Jones, M. Koffas**

**3:05 CHED 1915.** Implementation of a comprehensive, discovery-based experiment in nuclear chemistry. **J.C. Bryan, A.R. George, A. Staffaroni**

**3:25 CHED 1916.** Guided inquiry to the bromination of alkenes in the organic chemistry laboratory to foster student understanding of thin layer chromatography. **C.E. Wright, M.L. Grunert Kowalske, J.J. Kiddle**

**3:45 Intermission.**

**3:55 CHED 1917.** Discovery in large undergraduate biochemistry labs through homology modeling and functional annotation of paralogous genes. **B.J. McFarland, D. Wood**

**4:15 CHED 1918.** Genomics education partnership: Building and sustaining a large collaborative community around genomics research experiences in the undergraduate classroom. **A. Goodman, K. Saville, W. Leung, C. Shaffer, S. Elgin**



- 4:35 CHED 1919.** Assessment in CUREs: Ways to promote and assess student collaboration, creativity, and dissemination. **C.A. Thomas**, D. Gretch, D. Hitt, J.G. Rowley, C. Pharr
- 4:55** Discussion.

## Section F

Manchester Grand Hyatt San Diego Promenade B

### Curricular Innovations in Undergraduate Chemical Education Impacted by NSF

C. A. Burkhardt, *Organizer*  
R. K. Boggess, *Organizer, Presiding*

**1:30** Introductory Remarks.

- 1:35 CHED 1920.** National Science Foundation programs that support undergraduate chemistry education. **B. Driscoll**, T.B. Higgins, D. Rickey

- 1:55 CHED 1921.** National Science Foundation merit review principles and strategies for writing a successful proposal. **B. Driscoll**, T.B. Higgins, D. Rickey

**2:15** Intermission.

- 2:30 CHED 1922.** Let's focus on chemical thinking: A story of how an NSF funded idea grew from a seed to a tree. **J.R. Pollard**, V. Talanquer

- 2:50 CHED 1923.** Transform, interact, learn, and engage for success in STEM education. **R.S. Cole**, J. Emberger, S. Van Horne

- 3:10 CHED 1924.** Using needs analysis in the development of tools to help instructors enhance their content assessment. **T. Holme**, D. Hart

**3:30** Intermission.

- 3:40 CHED 1925.** Plugging the "leaky bucket" of early career science teacher attrition through the development of professional vision. **G.T. Rushton**, B.A. Criswell, M.L. Dean, D. Rosengrant, S.J. Polizzi

- 4:00 CHED 1926.** Implementation of an NSF S-STEM chemistry scholarship program at Winthrop. **C. Harris**, P.M. Owens, K.A. Snyder, T.F. Sumter

- 4:20 CHED 1927.** Elements of an NSF S-STEM program that promote retention. **K.J. Graham**, E.J. McIntee

**4:40** Concluding Remarks.

## Section G

Manchester Grand Hyatt San Diego Ocean Beach

### Chemistry Education Research

#### General Chemistry

K. J. Linenberger, S. Pazicni, J. R. Raker, *Organizers*

U. Kulatunga, *Presiding*

**1:30** Introductory Remarks.

- 1:35 CHED 1928.** Using the Toulmin's argumentation framework for the professional development of peer leaders in general chemistry. **U. Kulatunga**

- 1:55 CHED 1929.** Evaluating student attitudes towards self-directed learning and peer interactions in a flipped classroom environment using POGIL style activities and undergraduate learning assistants (LAs). **U. Swamy**

- 2:15 CHED 1930.** Study resources in general chemistry chosen by students with little time to study. **D.K. Dillner**, D. Bunce, R. Komperda, J. Hartman, S. Lin, M.J. Schroeder

- 2:35 CHED 1931.** Reading strategy leads to exam gains in chemistry: Implications for instruction. **J. Ross**

**2:55** Intermission.

- 3:10 CHED 1932.** Learning and studying strategies used by general chemistry students with different affective characteristics. **J. Chan**, C.F. Bauer

- 3:30 CHED 1933.** Enhancing learning: More evidence for evidence-based practices in high enrollment general chemistry. **C. Uvarov**, G. Allen, A. Guzman-Alvarez, M. Molinaro

- 3:50 CHED 1934.** Develop new learning materials and strategies for improving CHEM 1151 course. **A. Dutta**, M. Burkart, M. Attaya, J. Gonzalez-Roman, J. Blum

- 4:10 CHED 1935.** Chemistry supplemental instruction at a regional comprehensive state university. **C. Nicholson**

**4:30** Discussion.

## THURSDAY MORNING

### Section A

Manchester Grand Hyatt San Diego Mission Beach B

#### Chemistry Education Research

##### General Chemistry

K. J. Linenberger, S. Pazicni, J. R. Raker, *Organizers*

S. M. Underwood, *Presiding*

**8:00** Introductory Remarks.

- 8:05 CHED 1936.** Response process validity study of scale-themed assessments. **J.M. Trate**, A. Blecking, P. Geissinger, K.L. Murphy

- 8:25 CHED 1937.** From Bronsted to Lewis: A longitudinal study of student-constructed acid-base explanations. **H. Kouyoumdjian**, S.M. Underwood, M. Cooper

- 8:45 CHED 1938.** Semester long use of two different homework systems: Comparison of student learning, perceived learning, and attitudes. **C. Zumalt**, V.M. Williamson

**9:05 CHED 1939.** Withdrawn.

**9:25** Intermission.

- 9:40 CHED 1940.** Students' knowledge resources about rates of change and implications for understanding reaction kinetics. **S. Seethaler**, L. Stevens, L. Wynn

- 10:00 CHED 1941.** Inquiry representation in the Journal of Chemical Education. **F. Mumba**, S. Blankenship, W.J. Hunter, J.S. Carver

- 10:20 CHED 1942.** Assessment of student learning in general chemistry. **Z. Huang**

**10:40** Discussion.

### Section B

Manchester Grand Hyatt San Diego Mission Beach A

#### Instructors & Researchers Advancing Graduate Student Education

S. J. Hansen, S. Sandi-Urena, *Organizers*, *Presiding*

G. Bhattacharyya, *Presiding*

**8:00** Introductory Remarks.

- 8:05 CHED 1943.** But can they teach? **J.A. Parr**, R. Broyer

- 8:25 CHED 1944.** Graduate student pedagogic residency in inquiry-based course about concept of heat. **C.F. Bauer**, J. Chan

- 8:45 CHED 1945.** GTA-centered training to improve undergraduate motivation in a blended freshman general chemistry lab. **A. Pfaff**, S. Burchett, J.L. Hayes, K.H. Woelk

**9:05** Intermission.

- 9:20 CHED 1946.** CER synergy at Miami University: Building simultaneous expertise in chemistry and education research. **S. Bretz**, E.J. Yeziarski

- 9:40 CHED 1947.** Information seeking in the "Information Age": Case studies of organic chemistry graduate students. **G. Bhattacharyya**, L. Cain

- 10:00 CHED 1948.** Understanding the experiences of doctoral students from underrepresented minority groups. **M.G. Kowalske**, C.E. Wright

**10:20** Discussion.

### Section C

Manchester Grand Hyatt San Diego Solana Beach A/B

#### Supporting & Expanding Undergraduate Research in Chemistry

B. L. Gourley, *Organizer*

R. Jones, *Organizer, Presiding*

**8:00** Introductory Remarks.

- 8:05 CHED 1949.** Incorporating undergraduate research into the chemistry curriculum: A historical perspective. **B.E. Holmes**

- 8:25 CHED 1950.** Integrating undergraduate research with teaching and learning: Expanding opportunities and broadening participation. **L.E. Echegoyen**, S.B. Aley, C.E. Botez, G. Corral, H.H. Meeuwssen, D. Villagran

- 8:45 CHED 1951.** Integrating research into the curriculum: A low-cost strategy for promoting undergraduate research. **S. Hati**

- 9:05 CHED 1952.** Incorporating authentic research in an optional component of the second semester organic laboratory course. **T.L. Smith**, J.G. Gillmore

- 9:25 CHED 1953.** Transforming second semester organic chemistry laboratory into a research experience for all second year students. **S.L. Gould**, R.J. Felix, A.J. Carr

- 9:45 CHED 1954.** Translation of chemical biology research into the biochemistry laboratory: Chemical modification of proteins by diethylpyrocarbonate. **M. Konkle**, L. Hunsicker-Wang

**10:05** Intermission.

- 10:10 CHED 1955.** Broadening participation in STEM undergraduate research by targeting students at risk of leaving STEM. **P.M. Hare**, B.V. Bowling, D. Maureen, B. Brooke, J. Filaseta

- 10:30 CHED 1956.** Undergraduate research at the community college: Costs and benefits. **R.H. Jarman**

- 10:50 CHED 1957.** Undergraduate research at Armstrong State University: Authentic research experiences plus outcomes-based assessment. **S. Zingales**, W.E. Lynch

- 11:10 CHED 1958.** Establishing a forum for student dissemination of course-based research. **J.S. Kirk**, J. Roinila

- 11:30 CHED 1959.** Engaging early-career students in research using a tiered mentoring model. **S.M. Hayes**

- 11:50 CHED 1960.** Assessing undergraduate research in chemistry. **R.M. Jones**

- 12:10 CHED 1961.** Overview of a flexible curriculum and the impact on undergraduate research. **B.L. Gourley**

## Section D

Manchester Grand Hyatt San Diego Promenade A

### General Papers

S. A. Fleming, *Organizer*

R. Biggs, *Presiding*

**8:00** Introductory Remarks.

- 8:05 CHED 1962.** 3 R's (repetition, reinforcement, revelation) approach to teaching organic chemistry: A promising approach to helping students achieve their academic potential. **J.M. Quirke**

- 8:25 CHED 1963.** When can I teach that: How did freshmen and sophomores perform on multiple-choice items covering organic chemistry topics? **B. Barth**, E.C. Bucholtz, S. Sirmulla, N. Sanguantrakun

- 8:45 CHED 1964.** My two decades of teaching organic chemistry to high school students at a residential setting. **A. Rahman**

- 9:05 CHED 1965.** Improving student learning in a one-semester organic chemistry course. **A.M. Reeve**

**9:25** Intermission.

- 9:35 CHED 1966.** Design of a method to assess the effectiveness of open-ended mechanistic clicker questions for an introductory organic chemistry course. **R. Biggs**

- 9:55 CHED 1967.** CBS and CEC: Asymmetric synthesis and absolute configuration of an enantioenriched alcohol: A discovery-based undergraduate laboratory experiment. **S.M. King**, R. King

- 10:15 CHED 1968.** Improving synthetic, laboratory and instrumental skills via a series of organic synthetic and nanomaterial projects in the instrumental analysis lab. **K.S. Yamaguchi**, B. Kim

- 10:35 CHED 1969.** Development and use of Tap OChem, an organic chemistry animation application for the classroom. **N.T. Allison**, J.T. Allison

**10:55** Concluding Remarks.

## Section E

Manchester Grand Hyatt San Diego Mission Beach C

### General Papers

S. A. Fleming, *Organizer*

A. Primrose, *Presiding*

**8:00** Introductory Remarks.

- 8:05 CHED 1970.** Are we teaching chemistry by violating physics and math? **S. Mitrovski**

- 8:25 CHED 1971.** Developing an instrument to assess student attitudes towards interdisciplinary learning. **C. Addison**, F. Moosvi, J. Charbonneau

- 8:45 CHED 1972.** Withdrawn.

- 9:05 CHED 1973.** Withdrawn.

**9:25** Intermission.

- 9:35 CHED 1974.** Aspiring faculty professional development experiences at the University of California, San Diego (UCSD). **M.A. Boerneke**

- 9:55 CHED 1975.** Cigarette smoke and cancer cells: An interdisciplinary, collaborative, research-based laboratory initiative. **D.K. Hoover**, J. Fornagaglio

- 10:15 CHED 1976.** New student support for a flipped chemistry classroom. **A. Primrose**, D. Mckinzy, N. Cunanan

**10:35 CHED 1977.** Development of a sophomore-level cohort for chemistry majors to promote concurrent enrollment and success in analytical and organic chemistry. **K.P. Reber**, J.D. Sivey, T.J. Brunker, S.E. Stitzel, K.E. Kautzman, R.E. Sours

**10:55** Concluding Remarks.

### Section F

Manchester Grand Hyatt San Diego Promenade B

#### General Papers

S. A. Fleming, *Organizer*

P. Cohn, *Presiding*

**8:00** Introductory Remarks.

**8:05 CHED 1978.** Family matters: Structure-property studies in the undergraduate curriculum. **P. Cohn**

**8:25 CHED 1979.** Photochemical aging and oxidation: A discussion for undergraduate and high school students. **M. Minnis, A. Greer**

**8:45 CHED 1980.** Preparing future science teachers for southwestern Illinois. **S.D. Wiediger**, J.S. Krim, K. Barry, S. Locke

**9:05 CHED 1981.** Introducing research in a general chemistry course by faculty mentoring. **O.M. Primera**, M. A. Falero-Gil, L.F. de la Torre, S.P. Hernandez-Rivera

**9:25** Intermission.

**9:35 CHED 1982.** Mercer University's Chemical Commerce program. **K.M. Bucholtz**

**9:55 CHED 1983.** Integration chemistry laboratory instrumentation into the industrial internet. **D. Kosenkov**, N. Famularo, Y. Kholod

**10:15 CHED 1984.** Differentiated introductory chemistry courses for enhanced retention. **M.E. Hatcher**

**10:35 CHED 1985.** Chemistry in chemical engineering education. **Z. Tuiebakhova**, N. Celebi-Olcum

**10:55** Concluding Remarks.

## CHAS

### Division of Chemical Health and Safety

**D. Decker, F. Wood-Black and J. Pickel**,  
*Program Chairs*

### SUNDAY AFTERNOON

#### Section A

Hilton Gaslamp San Diego Marina Room

#### Safety Begins in the Classroom: Demonstrations, Awareness & Pre-Lab Planning

*Cosponsored by CCS and CHED*

D. M. Decker, F. K. Wood-Black, *Organizers*,  
*Presiding*

**1:30** Introductory Remarks.

**1:35 CHAS 1.** Wild, wild west to GHS: Reflections on my first year as a general chemistry laboratory coordinator. **R. Sansom**, M.B. Allen

**2:05 CHAS 2.** Safety education for early lab students: How do they learn it before they need it? **S.M. Kennedy**

**2:35 CHAS 3.** Chemical demonstrations: The good, the bad, the ugly. **D.A. Katz**

**3:05 CHAS 4.** Development of demonstrations – a collaborative project between the safety office and teaching assistants. **D.M. Decker**, **J.T. Greenfield**

**3:35** Concluding Remarks.

#### Section A

Hilton Gaslamp San Diego Marina Room

#### Ask Dr. Safety: About Incident Reporting

*Cosponsored by CCS*

H. J. Elston, N. R. Langerman, *Organizers*,  
*Presiding*

**3:50** Introductory Remarks.

**3:55 CHAS 5.** Anatomy of an incident report. **M.E. Cournoyer**

**4:15 CHAS 6.** When things go wrong ... Incident reporting. **H.J. Elston**,  
**N.R. Langerman**

### MONDAY MORNING

#### Cannabis: Exploring the Chemistry, History & Future

*Sponsored by AGFD, Cosponsored by CHAS and SCHB*

### MONDAY AFTERNOON

#### Section A

Hilton Gaslamp San Diego Marina Room

#### How Texas Tech & UCLA Have Affected Laboratory Safety Nationwide

*Cosponsored by CCS*

D. M. Decker, *Organizer*, *Presiding*

**1:30** Introductory Remarks.

**1:35 CHAS 7.** We better watch out: Prevention beats reparation. **K.P. Fivizzani**

**2:05 CHAS 8.** Digging deep: The response to cultural issues. **K.B. Jeskie**

**2:35 CHAS 9.** Changing a culture: The accident at Texas Tech; what happened in the next five years, and why you should develop a culture of safety: Thoughts from the department chair at the time. **D.J. Casadonte**

**3:05** Intermission.

**3:25 CHAS 10.** Developing a chemical safety program from lessons learned. **J.H. Wright**

**3:55 CHAS 11.** Developing standard operating procedures (SOPs): A tale of a really fun project (really!). **D.M. Decker**, **C.A. Jakober**

**4:25 CHAS 12.** Improving safety performance and compliance through web-based tools. **D.A. Harvey**

**4:55** Concluding Remarks.

#### Cannabis: Exploring the Chemistry, History & Future

*Sponsored by AGFD, Cosponsored by CHAS and SCHB*

### MONDAY EVENING

#### Section A

San Diego Convention Center Halls D/E

#### Sci-Mix

J. M. Pickel, *Organizer*

**8:00 - 10:00**

**CHAS 13.** Division of Chemical Health and Safety Information Poster. **J.M. Pickel**

**CHAS 14.** Safety in pictures: What message are you sending? **J.M. Pickel**

**CHAS 15.** Lessons learned in photos. **J.M. Pickel**, **M.R. Wilhelm**

**CHAS 16.** Lessons learned in photos: What went right. **M.R. Wilhelm**, **J.M. Pickel**

**CHAS 17.** iRAMP: A web-based model for laboratory chemical risk assessment. **R. Stuart**, **L. McEwen**

**CHAS 18.** Explosions and hazardous chemicals: Studying disaster preparedness with FEMA. **M.N. Heil**, **J. Sokatch**, **L. Daly**

### TUESDAY MORNING

#### Section A

Hilton Gaslamp San Diego Marina Room

#### Developing, Implementing & Teaching Hazard Assessment Tools

*Cosponsored by CCS and CHED*

S. B. Sigmann, R. Stuart, *Organizers*, *Presiding*

**8:30** Introductory Remarks.

**8:35 CHAS 19.** Creating a culture of safety: APLU recommendations and tools for universities and colleges. **E.A. Talley**

**8:55 CHAS 20.** Parsing the chemical risk assessment process for the laboratory. **R. Stuart**

**9:15 CHAS 21.** Incorporating hazard assessment into laboratory curricula: One pathway to growing a sustainable safety culture. **L.J. Tirri**

**9:35** Intermission.

**9:55 CHAS 22.** Risk analysis and crisis management in a research lab. **N. Bhatti**, **S. Singh**

**10:15 CHAS 23.** Software tools to assist and promote laboratory safety. **C.A. Merlic**, **S.M. Hussain**

**10:35 CHAS 24.** Using case studies and receiving ancillary benefits through instruction and use of what-if hazard reviews in an academic research environment. **K.W. Kretchman**

**10:55** Intermission.

**11:15 CHAS 25.** System to identify, analyze and control the hazards of laboratory researcher at Argonne National Laboratory. **S. Baumann**, **S. Rupkey**

**11:35 CHAS 26.** Hazard review and approval system at the national institute of standards and technology. **S.G. Ringen**

**11:55 CHAS 27.** Development of a database for hazard assessment and work approval in the Material Measurement Laboratory at the National Institute of Standards and Technology (NIST). **E. Mackey**, **C. Vogel**, **B. Brass**

**12:15** Concluding Remarks.

#### Cannabis: Exploring the Chemistry, History & Future

*Sponsored by SCHB, Cosponsored by AGFD, CHAS and ORGN*

### TUESDAY AFTERNOON

#### Section A

Hilton Gaslamp San Diego Marina Room

#### Developing, Implementing & Teaching Hazard Assessment Tools

*Cosponsored by CCS and CHED*

S. B. Sigmann, *Organizer*, *Presiding*

R. Stuart, *Presiding*

**2:00** Introductory Remarks.

**2:00 CHAS 28.** Introduction to bowtie methodology for a laboratory setting. **C. Boylan**, **R. Stuart**

**2:30 CHAS 29.** Application of barrier-based approach to enhance incident investigation. **M.E. Mulcahy**

### WEDNESDAY MORNING

#### Section A

Hilton Gaslamp San Diego Marina Room

#### Chemical, Sample & Asset Management Tools

*Cosponsored by CCS and CINF*

L. McEwen, J. M. Pickel, R. Stuart, *Organizers*,  
*Presiding*

**9:00** Introductory Remarks.

**9:10 CHAS 30.** Chemical inventories: What are they good for? **R. Stuart**

**9:35 CHAS 31.** How UNHCEMS® has evolved from a chemical inventory tracking system to an environmental management tool. **K. Myer**, **P. Collins**, **A. Glode**

**10:00 CHAS 32.** Use of RFID and scanning technologies for managing large chemical inventories. **J.M. Pickel**

**10:25** Intermission.

**10:50 CHAS 33.** Developing a cloud based chemical inventory application for the University of California system (UC Chemicals). **H. Weizman**

**11:15 CHAS 34.** Using a chemical inventory system to optimize safe laboratory research. **G. Baysinger**, **R. Creed**, **L.M. Gibbs**

**11:40 CHAS 35.** Chemical stockroom management: Lessons learned ten years in. **S.B. Sigmann**

### WEDNESDAY AFTERNOON

#### Section A

Hilton Gaslamp San Diego Marina Room

#### Chemical, Sample & Asset Management Tools

*Cosponsored by CCS and CINF*

L. McEwen, J. M. Pickel, R. Stuart, *Organizers*,  
*Presiding*

**1:30** Introductory Remarks.

**1:40 CHAS 36.** UC safety: An integrated approach to your chemical management needs. **S. Hussain**, **K. Smith**

- 2:05 CHAS 37.** Targeted safety assessments through technology. J. Crandall
- 2:30 CHAS 38.** Withdrawn.
- 2:55** Intermission.
- 3:20 CHAS 39.** PubChem's laboratory chemical safety summary (LCSS). S. Kim, J. Zhang, A. Gindulyte, P. Thiessen, L. McEwen, R. Stuart, E. Bolton, S. Bryant
- 3:45 CHAS 40.** Socio-legal issues in the application of semantic web technology to chemical safety. J.G. Frey, M.I. Borkum
- 4:10 CHAS 41.** Pre-competitive collaboration to advance laboratory safety. C.I. Nitsche

## CINF

## Division of Chemical Information

E. Davis and E. Alvaro, *Program Chairs*

## OTHER SYMPOSIA OF INTEREST:

**Fall 2015 InterCollegiate Cheminformatics Course** (see CHED, Sun)

**From Synthesis to Design: Modeling Tools for Medicinal Chemists** (see COMP, Sun)

**Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions** (see CHAL, Sun)

**Discovery, Pharmacology & Medicinal Chemistry of Rapidly Acting Antidepressants** (see MEDI, Mon)

**Advances in Computer-Aided Biologics Design** (see COMP, Wed)

**Computation & Cheminformatics in Polymers Research** (see PMISE, Tue, Wed, Thu)

## SOCIAL EVENTS:

**Reception**, 6:30 PM: Sun

**Luncheon**, 12:00 PM: Tue

**Data Summit Reception**, 6:30 PM: Wed

## BUSINESS MEETINGS:

**Business Meeting**, 1:00 PM: Sat

- 11:25 CINF 6.** Virtues and vicissitudes of curatorial data wrangling: The guide to pharmacology experience. C. Southan
- 11:55** Concluding Remarks.

## Section C

San Diego Convention Center  
Room 25A

## From Data to Prediction: Applying Structural Knowledge in Drug Discovery &amp; Development

J. Cole, *Organizer, Presiding*

- 8:40** Introductory Remarks.
- 8:45 CINF 7.** Finding better aim at a moving target by exploiting structural data. M. Verdonk
- 9:15 CINF 8.** Bridging the dimensions: Seamless integration of 3D structure-based design and 2D structure-activity relationships to guide medicinal chemistry. M. Gastreich, M.D. Segall, C. Detering, E. Champness, C. Lemmen
- 9:45 CINF 9.** Predicting binding affinity doesn't work, or does it? C. Lemmen
- 10:15** Intermission.
- 10:30 CINF 10.** Structural knowledge by prediction: Crystal structure prediction tests and progress. C. Groom, J. Cole, A.M. Reilly
- 11:00 CINF 11.** Using physicochemical data and predictions in the risk assessment of mutagenic impurities. S. Stalford
- 11:30 CINF 12.** Profile-QSAR generation 2: Perfection, the enemy of the good? V.R. Polyakov, E.J. Martin, L. Tian

## Ethics 101

*Sponsored by PROF, Cosponsored by CHED, CINF and ETHC*

## Fall 2015 InterCollegiate Cheminformatics Course

*Sponsored by CHED, Cosponsored by CINF and MPPG*

## From Synthesis to Design: Modeling Tools for Medicinal Chemists

*Sponsored by COMP, Cosponsored by CINF and MEDI*

## SUNDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 25B

## Global Initiatives in Research Data Management &amp; Discovery

## Global Landscape

*Cosponsored by ANYL, COMP, MEDI and PHYS*

L. McEwen, *Organizer*I. Bruno, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:15 CINF 13.** Open data is not enough: A look at the Research Data Alliance. M. Parsons
- 1:45 CINF 14.** Responses to the data revolution: CODATA on policy, data science, and capacity building. S. Hodson, J. Rumble
- 2:15 CINF 15.** Moving research forward with persistent identifiers and services. P. Cruise

- 2:45 CINF 16.** Discoverability and reusability of FAIR chemistry research data as a key outcome of registering persistent identifiers and standardized metadata with DataCite. H.S. Rzepa, M.J. Harvey, A. McLean

3:15 Intermission.

**3:30 CINF 17.** Surveying and tracking the biomedical data landscape. M.E. Martone

**4:00 CINF 18.** Data Observation Network for Earth: Earth and environmental science data management and discovery. A.E. Budden, W. Michener, D. Vieglais, R. Koskela, H. Soyka

**4:30 CINF 19.** California Digital Library: Advancing the digital transition of scholarly information. J. Chodacki

## Section B

San Diego Convention Center  
Room 24C

## Data Mining: Searching Non-covalent Interactions in Chemical Databases

*Cosponsored by COMP*

S. Sirimulla, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05 CINF 20.** Sigma-hole interactions for rational drug design. S. Sirimulla
- 1:30 CINF 21.** Deep convolutional neural networks for autonomous discovery of molecular interactions. A. Heifets, I. Wallach, M. Dzamba
- 1:55 CINF 22.** Crystallographic informatics: Similarity and statistics. S.J. Coles, G.J. Tizzard, P. Adler
- 2:20 CINF 23.** Chemical fragment analysis of halogen bonds in protein binding sites. A. Chan
- 2:45** Intermission.
- 3:00 CINF 24.** Mining interaction data in the Cambridge structural database: Getting the rewards and removing the risks! J. Cole, P.A. Wood, N. Feeder, R. Taylor, C. Groom
- 3:25 CINF 25.** Fast mining of adaptable interaction patterns in protein-ligand interface. T. Inhester, M. Rarey
- 3:50 CINF 26.** Dual nature of a halogen atom. M. Narayan
- 4:15 CINF 27.** Crystal clear: Using statistical descriptions and analysis to understand crystallisation. P. Adler, S.J. Coles, A.J. Norquist, J. Schrier, D. Woods, S. Friedler, L. Mapp
- 4:40** Concluding Remarks.

## Section C

San Diego Convention Center  
Room 25A

## From Data to Prediction: Applying Structural Knowledge in Drug Discovery &amp; Development

J. Cole, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35 CINF 28.** Towards a fully automated creation of large protein structure ensembles. S. Bietz, M. Rarey
- 2:05 CINF 29.** On our way to the automated search for ligand-sensing cores. T. Brinkjost, C. Ehart, P. Mutzel, O. Koch
- 2:35 CINF 30.** Deep learning in the 3rd dimension: Structure-based bioactivity prediction on novel targets. A. Heifets, I. Wallach, M. Dzamba
- 3:05** Intermission.

**3:20 CINF 31.** CDD vision: Advanced analytics, calculations, and visualization live in CDD vault. B.A. Bunin

**3:50 CINF 32.** Advances in data provisioning. M.R. Brodney, J. Klug-McLeod, G.A. Bakken, R. Stanton

**4:20 CINF 33.** Chemical Information on the web: Find and be found. A. Gindulyte

## Discussions with the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

## Fall 2015 InterCollegiate Cheminformatics Course

*Sponsored by CHED, Cosponsored by CINF and MPPG*

## SUNDAY EVENING

## Section B

San Diego Convention Center  
Room 3

## Scholarships for Scientific Excellence: Student Poster Competition

S. J. Chalk, *Organizer*

6:30 - 8:30

- CINF 34.** Quantifying the effect that chemical environment exerts upon changes in property in matched molecular pairs analysis. I. Lukac, A. Leach, E.J. Griffen, A. Dossetter
- CINF 35.** CSNAP: A new cheminformatics approach for target identification using chemical similarity networks. Y. Lo, S. Senese, C. Li, Q. Hu, Y. Huang, R. Darnoiseaux, J. Torres
- CINF 36.** Prediction and quantification of cation- $\pi$  interactions in ligand-bromodomain binding: Using quantum chemistry to capture electronic effects. W. Cortopassi, R.S. Paton
- CINF 37.** 3Dmol.js: Chemical structure visualization for the modern web. J.L. Collins, M. Ragoza, J. Jensen, D. Koes
- CINF 38.** General purpose 2D and 3D similarity approach to identify HERG blockers. P. Schyman, R. Liu, A. Wallqvist
- CINF 39.** Indexing techniques and algorithms to efficiently mine interaction patterns in large sets of protein-ligand-complexes. T. Inhester, M. Rarey
- CINF 40.** Development and application of multiclass QSAR models for predicting human skin sensitization. V.M. Alves, A. Zakharov, E. Muratov, D. Fourches, N. Kleinstreuer, J. Strickland, C.H. Andrade, A. Tropsha
- CINF 41.** Virtual screening in the cloud computing environment. A. Cooper, M.R. Koebel, G. Schmadeke, S. Sirimulla
- CINF 42.** Structural evolution of  $Tc_n$  ( $n = 4-20$ ) clusters from first-principles global minimization. C. Priest, D. Jiang

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## SUNDAY MORNING

## Section A

San Diego Convention Center  
Room 25B

## Tomayto vs. Tomahto: Overcoming Incompatibilities in Scientific Data

D. Deng, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 CINF 1.** Relational database file can take us beyond the plain text file format. T. O'Donnell
- 9:05 CINF 2.** Standard JSON molecule, a solution to a cross-vendor molecule file format? B. Cole
- 9:35 CINF 3.** Rule-based capture/storage of scientific data from PDF files and export using a generic scientific data model. S.J. Chalk, A. Bartholomew, B. Baraz, J. Turner
- 10:05** Intermission.
- 10:25 CINF 4.** Building linked-data, large-scale chemistry platform: Challenges, lessons, and solutions. V. Tkachenko, A. Pshenichnov, A. Day, C. Batchelor, P. Corbett
- 10:55 CINF 5.** Towards a functional database for enzyme data: STRENDA DB. C. Kettner, M.G. Hicks

### My Comments to the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

### My Experience with & Advice for Improving Diversity in Chemistry

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

### My Experiences in & Advice for Organic Chemistry Courses

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 25B

#### Global Initiatives in Research Data Management & Discovery

#### Role of Community & Standards

Cosponsored by ANYL, COMP, MEDI and PHYS

I. Bruno, *Organizer*

L. McEwen, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 CINF 43. PubChem BioAssay: A decade's practice for managing chemistry research data. Y. Wang

8:45 CINF 44. Data infrastructural design for informing critical evaluation. K. Kroenlein

9:15 CINF 45. Community-driven disciplinary data repositories: A case study. I. Bruno, C. Groom

9:40 CINF 46. ICSU World Data System: Trusted data services for global science. M. Mokrane, J. Minster, R. Edmunds

10:10 Intermission.

10:25 CINF 47. STRENDA and MIRAGE: Examples of community-based data reporting standardization initiatives. M.G. Hicks, C. Kettner

10:55 CINF 48. Standardizing the description of nanomaterials: The CODATA uniform description system. J. Rumble, S. Freiman, C. Teague

11:25 CINF 49. Scientific units in the electronic age. S.J. Chalk

### Section B

San Diego Convention Center  
Room 24C

#### Beyond Digitized Paper: The Next Generation of ELNs

E. Davis, D. Deng, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 CINF 50. Toward semantic representation of science in electronic laboratory notebooks (ELNs). S.J. Chalk

8:45 CINF 51. New cloud based ELN with built-in raw analytical data support and automatic structure confirmation capabilities. S. Dominguez Vivero, J.C. Cobas Gomez, S. Fraga Castro, F. Sardina

9:10 CINF 52. Mobile interfaces for a digital research notebook. J.G. Frey, C. Willoughby, S.J. Coles, R.J. Whitby, C.L. Bird

9:35 CINF 53. Not just another reaction database. A. Day, V. Tkachenko, A. Pshenichnov, L. McEwen, S.J. Coles, R.J. Whitby

10:00 Intermission.

10:15 CINF 54. Directly upload data from an ELN into PubChem. B. Shoemaker, A. Gindulyte, E. Bolton, S. Bryant

10:40 CINF 55. Intuitive collaboration platform: A Scilligence story. R. Hotchandani, J. Lee

11:05 CINF 56. ACAS LIMS simplifies diverse data loading, management, and querying. J. McNeil, G. Oshiro, B.C. Fielder, E. Gao, S. Meyer, B. Bolt, F. McNeil, M. Shaw, K. Carr

11:30 CINF 57. ChemEngine: An automated chemical data harvesting tool for molecular inventory and chemical computing from scientific literature. M. Karthikeyan, R. Vyas

11:55 Concluding Remarks.

### Section C

San Diego Convention Center  
Room 25A

#### Informatics & Quantum Mechanics: Combining Big Data & DFT in Pharma & Materials

A. Cho, *Organizer, Presiding*

8:40 Introductory Remarks.

8:45 CINF 58. Screening of materials for energy applications based on transport properties: Methods and data automation tools. B. Kozinsky

9:15 CINF 59. High-throughput chemical simulations and virtual screening for materials discovery. M. Halls, D. Giesen, T. Hughes, S. Kwak, T. Mustard, J. Gavartin, A. Goldberg, Y. Cao

9:45 CINF 60. Machine learning and high-throughput quantum chemistry methods for the discovery of organic materials. A. Aspuru-Guzik

10:15 Intermission.

10:30 CINF 61. Using drug discovery methods to accelerate the search for better battery materials. J. Schrier

11:00 CINF 62. Combining density functional theory with cheminformatics for development of a new-paradigm ligand screening method in computational drug discovery. A. Cho

11:30 CINF 63. Discovery through deterministic optimization: Navigating chemical space for effective material design. J.M. Elward, C.B. Rinderspacher

#### Is There a Crisis in Organic Chemistry Education?

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

#### Preparing for the Real World: Challenges Faced by Young Investigators

#### Choosing Grad Research Advisors & a Career in Academia or Industry

Sponsored by MPPG, Cosponsored by CHED, CINF, COMP, PHYS and YCC

## MONDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 25B

#### Global Initiatives in Research Data Management & Discovery

#### Technical Infrastructures: Enabling Cultural Shifts

Cosponsored by ANYL, COMP, MEDI and PHYS

I. Bruno, L. McEwen, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CINF 64. Authoring tools to automate data sharing in scientific publishing. J.R. Kitchin

1:35 CINF 65. Facilitating the inclusion of analytical raw data in the submission and review process. S. Dominguez Vivero, J.C. Cobas Gomez, F. Seoane, J.A. Garcia Pulido, A. Barba, J.A. Varela Carrete

2:00 CINF 66. Crystallography: A domain exemplar for chemistry data management. S.J. Coles

2:30 CINF 67. Are data management solutions developed for commercial organizations suitable for academic research? M.E. Vaschetto, T. Oldfield, M.J. Hartshorn

2:55 Intermission.

3:10 CINF 68. Data sharing in life sciences R&D: Pre-competitive collaboration through the Pistoia Alliance. C.I. Nitsche

3:30 CINF 69. The Royal Society of Chemistry and the data publication landscape. S. Dabb

3:50 CINF 70. Digital IUPAC: The need for global representation of chemistry and chemical information in the digital age. J.G. Frey

4:10 CINF 71. DIG chemistry: Establishing a research data interest group to address the many faces of chemical data management. L. McEwen

4:30 Panel Discussion.

### Section B

San Diego Convention Center  
Room 24C

#### Chemical Information for Small Businesses & Startups

Cosponsored by CPRM and SCHB

E. S. Simmons, *Organizer, Presiding*

1:00 Introductory Remarks.

1:15 CINF 72. Building a business with and without scientific computing: The five W's and one H. S.M. Muskal

1:40 CINF 73. Interactive cheminformatics for occasional use in SMEs. T. Inhester, M. Hilbig, M. Rarey

2:05 CINF 74. Playing by the rules: Knowing what applies and what information you have to maintain regarding your chemical inventory. F.K. Wood-Black

2:30 CINF 75. ChemSpider: Search and share chemistry... for free. S. Dabb

2:55 Intermission.

3:10 CINF 76. What chemists and other scientists need to know about their duty of disclosure under the new law governing the patenting process in the US. X. Pillai

3:35 CINF 77. Monitoring the minnows: Using IP information to understand what small businesses are doing. S.R. Adams

4:00 CINF 78. Patent information in PubChem for small businesses and startups. S. Kim, P. Thiessen, E. Bolton, S. Bryant

4:25 CINF 79. Open patent chemistry "big bang" presents large opportunities for small enterprises. C. Southan

4:50 Concluding Remarks.

### Section C

San Diego Convention Center  
Room 25A

#### Informatics & Quantum Mechanics: Combining Big Data & DFT in Pharma & Materials

A. Cho, *Organizer, Presiding*

1:30 CINF 80. *In silico*, high-throughput screening of non-fullerene acceptor materials for applications of organic photovoltaic devices: A Harvard clean energy project study. S.A. Lopez, E. Pyzer-Knapp, A. Aspuru-Guzik

2:00 CINF 81. Regioselectivity prediction of metabolic reactions based on *ab initio* derived descriptors. A.R. Finkelmann, A.H. Göller, G. Schneider

2:30 CINF 82. COSMO-based approach for the design of solvents to optimize reaction rates. N.D. Austin, N.V. Sahinidis, D.W. Trahan

3:00 Intermission.

3:15 CINF 83. Efficient, first-principles-based screening for high-charge carrier mobility in organic crystals. C. Schober, K.U. Reuter, H. Oberhofer

3:45 CINF 84. Data-driven chemistry: From small molecules to discovery of new functional materials. O. Isayev, A. Tropsha

4:15 CINF 85. Multi-agent approach for molecular modeling in chemical vapor deposition. L.E. Achenie

#### Diversity-Quantification-Success?

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

#### Computers in Chemistry: Bridging the Gap between Clients & Software

Sponsored by SCHB, Cosponsored by CINF and ORGN

#### Preparing for the Real World: Challenges Faced by Young Investigators

#### Research at PUI's

Sponsored by MPPG, Cosponsored by CHED, CINF, COMP, PHYS and YCC

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

E. Davis, *Organizer*

8:00 - 10:00

2, 13, 21, 29, 32-33, 57-58, 63, 81. See previous listings.

99, 105, 110, 116-117, 131, 139, 143, 147, 165. See subsequent listings.

## TUESDAY MORNING

### Section A

San Diego Convention Center  
Room 25B

#### Chemistry, Data & the Semantic Web: An Important Triple to Advance Science

##### Chemical Classification

E. Bolton, S. J. Chalk, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 CINF 86. Towards knowledge representation improvements in chemistry. E. Bolton

8:45 CINF 87. Chemical classifications for biology and medicine. M. Kanehisa

9:10 CINF 88. Withdrawn.

9:35 CINF 89. ChEBI database and ontology: A key resource for chemical biology and metabolomics. G. Owen

10:00 Intermission.

10:15 CINF 90. Classifying chemistry: Current efforts in Canada. D.S. Wishart

10:40 CINF 91. Classifying compounds in public databases. L. Weber

11:05 CINF 92. Automated structural and functional annotation of small molecules using integrated chemical ontologies: ClassyFire, ChemOnt, and downstream applications. Y. Djoumbou Feunang

11:30 CINF 93. Evaluation of machine-generated chemical ontologies for molecular information. S. Boyer, T. Griffin, E. Louie

### Section B

San Diego Convention Center  
Room 24C

#### Linking Big Data with Chemistry: Databases Connecting Genomics, Biological Pathways & Targets to Chemistry

R. J. Bienstock, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 CINF 94. Connecting 3D chemical data with biological information. I. Bruno, S. Ward, E. Thomas, C. Groom

9:55 CINF 95. PubChem BioAssay: Link chemical research to GenBank and beyond. Y. Wang

10:15 CINF 96. Withdrawn.

10:35 Intermission.

10:50 CINF 97. Predicting adverse drug events using literature-based pathway analysis. J. Rinker, T. Hoctor

11:10 CINF 98. Intersecting different databases to define the inner and outer limits of the data-supported druggable proteome. C. Southan

11:30 CINF 99. Applications of drug-target data in translating genomic variation into drug discovery opportunities. A. Gaulton

### Section C

San Diego Convention Center  
Room 25A

#### Driving Change: Impact of Funders on the Research Data & Publications Landscape

Cosponsored by MEDI and ORGN

A. B. Twiss-Brooks, *Organizer*

E. Alvaro, *Organizer, Presiding*

8:35 Introductory Remarks.

8:40 Update on NSF MPS Open Data Policies.

8:50 CINF 100. NIH public access policy. N. Thakur

9:15 CINF 101. U.S. Department of Energy public access plan. L. Biven

9:40 CINF 102. Helping authors and funders achieve open access goals at ACS Publications. D. Henderson

10:05 CINF 103. Libraries at the hub as the federally funded research wheel turns to open. S. Kipphut-Smith, B. Rozum, B. Thoms

10:30 Intermission.

10:45 CINF 104. SHARE phase II: Enhancing the dataset and engaging the community. J. Ruttenberg

11:10 CINF 105. Supporting openness and reproducibility in scientific research: The Center for Open Science. S. Bowman

11:35 CINF 106. Impact of open publishing: Scalability, sustainability, and success. A. Gabriel

#### Computer-Aided Drug Design

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

## TUESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 25B

#### Chemistry, Data & the Semantic Web: An Important Triple to Advance Science

##### Chemical Information

E. Bolton, S. J. Chalk, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CINF 107. Representing the chemistry of 800,000 crystal structures. S. Ward, I. Bruno, C. Groom

2:00 CINF 108. CHEMnetBASE and beyond: CRC handbooks and dictionaries in today's world. F. Macdonald, M. Eisenbraun

2:25 CINF 109. Collection, curation, and communication of thermophysical and thermochemical property data at the NIST Thermodynamics Research Center. A. Kazakov, R. Chirico, C.D. Muzny, V. Diky, E. Paulechka, A. Bazyleva, J. Magee, S.A. Townsend, K. Kroenlein

2:50 CINF 110. Building a better materials science database: Challenges and opportunities. R. Padilla, M. Klinge

3:15 Intermission.

3:30 CINF 111. TCI's approaches to chemical information for researchers. H. Taguchi, T. Barber

3:55 CINF 112. Presenting the latest scientific knowledge on an e-commerce website. J. Stephan

4:20 CINF 113. Beyond chemistry: Collect, organize, and visualize scientific data on the web. D. Deng, R. Hotchandani, J. Lee

### Section B

San Diego Convention Center  
Room 24C

#### Linking Big Data with Chemistry: Databases Connecting Genomics, Biological Pathways & Targets to Chemistry

R. J. Bienstock, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 CINF 114. How can genomic databases be linked to chemical structural information? R.J. Bienstock

2:25 CINF 115. Reactome pathway knowledgebase: Connecting pathways, networks, and disease. R.A. Haw

2:45 CINF 116. Competitive intelligence workbench: Getting access to information for decision making. H. Wang

3:05 Intermission.

3:15 CINF 117. Using systems biology in computational drug design workflows. G. Nicola, B. Kovacs

3:35 CINF 118. Combining semantic triples across domains to identify new and novel relationships and knowledge. M. Clark, F. van den Broek, A. Yuryev, M. Shkrob, S. Matis-Mitchell, T. Hoctor

3:55 Concluding Remarks.

### Section C

San Diego Convention Center  
Room 25A

#### Driving Change: Impact of Funders on the Research Data & Publications Landscape

Cosponsored by MEDI and ORGN

E. Alvaro, *Organizer*

A. B. Twiss-Brooks, *Organizer, Presiding*

2:00 CINF 119. Are we ready to define the scholarly commons? M.E. Martone

2:25 CINF 120. Research data curation services at UC San Diego library. H. Yoo, D. Minor

2:50 CINF 121. Is open science an inevitable outcome of e-science? J.G. Frey

3:15 CINF 122. Navigating the research data ecosystem. D. Valen

3:40 Intermission.

3:55 CINF 123. Funding mandates and policies: A database provider's response. I. Bruno, C. Groom, A. Sarjeant

4:20 CINF 124. Quest to find "broader impact": How funding bodies are using altmetrics to evaluate funded research and grant applications. S. Rouhi

4:45 Concluding Remarks.

#### Computer-Aided Drug Design

##### Computational Biophysics

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

## WEDNESDAY MORNING

### Section A

San Diego Convention Center  
Room 25B

#### Chemistry, Data & the Semantic Web: An Important Triple to Advance Science

##### Informatics Application

E. Bolton, S. J. Chalk, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 CINF 125. Analytical data, the web, and standards for unified laboratory informatics databases. G.A. Mc Gibbon, P.D. Wheeler

8:45 CINF 126. From molecular formulas to Markush structures: Different levels of knowledge representation in chemistry. M. Braden

9:10 CINF 127. Strategies for creating knowledge from chemistry and text data. T. Oldfield, M.E. Vaschetto, J. Naus

9:35 CINF 128. Combined structure and reaction retrieval in scientific content: What satisfied users in the past and what they demand for the future. G.F. Herrmann, J. Eiblmaier, V. Eigner-Pitto

10:00 Intermission.

10:15 CINF 129. Harnessing chemical and toxicological data for the evaluation of food ingredients and packaging. D.M. Schmit, T. Page, K.B. Arvidson, P. Volarath, L. Holt

10:40 CINF 130. Expansion of DSStox: Leveraging public data to create a semantic cheminformatics resource with quality annotations for support of U.S. EPA applications. C. Grulke, I. Thillainadarajah, A.J. Williams, D. Lyons, J. Edwards, A. Richard

11:05 CINF 131. Comparative toxicogenomics database: Advancing understanding of molecular connections among chemicals, genes, and diseases. C.J. Grondin, A.P. Davis, T.C. Weigers, C.J. Mattingly

11:30 CINF 132. Wikidata: Advancing science through semantic integration of genes, diseases, and drugs. B.M. Good, E. Mitraka, A. Waagmeester, S. Burgstaller-Muehlbacher, T. Putman, A. Su, L. Schriml

### Section B

San Diego Convention Center  
Room 24C

#### Reimagining Libraries as Innovation Centers: Enabling, Facilitating & Collaborating throughout the Research Life Cycle

V. F. Scaffani, *Organizer*

Y. Li, *Organizer, Presiding*

8:45 Introductory Remarks.

8:50 CINF 133. From dusty stacks to an information hub: Reimagining the UF libraries. N. Bharti, S. Gonzalez

9:15 CINF 134. Expanding the research commons model into disciplinary instances. J.R. Garritano

9:40 CINF 135. Libraries for the future: A digital economy perspective. J.G. Frey, S. Brewer

10:05 Intermission.

10:20 CINF 136. Leveraging the interdisciplinarity of chemistry: Building interdisciplinary collaborations. K. Deards

10:45 CINF 137. Predicting local trends in scholarly communication for decision-making in collection development: An exploration beyond citation analysis. Y. Li

11:10 CINF 138. Academic technologies: A new library service to offer advanced software training. V.F. Scaffani, M.F. Green

11:35 CINF 139. Enhanced chemical understanding through 3D-printed models. A. Sarjeant, P.A. Wood, I. Bruno, Y. Li, V.F. Scaffani, S. O'Grady

#### Big Data & Small Data

Sponsored by ANYL, Cosponsored by CINF and MPPG

#### Chemical, Sample & Asset Management Tools

Sponsored by CHAS, Cosponsored by CCS and CINF

#### Chemical Imaging: Applications, Advances & Challenges

Sponsored by ANYL, Cosponsored by CINF and MPPG

**Computer-Aided Drug Design****Real World Dynamics**

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

**WEDNESDAY AFTERNOON****Section A**

San Diego Convention Center  
Room 25B

**Chemistry, Data & the Semantic Web: An Important Triple to Advance Science****Knowledge Representation Evolution**

E. Bolton, S. J. Chalk, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 CINF 140.** IUPHAR/BPS guide to pharmacology (GtoPdb): Concise mapping for the triples of chemistry, data, and protein target classifications. C. Southan, J.L. Sharman, A.J. Pawson, E. Faccenda, J.A. Davies

**2:00 CINF 141.** Open PHACTS: Semantic interoperability for drug discovery. H. Van Vlijmen, O. Consortium

**2:25 CINF 142.** Representation of drug discovery knowledge in the ChEMBL and SureChEMBL databases. A. Gaulton

**2:50 CINF 143.** Chemical knowledge representation and access in Wolfram|Alpha and Mathematica. E.W. Weisstein

**3:15** Intermission.

**3:30 CINF 144.** Helping people navigate the changing seas of scientific information. D. Evans, P. Caduff, T. Geouli, J. Swienty-Busch

**3:55 CINF 145.** Characterization and categorization of novel knowns, unknowns, and the interface between physical and digital. G. Whitley, B. Berger, T. Adams

**4:20 CINF 146.** Semantic approaches for biochemical knowledge discovery. M. Dumontier

**Section B**

San Diego Convention Center  
Room 24C

**Reimagining Libraries as Innovation Centers: Enabling, Facilitating & Collaborating throughout the Research Life Cycle**

Y. Li, *Organizer*

V. F. Scalfani, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 CINF 147.** Leveraging the VIVO research networking system to facilitate collaboration and data visualization. M. Trimarchi, D. Bodrero Hoggan

**2:00 CINF 148.** Stanford profiles created to support the university's scholarly community. G. Baysinger

**2:25 CINF 149.** Managing researchers' reputations throughout the research life cycle. L. Galloway, A. Rauh

**2:50** Intermission.

**3:05 CINF 150.** Anatomy of the chemistry research enterprise in the academic sector: Serving the underserved in a large research institution. L. McEwen

**3:30 CINF 151.** Safety use case for chemical safety information. R. Stuart

**3:55 CINF 152.** PubChem BioAssay: Grow with the community. Y. Wang

**4:20** Discussion.**4:40** Concluding Remarks.

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**Big Data & Small Data**

Sponsored by ANYL, Cosponsored by BIOL, CINF, COMP, MEDI and MPPG

**Chemical, Sample & Asset Management Tools**

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**Computer-Aided Drug Design****New Modalities RNA**

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**Chemical Imaging: Applications, Advances & Challenges**

Sponsored by ANYL, Cosponsored by CINF and MPPG

**THURSDAY MORNING****Section A**

San Diego Convention Center  
Room 25B

**Chemistry, Data & the Semantic Web: An Important Triple to Advance Science****Informatics Evolution & Use**

E. Bolton, S. J. Chalk, *Organizers, Presiding*

**8:15** Introductory Remarks.

**8:20 CINF 153.** Linking chemical and non-chemical data in structured product labeling. Y. Borodina, B. Hess, C. Tsai, P. Phong, L. Smith

**8:45 CINF 154.** Ginas: A global effort to define and index substances in medical products. T.A. Peryea, L. Callahan

**9:10 CINF 155.** TranSMART Foundation: An open-data and open-science platform to integrate molecular and clinical data in translational research and precision medicine. R. Potenzoni

**9:35 CINF 156.** Leveraging RxNorm and drug classifications for analyzing prescription datasets. O. Bodenreider

**10:00** Intermission.

**10:15 CINF 157.** Evolution of digital and semantic chemistry at Southampton. J.G. Frey, S.J. Coles, C.L. Bird

**10:40 CINF 158.** Implementing chemistry platform for OpenPHACTS: Lessons learned. C. Batchelor, A. Pshenichnov, J. Steele, V. Tkachenko

**11:05 CINF 159.** Representation of molecular structures and related computations on the semantic web: A universal data model and its ontology. M. Sopek, S.J. Chalk, N.S. Ostlund, J.W. Bloom

**11:30 CINF 160.** GlyYouCan international glycan structure repository using semantic web technologies. I. Yamada, K. Aoki-Kinoshita, N. Aoki, D. Shinmachi, M. Matsubara, A. Fujita, S. Tsuchiya, S. Okuda, N. Fujita, H. Narimatsu

**Section B**

San Diego Convention Center  
Room 24C

**General Papers**

E. Alvaro, E. Davis, *Organizers, Presiding*

**9:00** Introductory Remarks.

**9:05 CINF 161.** Progress toward a conformational database for sesquiterpene reaction pathways. J.D. Zehr, D.J. Tantillo, C.S. Hamann

**9:35 CINF 162.** OMPOL: Visualization of large chemical spaces. P. Corbett, C. Batchelor, A. Pshenichnov, V. Tkachenko

**10:05 CINF 163.** Comparison of machine learning algorithms for the prediction of critical values and acentric factors for pure compounds. W. Carande, A. Kazakov, K. Kroenlein

**10:35** Intermission.

**10:50 CINF 164.** Optimal superposition of arbitrarily ordered molecules using the Kuhn-Munkres algorithm. B. Temelso, J. Mabey, T. Kubota, G.C. Shields

**11:20 CINF 165.** Predicting drug-induced hepatic systems' toxicity by integrating transporter interaction profiles. E. Kotsampasakou, G.F. Ecker

**Big Data Science****Accessing Chemical Space & Better Modeling**

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

**Chemical Imaging: Applications, Advances & Challenges**

Sponsored by ANYL, Cosponsored by CINF and MPPG

**Computer-Aided Drug Design****New Modality Therapeutics**

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

**THURSDAY AFTERNOON****Section A**

San Diego Convention Center  
Room 25B

**Chemistry, Data & the Semantic Web: An Important Triple to Advance Science****Ontology Evolution & Use**

E. Bolton, S. J. Chalk, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 CINF 166.** Ontology for biomedical investigations (OB). B. Peters, J.A. Overton, R. Vita, O. Consortium

**2:00 CINF 167.** Protein ontology: Fostering connections in chemical biology. D. Natale

**2:25 CINF 168.** Ontologies for classifying and modeling drug discovery data. S. Schuerer, A. Lin, S. Mehta, H. Küçük McGinty, Q.C. Cheng, A. Koletli, N. Zadeh, D. Vidovic

**2:50** Intermission.

**3:05 CINF 169.** Immune Epitope Database (IEDB) and its use of formal ontologies. R. Vita, J.A. Overton, B. Peters

**3:30 CINF 170.** PubChemRDF: Semantic annotation and search. G. Fu, E. Bolton

**3:55 CINF 171.** Generic scientific data model and ontology for representation of chemical data. S.J. Chalk

**Big Data Science****Interpreting Pharmacology**

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

**CHAL****Division of Chemistry and The Law**

K. Bianco, J. Kennedy and J. Hasford, *Program Chairs*

**SOCIAL EVENTS:**

**Reception**, 6:00 PM: Mon

**Luncheon**, 12:00 PM: Mon

**BUSINESS MEETINGS:**

**Business Meeting**, 5:00 PM: Sun

**SUNDAY AFTERNOON****Section A**

San Diego Convention Center  
Room 22

**Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions**

A. H. Berks, X. Pillai, *Organizers, Presiding*

**12:00 CHAL 1.** Review of recent Federal Circuit decisions relevant to what scientists need to know about patent filing and prosecution. X. Pillai, A. Berks

**1:30** Panel Discussion.**Section A**

San Diego Convention Center  
Room 22

**Patenting Gene Sequences: What Is Patentable in Australia, Europe, Mexico & the U.S.**

J. L. Kennedy, *Organizer, Presiding*

D. Lorentzen, *Presiding*

**2:00 CHAL 2.** "Human ingenuity" vs. "application of laws of nature": Patenting gene sequences in Australia. M. Roberts

**2:45 CHAL 3.** "Human ingenuity" vs. "application of laws of nature": Patenting gene sequences in Europe. H. Tostmann

**3:30 CHAL 4.** "Human ingenuity" vs. "application of laws of nature": Patenting gene sequences in Mexico. M. Samano

**4:15 CHAL 5.** "Human ingenuity" vs. "application of laws of nature": Patenting gene sequences in the U.S.. D. Lorentzen

**MONDAY MORNING****Section A**

San Diego Convention Center  
Room 22

**Symposium on the Generic Drug User Fee Program (GDUFA) of 2012 & ANDA Review Process**

K. E. Bianco, *Organizer*

R. Randad, *Organizer, Presiding*

**8:30 CHAL 6.** Hatch-Waxman 101: A practical guide on the regulatory impact of exclusivity, patents, and patent litigation on generic drug development and approval. M.W. Toufanian

**9:00 CHAL 7.** Type II active pharmaceutical ingredient (API) drug master files (DMFs) under the Generic Drug User Fee Act of 2012 (GDUFA). R. Randad

**9:30 CHAL 8.** Regulatory science under the Generic Drug User Fee Act of 2012 (GDUFA), including FDA's consideration of complex drug substances and innovative analytical method development. X. Jiang

**10:00** Intermission.

**10:15 CHAL 9.** Policy development in the area of generic drug quality. A. Boam

**10:45 CHAL 10.** Quality assessment of generic drug products. S. Rosencrance

**11:15 CHAL 11.** Office of Process and Facilities role in generic drug review. R. Iser

**11:45** Panel Discussion.

## MONDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 22

#### The Role of Scientific Patent Information in the Innovation Process

E. N. Cheeseman, M. McBride, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 CHAL 12.** Techniques for searching for scientific information. E.N. Cheeseman

**2:05 CHAL 13.** Vital role of scientific patent information in the innovation process. L. Yu

**2:35 CHAL 14.** CAS: Innovative product solutions for faster, easier access to chemistry and related scientific information. S.P. Kuhn

**3:05 CHAL 15.** Resources for searching biological sequence patent information. K.L. Hoppe

**3:35 CHAL 16.** Cost-effective patent searching in small molecule drug development. J. Mallon, K. Miller

**4:05 CHAL 17.** Precision searching in STN's patent databases: Discover numeric properties. J. Brown

## MONDAY EVENING

### Section A

San Diego Convention Center  
Hall D/E

#### Sci-Mix

K. E. Bianco, J. L. Kennedy, *Organizers*

**8:00 - 10:00**

**CHAL 18.** Chocolate: Food of the gods. H.M. Peters, S.B. Peters

**CHAL 19.** National Inventors Hall of Fame 2016. H.M. Peters, S.B. Peters

**CHAL 20.** Use of bovine milk for the generation of LacDiNAc (LDN) bearing N-glycans for the chemenzymatic synthesis of schistosoma-type antigenic N-glycans. K.K. Robinson

## TUESDAY MORNING

### Section A

San Diego Convention Center  
Room 22

#### Recent Developments in Chemical & Pharmaceutical Patent Law

K. E. Bianco, *Organizer*

J. MacAlpine, E. M. Sommers, *Presiding*

**9:00 CHAL 21.** Hatch-Waxman and the orange book. J. MacAlpine

**9:45 CHAL 22.** Anticipation of challenges in pharmaceutical litigations. E.M. Sommers

**10:30 CHAL 23.** Post-grant challenges to pharmaceutical patents. K.E. Bianco, J. MacAlpine

**11:15** Panel Discussion.

## TUESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 22

#### Recent Developments in Chemical & Pharmaceutical Patent Law

**Challenges to Patentability**

K. E. Bianco, *Organizer*

R. C. Smith, *Organizer, Presiding*

**1:30 CHAL 24.** Methyl, ethyl, propyl, butyl, futile: The law of chemical obviousness. V. Capuano

**2:00 CHAL 25.** Indefiniteness in biotechnology and chemistry patents. R. Prince

**2:30 CHAL 26.** It's harder to get a patent than a Nobel Prize. V. Norton

**3:00** Panel Discussion.

## WEDNESDAY MORNING

### Section A

San Diego Convention Center  
Room 22

#### Building & Protecting Intellectual Property

K. E. Bianco, *Organizer*

R. C. Smith, *Organizer, Presiding*

**9:00 CHAL 27.** Under the microscope: Your workplace. J. Kearns

**9:45 CHAL 28.** Processing invention disclosures at a university technology transfer office. R.C. Smith

**10:30 CHAL 29.** Lab notebook: Friend or foe? J. Kearns

**11:15** Panel Discussion.

## WEDNESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 22

#### Chemistry of Peace

J. L. Kennedy, A. Usman, *Organizers, Presiding*

**1:00 CHAL 30.** Chemical and explosives terrorism: Domestic and international implications. V. Zaitsev

**2:00 CHAL 31.** Countering terrorism and attaining peace: Chemistry of peace. J. Forman

**3:00 CHAL 32.** Chemistry and human rights: Hand in hand for peace and stability.

A. Usman

## THURSDAY MORNING

### Section A

San Diego Convention Center  
Room 22

#### The Many Faces of CHAL: Where Chemistry Meets the Law

K. E. Bianco, J. L. Kennedy, *Organizers*

G. M. Halpenny, *Presiding*

**9:30 CHAL 33.** Opportunities in pharmaceutical pricing policies. G.M. Halpenny

## COLL

### Division of Colloid and Surface Chemistry

R. Nagarajan, *Program Chair*

#### OTHER SYMPOSIA OF INTEREST:

**Detection of Engineered Nanomaterials in Environmentally Relevant Media** (see ENVR, Sun)

**Functional Lignocellulosics & Nanotechnology** (see CELL, Sun, Mon, Tue, Wed)

**Applications of Polymer Surfaces & Interfaces** (see POLY, Sun, Mon, Tue, Wed, Thu)

**Physical Chemistry of Complex Environmental Interfaces** (see PHYS, Sun, Mon, Tue, Wed, Thu)

**Computers in Nanoscience & Nanotechnology** (see MPPG, Mon)

**Nanomaterials for Energy Conversion & Storage** (see ENFL, Mon, Tue, Wed)

**Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials** (see PHYS, Mon, Tue, Wed, Thu)

#### SOCIAL EVENTS:

**Social Hour, 6:00 PM:** Sun

**Luncheon, 12:00 PM:** Tue

#### BUSINESS MEETINGS:

**Executive Committee Meeting, 5:00 PM:** Sat

**Open Business Meeting, 5:30 PM:** Sun

## SUNDAY MORNING

### Section A

San Diego Convention Center  
Room 7A

#### ACS Award in Colloid & Surface Chemistry: Symposium in honor of Nicholas L. Abbott

##### Emulsions

P. Alexandridis, *Organizer*

M. E. Helgeson, Y. Kondo, *Presiding*

**9:00 COLL 1.** Structuring materials through droplet templating. D. Weitz

**9:30 COLL 2.** Behaviors of thermotropic liquid crystals 'caged' inside partially filled polymer capsules. D.M. Lynn

**10:00 COLL 3.** Thermoresponsive nanoemulsions: Quenchable colloids through molecular self-assembly. M.E. Helgeson

**10:30 COLL 4.** Photoinduced demulsification and two findings from the study. Y. Kondo

**11:00 COLL 5.** Complex emulsions as stimuli-responsive soft materials. V. Sresht, L. Zarzar, E. Sletten, J.A. Kalow, T.M. Swager, D. Blankschtein

### Section B

San Diego Convention Center  
Room 7B

#### Biomembrane Synthesis, Structure, Mechanics & Dynamics

##### Characterization

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, N. Sridivya, *Organizers*

D. Y. Sasaki, *Presiding*

**8:30 COLL 6.** Benzoic acid penetration of surfactant interfaces in the context of *Mycobacterium tuberculosis*. D.C. Crans, B.J. Peters, A. Groninger, D.C. Crick

**9:00 COLL 7.** From thermal fluctuations to extreme mechanics of polymer vesicles. H. Jang, K. Lou, K. Kim, C. Yu, K. Chen, S. Granick

**9:30 COLL 8.** Optimizing fluidity versus stability in planar supported and suspended lipid bilayers using mixtures of polymerizable and fluids lipids. C. Smith, M. Fonseca, K.S. Orosz, S. Saavedra

**10:00** Intermission.

**10:10 COLL 9.** Spontaneous lipid transfer and its implication of membrane lateral organization and structural stability. Y. Xia, K. Charubin, F. Heberle, D. Marquardt, J. Katsaras, J. Tian, X. Cheng, M. Nieh

**10:40 COLL 10.** Studying intracellular pathways of cationic liposome-nucleic acid nanoparticle assemblies with applications in gene delivery. K.K. Ewert, R.N. Majzoub, E.A. Wonder, V. Steffes, C.R. Safinya

**11:10 COLL 11.** Confocal Raman microscopy for *in situ* characterization of hybrid supported phospholipid bilayers within individual C<sub>18</sub>-functionalized chromatographic particles. J.P. Kitt, J.M. Harris

**11:40 COLL 12.** Photo-induced vesicle formation using "click" chemistries. D. Konetski, T. Gong, C. Bowman

### Section C

San Diego Convention Center  
Room 8

#### Nanomedicines: Targeting & Clearance Targeting

Z. Gu, Z. Wang, J. Xie, *Organizers*

G. Han, J. Zheng, *Organizers, Presiding*

**8:30 COLL 13.** Renal clearable luminescent gold nanoparticles. J. Zheng

**9:00 COLL 14.** Direct delivery of proteins and nucleic acids to the cytosol. V.M. Rotello

**9:30 COLL 15.** Enhancing tumor delivery and targeting with sub-5 nm ultrafine magnetic nanoparticles and anti-bio-fouling coating. H. Mao, J. Huang, Y. Li, L. Wang, L. Yang

**10:00 COLL 16.** Nanolayered delivery for synergistic tumor therapies. P.T. Hammond

**10:30 COLL 17.** One-component nanomedicine. R. Lin, H. Su, P. Zhang, H. Cui

**11:00 COLL 18.** Mageto-optical nanoparticles for ultrasensitive tumor imaging. X. Gao

**11:30 COLL 19.** Surface chemistry effect: Renal clearance and tumor targeting of NIR-emitting gold nanoparticles. J. Liu, M. Yu, X. Ning, J. Zheng

**11:50 COLL 20.** B-glucan/ODN carrier conjugated with TAT peptide: Specific delivery to cytosol. N. Miyamoto, S. Mochizuki, K. Sakurai

## Section D

San Diego Convention Center  
Room 9

### Nanometal: Synthesis, Structure, Property & Application

#### Nanoclusters

Y. Han, J. Zheng, *Organizers*

D. Jiang, *Organizer, Presiding*

Q. Wang, *Presiding*

**8:30** Introductory Remarks.

**8:35 COLL 21.** Ligand-protected gold superatoms and superatomic molecules. T. Tsukuda

**9:10 COLL 22.** Controlling colloidal gold nanoparticles with atomic precision: Fundamentals and opportunities. R. Jin

**9:45 COLL 23.** Gold and silver in nanoscale, dispersed by ligands to molecular precision. H. Hakkinen

**10:20** Intermission.

**10:50 COLL 24.** High-resolution separation of thiolate-protected gold clusters by reversed-phase high-performance liquid chromatography. Y. Negishi

**11:25 COLL 25.** Comparative studies on ligand binding stability on Au(111) surface. Q. Tang, D. Jiang

**11:45 COLL 26.** Controlling synthesis of atomic precision alloy nanoclusters and their structure related properties. M. Zhu, S. Wang, Y. Song, S. Jin, J. Xiang

## Section E

San Diego Convention Center  
Room 10

### Frontier of the Interface of Materials & Biology: Protein Based Nanomaterials Virus Based Chemistry & Materials Sciences

Q. Wang, *Organizer*

H. Yi, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 COLL 27.** What do you get when you cross a virus with a polymer? M. Hovlid, C. Scheibe, J.K. Pokorski, C.J. Higginson, M. Finn

**9:05 COLL 28.** Water at the tobacco mosaic virus. A. Bittner

**9:35 COLL 29.** Protein-templated self-assembly of hierarchical nanoarchitectures. Q. Wang

**10:05 COLL 30.** Engineering virus-like nanotubes and rods. J.N. Culver

**10:35 COLL 31.** Rod-like plant virus: Functionalization, self-assembly, and bioapplications. Z. Niu, Y. Tian

**11:05 COLL 32.** Dynamic assemblies of virus-like particles in solution and on surfaces. J.J. Cornelissen

**11:35 COLL 33.** Frame-guided assembly. D. Liu

## Section F

San Diego Convention Center  
Room 11A

### Colloids for Medical Imaging

#### Cellular Labeling, Tracking & Delivery

J. M. Berlin, *Organizer*

P. del Pino, W. Parak, *Organizers, Presiding*

J. Berlin, *Presiding*

**8:30** Introductory Remarks.

**8:35 COLL 34.** Degradation of colloids *in vitro* and *in vivo*. W. Parak

**8:45 COLL 35.** Biological interactions of layer-by-layer engineered particles. F. Caruso

**9:15 COLL 36.** Peptide-mediated cytosolic internalization of luminescent quantum dots. A. Kapur, W. Wang, S. Medina, J. Schneider, H.M. Mattoussi

**9:45 COLL 37.** Co-precipitation of SPIONs for stem cell tracking: How synthesis conditions affect particle properties, stem cell labelling, and MR contrast. M. Barrow, A. Taylor, J. Garcia Carrion, P. Mandal, H. Poptani, P. Murray, M. Rosseinsky, D. Adams

**10:05** Intermission.

**10:35 COLL 38.** Multicompartmental particles for combined imaging and release. J. Lahann

**11:05 COLL 39.** Perfluorocarbon-loaded polymeric nanoparticles for cell tracking using multimodal *in vivo* imaging. O. Koshkina, E. Swider, M. Boerman, J. van der Weijden, S. Xiaofeng, J. van Hest, E. van Dinther, C. Figdor, J. de Vries, M. Srinivas

**11:25 COLL 40.** Gold nanocages for imaging and therapy of prostate cancer by active targeting of neuropeptide Y-receptor. S. Avakumova, E. Galbiati, L. Sironi, S.A. Locarno, C. Macchi, M. Ruscica, P. Magni, S. Romeo, D. Prosperi

**11:55 COLL 41.** Mesoporous silica nanoparticles for ultrasound/magnetic resonance imaging and therapeutic drug delivery for stem cell therapy. P. Kempen, J. Campbell, S. Greasley, J. Jones, S. Gambhir, R. Sinclair, J.V. Jokerst

## Section G

San Diego Convention Center  
Room 11B

### Basic Research in Colloids, Surfactants & Nanomaterials

#### Metal & Metal Oxide Nanoparticles

R. Nagarajan, *Organizer*

J. E. Whitten, *Presiding*

**8:30 COLL 42.** Direct measurement of the functionalization of metal oxide nanoparticles through radioanalytical methods. K. Davis, J. Mayer, M. Witmer, B. Qi, B.A. Powell, C.L. Kitchens, O.T. Mefford

**8:50 COLL 43.** Synthesis and optical characterization of cysteine- and cystine-coated metal nanoparticles. A. Thomas

**9:10 COLL 44.** Synthesis of Co-based bimetallic nanocrystals with rod-like branches for selective hydrogenation of CO. Y. Zhu

**9:30 COLL 45.** Fluorescence properties of hybrid core-shell superparamagnetic Fe@C-CNx nanoparticles. S. Murugesan, O. Kuznetsov, Z. Zhou, V.N. Khabashesku

**9:50 COLL 46.** 2D Cu<sub>2</sub>xS nanocrystals from thermolysis of a lamellar template. W. Bryks

**10:10 COLL 47.** Electrochemical control of vanadium dioxide nanocrystal films. G. LeBlanc, A. Bergerud, C.J. Dahlgren, D.J. Milliron

**10:30 COLL 48.** Palladium nanoparticle seed mediated growth of palladium nanoshell on silica core. K. Bandyopadhyay, J. Jeffries, R. Teh

**10:50 COLL 49.** Temperature dependence of the nanocrystal nucleation revealed through plasmon resonance of bimetallic nanoparticles. N. Razgoniaeva, M. Zamkov

**11:10 COLL 50.** Photoluminescent zinc oxide nanoparticles: Surface chemistry and gas sensing. J.E. Whitten

**11:30 COLL 51.** Remediation of organophosphates by mixed metal oxide nanocomposites. M.M. Allard, K. Gates, R.S. Kellow, B. Figueroa, V. Liu, J. Song, K. Nick, C.C. Perry

## Section H

San Diego Convention Center  
Room 24B

### Basic Research in Colloids, Surfactants & Nanomaterials

#### Nanomaterials Design & Applications

R. Nagarajan, *Organizer*

J. V. Jokerst, *Presiding*

**8:30 COLL 52.** Engineering cascade reactions via supraparticle assemblies. N. Ramesar, N. Kotov

**8:50 COLL 53.** Saporin magnetic nanodriv-ers for suicide breast cancer therapy. R. Vago, V. Collicco, S. Zuppono, M. Colombo

**9:10 COLL 54.** Ternary sol-gel nanoparticle for ultrasound imaging of mesenchymal stem cells. F. Foroutan, J. Knowles, J.V. Jokerst

**9:30 COLL 55.** Molecular imprinted bio-sensor for rapid detection of CEA from pancreatic fluid cysts. Y. Yu

**9:50 COLL 56.** Light responsive supra-molecular nanoparticles. E. Cavatorta, J. Voskuhl, J. Brinkmann, D. Wasserberg, J. Huskens, P. Jonkheijm

**10:10 COLL 57.** Copper sulfide nanodisks are photoacoustic imaging contrast agents. J. Wang, B. Marin, A.R. Tao, J.V. Jokerst

**10:30 COLL 58.** Synthesis and characterization of ash rice husk supported manganese nanocomposite and its application for adsorption of Cd(II), Pb(II) and Cu(II) ions. O.A. Dada, F.A. Adekola, E.O. Odebummi

**10:50 COLL 59.** Design and preparation of surface Au-Pd alloy nanocatalysts for alkyne semihydrogenation. M. Jin, X. Li

**11:10 COLL 60.** Synthesis, characterization, viability assessment and silica encapsulation of thiol- capped CdSe quantum dots. M.R. Rodriguez, O. Rivera, J.G. Medina, J. Lopez-Colon, G.J. Ortiz-Torres, O.M. Primera

**11:30 COLL 61.** Echogenicity of mesoporous and nonporous silica nanoparticles. F. Chen, J.V. Jokerst

### Applications of Polymer Surfaces & Interfaces

#### New Processes & Surface Functionalization

*Sponsored by POLY, Cosponsored by COLL and PMSE*

#### Physical Chemistry of Complex Environmental Interfaces

*Sponsored by PHYS, Cosponsored by COLL*

## SUNDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 7A

#### ACS Award in Colloid & Surface Chemistry: Symposium in honor of Nicholas L. Abbott

#### Stimuli-Responsive Interfaces

P. Alexandridis, *Organizer*

J. Frechette, J. Texter, *Presiding*

**2:00 COLL 62.** Redox-mediated electro-sorption for chemical and environmental separations. T. Hatton

**2:30 COLL 63.** Engineering responsive liquid crystal interfaces with surfactants, lipids, and nucleic acids. D.K. Schwartz

**3:00 COLL 64.** Surface engineering using vapor-deposited polymers. J. Lahann

**3:30 COLL 65.** Programming polymeric nanomaterials with enzymes, peptides and nucleic acids. N.C. Gianneschi

**4:00 COLL 66.** Stimuli-responsive surfactants, polymers, and materials. J. Texter

**4:30 COLL 67.** Approach to contact of soft or structured surfaces in fluids. J. Frechette

### Section B

San Diego Convention Center  
Room 7B

#### Biomembrane Synthesis, Structure, Mechanics & Dynamics

#### Spectroscopy & Microscopy

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

M. L. Longo, *Presiding*

**2:00 COLL 68.** Molecular interactions between cell membranes and biological molecules. Z. Chen

**2:30 COLL 69.** Quantifying molecular transport through cell membranes by nonlinear light scattering. H. Dai

**3:00 COLL 70.** Molecular origins of cholesterol accelerated lipid flip-flop. J.C. Conboy, J. Allhusen

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3:30 Intermission.

3:40 **COLL 71.** Fluorescent lipids with selective partitioning to liquid ordered membrane domains. **D.Y. Sasaki**, S. Bordovsky, J. Stachowiak, G.D. Bachand

4:10 **COLL 72.** Kinetics of peptide-membrane interactions. **F. Gai**

4:40 **COLL 73.** NMR structural studies on functional cannabinoid type II receptor in a lipid matrix. **T. Kimura**, K. Vukoti, D.L. Lynch, D.P. Hurst, A. Grossfield, M.C. Pitman, P.H. Reggio, A.A. Yeliseev, K. Gawrisch

5:10 **COLL 74.** Correlating lipid-protein interactions with single particle tracking and PIE-FCCS. **A.W. Smith**, X. Shi, X. Li

## Section C

San Diego Convention Center  
Room 8

### Nanomedicines: Targeting & Clearance Delivery

Z. Gu, G. Han, Z. Wang, *Organizers*

J. Xie, J. Zheng, *Organizers, Presiding*

2:00 **COLL 75.** Coating nanoparticles with cell membranes for targeted drug delivery. **L. Zhang**

2:30 **COLL 76.** Nucleic acid delivery systems for RNA therapy and gene editing. **D.G. Anderson**

3:00 **COLL 77.** Enzyme-instructed assembly to form nanostructures for selectively inhibiting cancer cells. **B. Xu**, J. Zhou, X. Du, J. Shi, J. Li, H. Wang, Z. Feng

3:30 **COLL 78.** Surfactant additives to improve the distribution of inhaled drugs in the lungs. **T.E. Corcoran**, R. Sharma, A. Khanal, A. Stetten, T.M. Przybycien, R.D. Tilton, S. Garoff

4:00 **COLL 79.** Leveraging physiology for programmed precision nanomedicine. **Z. Gu**

4:30 **COLL 80.** Neutrophil-mediated transport of nanoparticles across blood barriers. **Z. Wang**

5:00 **COLL 81.** Nano-theranostics for photothermally triggered immunotherapy against cancer. **Z. Liu**

5:30 **COLL 82.** Using neural stem cell: Nanoparticle constructs to selectively deliver therapeutics to ovarian cancer. **P. Cao**, R. Tirughana-Samban, S. Aramburo, U. Nwokafor, K. Aboody, J. Berlin

## Section D

San Diego Convention Center  
Room 9

### Nanometal: Synthesis, Structure, Property & Application

#### Nanoclusters

Y. Han, D. Jiang, J. Zheng, *Organizers*

H. Hakkinen, T. Tsukuda, *Presiding*

2:00 **COLL 83.** Distinguishing superatomic, metallic, and ligand-state electron dynamics in monolayer protected nanoclusters using femtosecond nonlinear spectroscopy. **K.L. Knappenberger**

2:35 **COLL 84.** New design strategies for highly luminescent gold nanoclusters. **D. Lee**

3:10 **COLL 85.** Modulation of optical property and response of small gold clusters through the design of surface organic ligands. **K. Konishi**

3:45 Intermission.

4:15 **COLL 86.** Chirality of nanoscale gold particles and clusters. **T. Bürgi**

4:50 **COLL 87.** Nonlinear optical properties of thiolate-protected gold clusters: Second-harmonic scattering. **S. Knoppe**, T. Verbiest

5:10 **COLL 89.** Jahn-Teller effects in thiol protected gold nanoclusters and doped thiol protected gold nanoclusters. **C.J. Ackerson**, M.A. Tofanelli, T.W. Ni

5:45 **COLL 88.** Interconversion between superatomic electron configurations of  $M@Au_{24}(SR)_{18}$  ( $M = Au, Pd, Pt$ ) clusters. **K. Kwak**, Q. Tang, M. Kim, D. Jiang, D. Lee

## Section E

San Diego Convention Center  
Room 10

### Frontier of the Interface of Materials & Biology: Protein Based Nanomaterials

#### Virus Based Chemistry & Materials Sciences

H. Yi, *Organizer*

Q. Wang, *Organizer, Presiding*

1:30 **COLL 90.** From pathogen to cure: Plant virus-based therapeutics. **N. Steinmetz**

2:00 **COLL 91.** Dynamics of the adsorption and reduction of palladium on plant viruses. **O.O. Adigun**, E.L. Retzlaff-Roberts, G.D. Novikova, **M.T. Harris**

2:30 **COLL 92.** Viral templated palladium nanocatalysts. **H. Yi**

2:50 **COLL 93.** Effect of nanotopography created by plant virus nanoparticles on osteogenic differentiation of bone derived mesenchymal stem cells. **K. Metavarayuth**, P. Sitasuwan, J. Luckanagul, Q. Wang

3:10 **COLL 94.** Virus-like-particles in advanced materials applications. **J.J. Gassensmith**

3:30 **COLL 95.** Virus bionanomaterials development and potential clinical applications. **P. van Rijn**

4:00 **COLL 96.** Plasmonically active filamentous viruses as protein sensors. **J. Cha**

4:30 **COLL 97.** Influencing material properties using biomolecular interactions. **R.R. Naik**

5:00 **COLL 98.** Synthesis and characterization of metal-organic frameworks coated virus particle. **S. Li**, M. Dharmawardana, R. Welch, J.J. Gassensmith

## Section F

San Diego Convention Center  
Room 11A

### Colloids for Medical Imaging

#### Targeted Imaging & Therapy

J. M. Berlin, P. del Pino, W. Parak, *Organizers, Presiding*

2:00 **COLL 99.** Layer-by-layer near-IR II theranostic systems for ovarian cancer. **L. Gu**, X. Dang, J. Qi, S. Correa, G. Zhang, A.M. Belcher, **P.T. Hammond**

2:30 **COLL 100.** Theranostics of tumoral cells with nanoparticles. **P. Taboada Antelo**, A. Topete, E. Villar-Alvarez, S. Barbosa

3:00 **COLL 101.** Tumor-specific nuclear targeting *in vivo* of graphene quantum dots via a mesoscopic interstitial fluid. **Y. Wang**, C. Yao, L. Ding, C. Li, D. Pan, M. Wu

3:30 **COLL 102.**  $^{99m}Tc$ -labeled multifunctional low-generation dendrimer-entrapped gold nanoparticles as a platform for targeted dual mode SPECT/CT imaging of tumors. **X. Shi**, X. Li, C. Peng, X. Xu, Y. Luo, M. Shen

3:50 **COLL 103.** Improved contrast in whole-body imaging with targeted colloids and membrane-impermeable quenchers and etchants. **G.B. Braun**, X. Liu, K. Sugahara, E. Ruoslahti

4:10 Intermission.

4:40 **COLL 104.** Size-selected imageable nanoparticles for effective image-guided vaccine delivery and cancer immunotherapy. **J.C. Mareque-Rivas**, **A. Ruiz de Angulo**, **N. Gomez Blanco**, **A. Zabaleta**, **A. Garaikoetxea Arguinzoniz**, **A. Bocanegra**, **V. Gómez Vallejo**, **D. Pedro**, **B. Szczupak**

5:10 **COLL 105.** Two-step Raman imaging-guided chemo-photothermal cancer therapy. **N.M. Khashab**

5:40 **COLL 106.** Targeting polydopamine-coated gold nanocages to tumor cells using the anti-angiogenic peptide anginex. **S.V. Jenkins**, R.P. Dings, J. Chen, R.J. Griffin, D. Nedosekin

6:00 **COLL 107.** Labelling of mesenchymal stem cells with gold nano: An initial *in vitro* study towards future *in vivo* tracking of mesenchymal stem cells. **W. Parak**, N. Feliu, P. Nold, K. Kantner, R. Hartmann, M. Gamal, B. Pelaz, M. Lim, S. Sjöqvist, P. Jungebluth, P. del Pino, H. Hackstein, P. Macchiarini, C. Brendel

## Section G

San Diego Convention Center  
Room 11B

### Basic Research in Colloids, Surfactants & Nanomaterials

#### Gold Nanoparticles & Plasmonics

R. Nagarajan, *Organizer*

K. Bandyopadhyay, *Presiding*

2:00 **COLL 108.** Impact of the gold nanoparticle stabilizing ligands on catalysis. **S.M. Ansar**, C.L. Kitchens

2:20 **COLL 109.** Probing the surface chemistry of ligand capped gold nanostructures by nuclear magnetic resonance (NMR) spectroscopy. **C. Guo**, B. Cherry, S. Amin, J.L. Yarger

2:40 **COLL 110.** Changes in alkanethiolate chain length result in large changes to the electronic properties of the metallic core in gold nanoparticles, as probed by conduction electron spin resonance. **B.J. Lear**, A. Cirri

3:00 **COLL 111.** Evaluation of thiolated ligand exchange on gold surfaces by using surface-enhanced Raman scattering. **W. Qian**

3:20 **COLL 112.** Synthesis of carbon-based nanomaterials loaded with silver and gold and their Raman and SERS characterization. **T.A. Saleh**, A. Alabsi

3:40 **COLL 113.** Controlling gold nanorod synthesis via surface acoustic waves. **J. Hartanto**, M. Miansarigavzan, J. Wang, J. Friend, J.V. Jokerst

4:00 **COLL 114.** Synthesis and characterization of nanodiamond based hybrid nanostructures. **J. Gong**, N. Steinsultz, M. Ouyang

4:20 **COLL 115.** *In situ* spectroscopy of the ligand exchange at the surface of colloidal Au nanoparticles. **R. Dinkel**, B. Braunschweig, W. Peukert

4:40 **COLL 116.** Withdrawn.

5:00 **COLL 117.** Aryl bisthiolate functionalized plasmonic nanoporous discs: New direction for detecting polycyclic aromatic hydrocarbons using surface-enhanced Raman spectroscopy. **O. Zenasni**, F. Zhao, Y. Sung, G. Santos, T. Lee, W. Shih

## Section H

San Diego Convention Center  
Room 24B

### Proteins & Polymers Under Confinement

R. G. Toomey, R. S. Tu, *Organizers, Presiding*

2:00 Introductory Remarks.

2:05 **COLL 118.** Sequence-dependent self-assembly of peptide amphiphiles via molecular simulations. **H. Nguyen**

2:35 **COLL 119.** Recognition in tight spaces. **D.E. Leckband**, N. Shashikanth

3:05 **COLL 120.** Colloid-enhanced poly-peptide polydispersities: Synthesis of self-assembling, amphiphatic  $\beta$ -sheets. **M.B. Kubiilus**, R.S. Tu

3:25 **COLL 121.** Interactions between water-soluble peptoids and silica surfaces studied by second harmonic generation. **G.Y. Stokes**, A.L. Calkins, A.A. Fuller

3:45 **COLL 122.** Use of a unique protein model system to explore the effects of crowding by sol-gel confinement, polymeric crowding and small-molecule osmolyte crowding on different levels of protein structure. **V. Krejci**, K. Christensen, K. Lozier, J. Caballero, M.V. Wilson, E.E. Wilson

4:05 **COLL 123.** Dynamics of periodically sequenced polypeptides at the aqueous/liquid crystal interface. **R.S. Tu**

4:25 **COLL 124.** Scaling of polymer dynamics at an oil-water interface in regimes dominated by viscous drag and desorption-mediated flights. **D. Wang**, D.K. Schwartz

4:45 **COLL 125.** Surface tension of nano-confined lattice polymers. **P. Zhang**, **Q. Wang**

5:05 **COLL 126.** Frustration by shape design: A colloidal glass of hard Brownian kites. **T.G. Mason**

5:25 **COLL 127.** Nanoscale surface creasing induced by post-polymerization modification. **K. Brooks**, J. Razavi, X. Wang, J.J. Locklin

### Discussions with the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINP, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

### Applications of Polymer Surfaces & Interfaces

#### New Processes & Surface Functionalization

*Sponsored by POLY, Cosponsored by COLL and PMSE*

### Environmental Interfaces

#### Surface Structures

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG†*

### Physical Chemistry of Complex Environmental Interfaces

*Sponsored by PHYS, Cosponsored by COLL*

## SUNDAY EVENING

## Section A

San Diego Convention Center  
Hall E

## Fundamental Research in Colloids, Surfaces &amp; Nanomaterials

R. Nagarajan, *Organizer*

6:00 - 8:00

- COLL 128.** Synergistic enhancement of antibiotic activity with silver nanoparticles. G. Vildor, K. LaiHing
- COLL 129.** Enhanced solid state fluorescence of nano-colloid and its application on a immunofluorescence labeling. H. Kim
- COLL 130.** Maneuvering the growth pathways of silver nanoplates in kinetically controlled synthesis. M. Kim
- COLL 131.** Synthesis of multilayer organic thin film with variable densities by layer-by-layer (LBL) deposition technique. M. Rashed, M. Hara, S. Nagano, Y. Nagao
- COLL 132.** High throughput protein biomarker studies for early cancer detection. D. Angrish, M.L. Stolowitz, R. Elison, S.S. Datwani
- COLL 133.** Tobacco mosaic virus stabilized by coordination polymers. R. Welch, S. Li, M. Dharmawardana, J.J. Gassensmith
- COLL 134.** Synthesis of PbS/CdS core/shell nanocrystals for emerging optoelectronics applications. S. Krishnamurthy, S. Rupich, J.A. Hollingsworth, A. Malko
- COLL 135.** Optical detection of phosphatase activity with fluorescent graphene oxid. J. Ju, S. Jeon, T. Kang, H. Kim, J. Kim
- COLL 136.** Behavior of nanoscopic quantities of water in reverse micelles using NMR and fluorescence spectroscopies. B. Shone, B.L. Gourley
- COLL 137.** Preparation of octanoic acid coated  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> nanoparticles monolayers using a mixed solvent system. J. Feng, H. Jayathilake
- COLL 138.** What controls the biological stability of RNA immobilized on nanoparticle surfaces? S.N. Barnaby, G. Perelman, C.A. Mirkin
- COLL 139.** PbS/CdS and PbS/ZnS all inorganic quantum dot thin films for solar cells. J.G. Beltran
- COLL 140.** Morphologies of poly(vinyl alcohol) films adsorbed on polydimethylsiloxane substrates with and without plasma treatment. Y. Yan, A. Karki, W. Chen
- COLL 141.** XPS and SERS characterization of plasma-treated Ag colloids. S. Lee, Z. Yang
- COLL 142.** Performance of a new anti-fouling coating on biofilm growth on nanofiltration membranes. Y. Li, W. Hui, K. Yeung
- COLL 143.** Synthesis and biomedical applications of carbon nanomaterials: Investigation of PEG-HCCs in the treatment of ROS-mediated conditions and glioblastoma. L.G. Nilewski, M.A. Sharpe, W. Sikkema, A.S. Jallio, D. Baskin, J.M. Tour
- COLL 144.** Partitioning of organics into surfactant bilayers. R.K. Lindsey, S.N. Jamadagni, D. Eike, P.H. Koenig, J.I. Siepmann
- COLL 145.** Modified atomic layer deposition of ZnS on CdSe quantum dot thin films. F. Al-Quaiti, D. Khon, P. Moroz, A. Lahey, M. Zamkov
- COLL 146.** Size-tunable interfacial charge transfer with CdSe/CdS nanorod photocatalysts. V.L. Bridewell, R. Alam, P.V. Kamat
- COLL 147.** Room temperature growth of CdS monolayers on spherical quantum dots. L.J. Carrillo, D. Khon, N. Razgoniaeva, M. Zamkov
- COLL 148.** Probing nano-bio interactions via a multipronged approach. F. Geiger, H. Fairbrother, J.A. Pedersen, J. Troiano, T. Kuech, A. McGeachy, L.L. Olenick, E. Melby, R. Lankone, E. Ehimighe
- COLL 149.** Characterizing the aggregation of chromonic dyes in the isotropic phase via prodan, an extrinsic fluorophore. Z. Evans, A. Zhang, K.K. Karukstis
- COLL 150.** Synthesis of unusually large magnetic nanospheres and their novel applications in protein detection. Y. Chen, S. Xu, T. Lee
- COLL 151.** Long-range hydrophobic interaction and contact mechanic between rough polymer films in H<sub>2</sub>O, D<sub>2</sub>O, and electrolyte solutions. D. Kienle, J. Ventrici de Souza, T. Kuhl
- COLL 152.** Characterizing divalent metal ion binding sites in graphene oxide with Mn(II) ions. G.E. Decker, L. Nolasco, K. Gesuelli, D.J. Hirsh
- COLL 153.** Method for attaching thiol groups on a silicon (111) substrate. X. Zhang, D. Brodus, V. Hollimon
- COLL 154.** Fabrication of thermoresponsive PEGMA colloids for controlled drug delivery. M. Atas, A. Ozkaya Balci, M. Yavuz
- COLL 155.** Iron oxide nanocages for medical applications. H. Matsui, S. Rampersaud, J. Fang
- COLL 156.** Adsorption of amphoteric polyacrylamide on silica and cellulose surfaces monitored by QCM. Y. Zhu, F. Yang, E. Jin, J. Song
- COLL 157.** Withdrawn.
- COLL 158.** Surface oxidation-reduction of CuOx nanoparticles for the catalytic oxidative reaction. D. Tsai, Y. Lu, C. Lin, F. Chiou, F. Lee
- COLL 159.** Amyloid targeting polymeric nanoparticles which inhibit the enhancement of HIV infectivity related to binding and internalization of HIV virions by SEVI amyloid fibril-mediated mechanisms. D. Sheik, L. Brooks, K. Frantzen, S. Dewhurst, J.C. Yang
- COLL 160.** Zeta potential measurements for the characterization of polymer surfaces with varying amide/amine contents. Z. Zhang, A. Kelly, I. Mühlbacher, F. Stelzer, F. Wiesbrock
- COLL 161.** Modeling the effect of varying surface thickness on the photomobilities of Si slabs. R. Hembree, T. Vazhappilly, D.A. Micha
- COLL 162.** Fluorescently multiplexed proteinase K: Non-mesoporous silica nanoparticle. N. Ledra, T. McCaffrey, J. Cabrera
- COLL 163.** Targeting the role of tyrosine in amot protein-lipid binding events. N. Abufares
- COLL 164.** Withdrawn.
- COLL 165.** Cross-linked polystyrene sulfonic acid and polyethylene glycol as a low-fouling material. A. Alghunaim, B.M. Zhang Newby
- COLL 166.** Development and characterization of surface modified metal oxide nanoparticles. A. Torres, O. Santillan, B. Veldman
- COLL 167.** Gas-phase synthesis of functional nanoparticles for energy applications. D. Tsai, F. Lee, Y. Lu
- COLL 168.** Understanding and controlling the magnetic properties of chemically modified graphene oxide flakes using sulfates. D. Lee, D. Litvinov, T. Lee
- COLL 169.** Probing the conductivity peak of organic electrolyte gated transistors. R. Enright, E. Schmidt, S. White, C.D. Frisbie
- COLL 170.** Structural characterization of red light photoreceptors isolated from *Stigmatala aurantiaca* using atomic force microscopy. R. Rebiai, A. Frost, E.A. Stojkovic, S. Tsonchev, K.T. Nicholson
- COLL 171.** Sol-gel synthesis of modified silica gels containing incorporated heteropolyacids. O. Adetola, L. Golovko, A. Vasiliev
- COLL 172.** ZnO/TiO<sub>2</sub> bilayer film: Energy storage and photocatalytic properties. P. Rangsunwigit, U. Sitthiwong, S. Buama, P. Ngoatrankanwivat
- COLL 173.** Interfacial control of highly absorbent polymers for hemostatic and drug-releasing properties. J. Lundin, B. Streifel, G. Daniels, R. Baumann, J. Duncan, M.G. Stockelman, C.M. Watters, J.A. Stanbro, B.T. Rasley, J.H. Wynne
- COLL 174.** Understanding interactions of organophosphates and thioethers with polyoxometalate clusters. S.L. Giles, J. Lundin, J.H. Wynne, P. Pehrsson, W. Gordon, G.W. Peterson
- COLL 175.** Thiol-functionalized substrates for protein immobilization. S. Xu, W. Chen
- COLL 176.** Hydrotreating properties of nickel phosphide on modified oxide supports. T.R. Clinkingbeard, C.E. Miles, P. Topalian, S.J. Danforth, M.E. Bussell
- COLL 177.** Effects of colloidal C<sub>60</sub> particle size on zeta potential. K. Fujimoto, S. Cates, K. Ausman
- COLL 178.** Phosphatidylserine-containing supported lipid bilayer as a separation medium for copper binding compounds. C.F. Monson, C. Reynolds
- COLL 179.** Holographic imaging of protein aggregates, slurry agglomerates, and waste water contaminants. D.B. Ruffner, D.G. Grier, L.A. Phillips
- COLL 180.** Effect of molecular topology on hydrocarbon surfactant performance. J.A. Clark, M. Ritz, E.E. Santiso
- COLL 181.** Photothermal lens characterization of Ag nanoparticle colloids and films. B. Gebear-Eigzabher, D.R. Radu, C. Lai, A. Marciano
- COLL 182.** CRISPR-Cas9 delivery by DNA nanoclews for efficient genome editing. W. Sun, W. Ji, J.M. Hall, Q. Hu, C. Wang, C. Beisel, Z. Gu
- COLL 183.** Size-tunable dendritic nanoparticles through thiol-yne click chemistry. O. Munkhbat, J. Guo, S. Thayumanavan
- COLL 184.** Layer-by-layer low-temperature passivation of semiconductor nanocrystals with transition metal chalcogenides. P. Moroz, M. Zamkov
- COLL 185.** Fabrication and characterization of germanane as a lithium-ion battery anode. A. Serino, J. Ko, M. Yeung, J. Schwartz, R.B. Kaner, B. Dunn, P.S. Weiss
- COLL 186.** Withdrawn.
- COLL 187.** Flash sintering of solution synthesized Bi<sub>2</sub>Te<sub>3</sub> nanoplatelets. S. Chou, B. Kaehr, B. Swartzenruber, A. Cook, M. Janish, T. Beechem, C. Carter, C. Brinker, D. Ingersoll
- COLL 188.** Convenient bio-inspired approach to the synthesis of multifunctional, stable fluorescent silica nanoparticles. G.W. Chi, C. Bauer
- COLL 189.** Fabrication of mesoporous gold-coated polystyrene particles for enzyme immobilization. S. Choi, O. Graeve
- COLL 190.** Application of soy protein flour as a novel detackifier agent in the recycled pulp. A.H. Tayeb, O.J. Rojas, K.D. Wing, C.L. Salas
- COLL 191.** Effect of incorporation of lysolipid on the stability of dipalmitoyl phosphatidyl choline bilayer membrane at various temperatures: Molecular dynamics simulation approach. K. Lee, H. Yoon, S.S. Jang
- COLL 192.** Single-molecule chemical investigations on DNA nanostructures. M. Freeley, N. Ahlsten, I. Larrosa, M. Palma
- COLL 193.** Nonlinear optical interactions between silver nanoplatelet surface plasmons and various organic/inorganic excitons. Z. Zander, B.G. DeLacy
- COLL 194.** Study of mobility of tri-metallic alloyed nanocrystal in a glassy silica nanosphere. J. Choi, K. Jeon, I. Lee
- COLL 195.** Designing and building an effusive molecular beam doser for methane sticking on vanadium. E. Gabilondo, H. Abbott-Lyon
- COLL 196.** Wettability and packing structure of partially fluorinated  $\omega$ -alkylated self-assembled monolayers. M.D. Marquez, O. Zenasni, T. Lee
- COLL 197.** Deoxygenation properties of bimetallic phosphide catalysts. P.M. Cochran, P. Topalian, B. Carrillo, M.E. Bussell
- COLL 198.** Investigating polymer mediated depletion stabilization of gold nanoparticles in nonpolar solvents. L.B. Thompson, K.T. Lerner
- COLL 199.** Novel nano-drug carrier based on ginsenoside Rb1. J. Lei
- COLL 200.** Quantum chemical studies on the adsorption of DNA bases on Ge(100). D. Kim, Y. Youn
- COLL 201.** Oils derived from native plants to generate a naturally-derived wound dressing. K. Velez, J.J. Rizzo
- COLL 202.** Multifunctional coatings created using an antimicrobial polymer as a platform for titania precipitation on cotton. J.S. Lum, S. Salinas, S. Filocamo
- COLL 203.** Surface assembly of octadecyltrimethoxysilane and 2-[methoxy(polyethyleneoxy)propyl]trichlorosilane nanostructures for the deposition of metal nanoparticles. A.M. Taylor, J.C. Garno
- COLL 204.** Factors affecting morphologies and hydrophilicity of poly(vinyl alcohol) thin films spin-cast on polydimethylsiloxane substrates. K. Lim, W. Chen
- COLL 205.** Synthesis of diphosphine-protected Au<sub>22</sub>(C<sub>28</sub>H<sub>28</sub>OP)<sub>4</sub> nanocluster. Q. Zhang, P.G. Williard, L. Wang
- COLL 206.** Molecular adsorption and surface coverage effects on the morphology of gold nanoparticle. K. Kim, J. Han

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- COLL 207.** Graphene quantum dot-Titania composite materials for photocatalytic water splitting and photovoltaic applications. **S. Chinnusamy Jayanthi, R. Kaur, F. Erogbogbo**
- COLL 208.** Synthesis, characterization, and cellular uptake of cholesterol-modified poly(ethylene glycol)-poly(D,L-lactic acid) polymeric micelles for effective delivery of curcumin in cancer. **P. Kumari, O. Muddineti, B. Ghosh, S. Biswas**
- COLL 209.** Transferrin modified vitamin E: Conjugated lipidic mixed micellar system as nanocarrier for the delivery of curcumin in cancer. **O. Muddineti, P. Kumari, B. Ghosh, S. Biswas**
- COLL 210.** 2-photon fluorescence of quantum dots for investigations of nanoparticle formation and growth. **R. Dinkel, B. Braunschweig, W. Peukert**
- COLL 211.** Effects of defective graphene on the enhanced gas sensing: A density functional theory study. **A. Cho, K. Kim, J. Han**
- COLL 212.** Development of a multiplexed point-of-care SERS immunoassay based on antigen mediated aggregation of gold nanoparticles. **S. Filbrun, Y. Lai, A. Lopez, J. Driskell**
- COLL 213.** Asymmetric functionalization of gold nanoparticles to produce controlled dimers: A novel approach to aggregation based immunoassays. **A.B. Mandl, S. Filbrun, Y. Lai, F. Lovato, J. Driskell**
- COLL 214.** Graphene quantum dots enhanced microfluidics based paper analytical device ( $\mu$ pads) for glucose detection. **N. Gobi, D. Vijayakumar, F. Erogbogbo**
- COLL 215.** Structural conformation of methacrylate-based functionalized monomers and polymer thin films at the air interface. **K.A. Cimatu, S.C. Chan, N.M. Adhikari**
- COLL 216.** Detection and identification of negatively-charged gold nanoparticles using pH indicator arrays. **J.C. Williams, S.E. Lohse**
- COLL 217.** Layer-by-layer assembly and catalysis from polymer-capped Au nanoparticles. **N. Siepsner, D.A. Rider**
- COLL 218.** Mechanism and characterization of inorganic mineralization of palladium on virus templates. **O. Adigun, M.T. Harris**
- COLL 219.** Elucidating the mechanism behind spin-dependent charge transport through DNA monolayers. **J.M. Abendroth, P.S. Weiss**
- COLL 220.** Colloidal self-assembly of multi-fluorescent hybrid silsesquioxane particles. **H.P. Rathnayake**
- COLL 221.** Lithium fluoride nanoparticles injected with hyaluronic acid for management of osteoarthritis pain. **T. Todd, Z. Zhen, H. Chen, J. Xie**
- COLL 222.** Four criteria demonstrating cross-linking of ultrasmall superparamagnetic iron oxide (USPIO) nanoparticles. **E.V. Groman**
- COLL 223.** Emulsion properties depend on the equilibrium phase behavior and structure encountered during the emulsification process. **K. Kaizu, P. Alexandridis**
- COLL 224.** Tracking and aiding the survival of stem cells by indocyanine green- and insulin growth factor-loaded mesoporous cellular foam. **F. Chen, J. Wang, F. Wang, J.V. Jockerst**
- COLL 225.** Nanoporous materials genome center: Methods and software to optimize gas storage, separation, and catalysis. **J.J. Siepmann, L. Gagliardi**
- COLL 226.** Solvent and ligand effect on ultrafast and temperature-dependent optical properties of bi-icosahedral Au<sub>25</sub> clusters. **V.D. Thanthirige, A. Chaffee, R. Guda, E. Sinn**
- COLL 227.** Microdroplet traps for the investigation of nanocrystal interactions in small volumes. **B. Rossi, M. Stoller, S. Morin**
- COLL 228.** Novel polymeric silsesquioxane nanocolloids and their assembly. **P.M. Huzyak, J. Sharpsteen, H.P. Rathnayake**
- COLL 229.** Chiral ceramic nanoparticles. **S. Jiang, N. Kotov, A. Yelitik**
- COLL 230.** Interferences in reflected infrared extinction spectra from a gold-coated periodic particle array. **A. Carrillo, E. Miller, D.E. Thompson**
- COLL 231.** Silver nanoparticles synthesis as SERS substrates for ketoconazole determination. **M. Alshalfah, A.A. Al-Saadi, T.A. Saleh**
- COLL 232.** Localization of porphyrins to spatially confined sites of self-polymerized 4-(chloromethyl)phenyltrichlorosilane studied with atomic force microscopy. **P.C. Chambers, J.C. Garno**
- COLL 233.** One-step and one-pot preparation of ampicillin-functionalized antibacterial gold and silver nanoparticles. **Y. Park, S. Cho**
- COLL 234.** Optical and structural characterization of stoichiometric and indium-rich CuInS<sub>2</sub>/ZnS colloidal quantum dots. **A. Nguyen, C. Robinson, C.D. Heyes**
- COLL 235.** Ultrasmall metal nanoclusters as electrocatalysts for hydrogen evolution reaction. **W. Choi, K. Kwak, M. Kim, D. Lee**
- COLL 236.** Effects of antifreeze polypeptides on calcium carbonate crystallization. **J. Lugo, A.A. Kishishita, Y. Bagdagulyan, A. Morita, X. Wen**
- COLL 237.** Green silver nanoparticles synthesized by *Caesalpinia sappan* extract and their antibacterial activities against methicillin-resistant *Staphylococcus aureus*. **Y. Park, S. Cho**
- COLL 238.** Catechin-capped gold nanoparticles: Eco-friendly synthesis and catalytic activity toward 4-nitrophenol reduction. **Y. Park, S. Cho**
- COLL 239.** Green gold nanoparticles synthesized with earthworm extracts and their enhancement on anticoagulant activities of heparin. **Y. Park, S. Cho**
- COLL 240.** Resveratrol-capped gold and silver nanoparticles and their antibacterial activity against *Streptococcus pneumoniae*. **Y. Park, S. Cho**
- COLL 241.** Ultrasound signal of mesocellular foam and mesoporous nanoparticles. **F. Wang, F. Chen, J.V. Jockerst**
- COLL 242.** Gold nanostructures stabilized with peptide self-assembly for chemical and biological applications. **S. Lee**
- COLL 243.** Electrocatalytic behaviors of metal nanoparticles for CO<sub>2</sub> reduction. **Y. Lee, S. Im, D. Lee**
- COLL 244.** Charge anisotropy of gold nanorods. **J. Kim, M. Han, Y. Zhu, N. Kotov**
- COLL 245.** Bio-activity of a series of novel multi-functional bio-compatible polymers. **P. Fulmer, B. Streifel, J. Duncan, J. Lundin, J.H. Wynne**
- COLL 246.** Few-layered 2D nanosheets generated by green liquid-phase exfoliation methods. **S. Ravula, G.A. Baker**
- COLL 247.** Plasmonic coupling in nanoparticle cluster and random arrays. **J. Jenkins, X. Tian, Y. Zhou, S. Thota, S. Zou, J. Zhao**
- COLL 248.** Nano-confinement induced phase transitions of dithiol monolayers with applications in directing the assembly of electro-active porphyrin molecules. **A. Pawlicki, E. Avery, M.J. Jurow, B. Ewers, A. Vilan, C.M. Drain, J.D. Batteas**
- COLL 249.** Surface patterns of inorganic nanoparticles characterized with force modulation atomic force microscopy. **D. Alexander, X. Zhai, J.C. Garno**
- COLL 250.** Dynamic surface on gold nanorods for reversible Raman enhancement. **J. Li, K.G. Schmitt, C.J. Murphy**
- COLL 251.** Langmuir monolayer and AFM analysis of a collagen/phospholipid/titanium model membrane system for the investigation of osteoblast affinity to titanium rods. **M. Gulley, K.B. Eskandar, L.J. Moore, A. Sostarecz**
- COLL 252.** Using AFM to study transcription factor binding. **K.B. Eskandar, M.M. Ahmad, A. Sostarecz, L.J. Moore**
- COLL 253.** Synthesis and AFM characterization of designed nanostructures of transition metal-doped-ceria. **A. Francis, S.M. Deese, J.C. Garno**
- COLL 254.** Patterning proteins at the nanoscale using spatially selective surfaces prepared by particle lithography. **C.N. Leegwater, Z.L. Highland, J.C. Garno**
- COLL 255.** Designed synthesis of lanthanide doped core-shell nanoparticles with excitation at a benign wavelength. **C.A. Arboleda, S. He, N.J. Johnson, A. Almutairi**
- COLL 256.** Adsorption of methanol on ZIF-8 thin films under low temperature and low pressure conditions. **F. Tian, A. Mosier, H. Larson, E. Webster, M. Ivos, L.B. Benz**
- COLL 257.** Influence of surface chemistry on gold nanoparticle biostability. **J. Delaney, S.E. Lohse**
- COLL 258.** Characterization of nanofoam collapse in response to exposure to volatile organic compounds. **C. Tysinger, N. Borodinov, B.V. Zdyrko, A.E. Soliani, Y.D. Galabura, J.M. Giammarco, I.A. Luzinov**
- COLL 259.** Examination of 4',6-diamidino-2-phenylindole in silica gels through surface-enhanced Raman spectroscopy and fluorometry. **N. Trujillo, E.J. Atkinson**
- COLL 260.** Adsorption and surface reactivity of Zn<sub>x</sub>Ce<sub>1-x</sub>O<sub>2-y</sub> nanoparticles. **T.H. James, M.L. Kumbier, D. Wilson, M.A. Langell**
- COLL 261.** Withdrawn.
- COLL 262.** Fabrication of superhydrophobic wood surfaces with micro-/nano-composite particles. **X. Zhai, Z. Gao, C. Wang**
- COLL 263.** Reduction of CO<sub>2</sub> on Cu and Au/W electrode surfaces: A study by differential electrochemical mass spectrometry. **A. Javier, J.H. Baricuatro, Y. Kim, M.P. Soriaga**
- COLL 264.** Synthesis and characterization of magnetic Fe and Fe-Co polypyrrole-encapsulated nanoparticles. **N. Longoria, R. Morales**
- COLL 265.** Elucidating the structure and assembly of amino acids on silica nanoparticles. **H.L. Swanson, C. Guo, S.K. Davidowski, G.P. Holland**
- COLL 266.** Tethering of lipids leads to increased resistance to membrane leakage at elevated temperature. **G. Leriche, Y.H. Kim, T. Koyanagi, K. Diraviyam, K. Gao, O. Eggenberger, D. Onofrei, J. Patterson, N.C. Gianneschi, G.P. Holland, M.K. Gilson, D. Sept, M. Mayer, J.C. Yang**
- COLL 267.** Characterization of CdSSe and CdS<sub>2</sub> quantum dots prepared via microwave assisted synthesis. **C. Aviles, I.N. Leon Feliciano, G. Rivera Rodriguez, L. Alamo Nole**
- COLL 268.** Polarization mapping sum frequency generation vibrational spectroscopy of methacrylate based functional polymer thin film on dielectric substrate. **N.M. Adhikari, K.A. Cimatu, S.C. Chan**
- COLL 269.** Modifying lipid bilayer permeability with inorganic nanoparticles. **S.M. Ansar, C.L. Kitchens**
- COLL 270.** Computational study of lumazine assembly around single-walled carbon nanotubes. **E. Karunarathne, M. Mollahosseini, F. Papadimitrakopoulos**
- COLL 271.** Morphology-tunable synthesis, growth and optimization of copper nanowires. **M. Ghabadi, S. Darmakolla, S.B. Rananavare**
- COLL 272.** Controlling void development in phenolic composites. **A. Hollcraft, D.A. Rider, C. Grubb**
- COLL 273.** Solution phase investigation of free charge carriers in single-walled carbon nanotubes. **A. Sykes**
- COLL 274.** Colloidal nanocrystals for self-assembled optical nanotenna. **T. Dill, D. Zwisler, S. Palani, A.R. Tao**
- COLL 275.** Preparation of (Cu-ZnO)/C core- and yolk-shell nanoparticles. **C. Hong, J. Wang, Y. Wei, W. Lin, H. Wang**
- COLL 276.** Withdrawn.
- COLL 277.** Robust hybrid membrane-coated nanoparticles for targeting tumors. **M.R. Mackiewicz, P.J. Sanchez**
- COLL 278.** Withdrawn.
- COLL 279.** ROS-responsive nanoparticles to extend the lifetime of anti-angiogenic drug. **V. Nguyen Huu, J. Zhu, G. Collet, S. Patel, C. de Gracia Lux, K. Zhang, A. Almutairi, J. Luo**

### My Comments to the President's Task Force on Employment

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### My Experience with & Advice for Improving Diversity in Chemistry

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## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 7A

### ACS Award in Colloid & Surface Chemistry: Symposium in honor of Nicholas L. Abbott

#### Self-Assembly

P. Alexandridis, *Organizer, Presiding*

P.R. Van Tassel, *Presiding*

**8:30 COLL 280.** Dynamics of colloidal particles in liquid crystals. **O. Lavrentovich**

**9:00 COLL 281.** Engineering interfaces and particles through the assembly of metal-phenolic networks. **F. Caruso**

**9:30 COLL 282.** Spontaneous vs. on-demand degrafting of polymer brushes and organosilane monolayers from silica surfaces. J. Genzer

**10:00 COLL 283.** Stimuli responsive materials from lipids: Applications into drug delivery systems and diagnostics. B.J. Boyd

**10:30 COLL 284.** Layer-by-layer assembled polyelectrolyte films as porous biomolecular delivery systems. A. Gand, M. Hindie, E. Pauthe, P.R. Van Tassel

**11:00 COLL 285.** Amphiphilic polymer self-assembly and disassembly. P. Alexandridis

**11:30 COLL 286.** Molecular packing and self-assembly. R. Nagarajan

## Section B

San Diego Convention Center  
Room 7B

### Biomembrane Synthesis, Structure, Mechanics & Dynamics

#### Model Systems

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

D. L. Daleke, *Presiding*

**8:30 COLL 287.** Simple routes to all-polymeric corrals, flow-channels and traps for studies of lipid and protein diffusion in supported lipid bilayers. G.J. Leggett, A. Johnson, P. Bao, E. Leeds, S.P. Armes, M. Cartron, C. Hunter

**9:00 COLL 288.** Characterizing the interactions of lipid bilayers with antimicrobial peptides and magnetic fields. S.L. Biswal, J. Wang

**9:30 COLL 289.** Nanolipoprotein particles: Encapsulated in silica gel or targeted to lipid phases. W. Zeno, S.H. Risbud, M.L. Longo

**10:00** Intermission.

**10:10 COLL 290.** Designing beta solenoid proteins for nanoscale materials and devices. M. Peralta, Z. Peng, A. Karsai, A. Ngo, C. Sierra, K. Ravikumar, N.R. Hayre, X. Chen, G. Liu, M. Toney, D. Cox, R.R. Singh, K. Fong, A. Kluber, N. Mirzaee

**10:40 COLL 291.** Dissipative and dynamic self-assembly: Spontaneous osmoregulation in giant vesicles. A.N. Parikh

**11:10 COLL 292.** En route to tunable membrane topography: Induced domain reorganization and switchable protein binding. R. Ashkar

**11:40 COLL 293.** Colloidal properties of nanoerythrocytes derived from bovine red-blood-cells. S.R. Raghavan, Y. Kuo

## Section C

San Diego Convention Center  
Room 8

### Nanomedicines: Targeting & Clearance Therapy

G. Han, Z. Wang, J. Zheng, *Organizers*

Z. Gu, J. Xie, *Organizers, Presiding*

**8:30 COLL 294.** Liposomal spherical nucleic acids: Nanostructures enabling the potential of therapeutic nucleic acids. C.A. Mirkin

**9:00 COLL 295.** Chemoradiotherapy with nanoparticle therapeutics: Improving targeting and reducing toxicity. A. Wang

**9:30 COLL 296.** Self-assembly of nano-conjugates on the cell surface triggers apoptosis. J. Kopeček, J. Yang, J.M. Hartley, R. Zhang, T. Chu

**10:00 COLL 297.** Hybrid nanoparticles for treating resistant cancers. W. Lin

**10:30 COLL 298.** Formulation of nanoparticles through controlled chemistry for drug delivery application. Q. Yin, L. Tang, J. Cheng

**11:00 COLL 299.** Macrophage recognition of 'self' for nano- and micro-medicine. D.E. Discher

**11:30 COLL 300.** Synergistic photothermal and antibiotic eradication of *S. aureus* biofilms using targeted, drug-loaded nanoparticle. S.V. Jenkins, D.G. Meeker, E.K. Miller, M.S. Smeltzer, J. Chen

**11:50 COLL 301.** Kras/P53 targeted RNAi combination nano-therapeutics for treating non-small cell lung cancer. L. Gu, Z. Deng, P.T. Hammond

## Section D

San Diego Convention Center  
Room 9

### Nanometal: Synthesis, Structure, Property & Application

#### Nanoclusters

Y. Han, D. Jiang, J. Zheng, *Organizers*

T. Bürgi, Q. Wang, *Presiding*

**8:30 COLL 302.** Toward synthesis of the Au<sub>20</sub> pyramid and other atom-precise gold nanoclusters using phosphine ligands. J. Chen, Q. Zhang, P.G. Williard, L. Wang

**9:05 COLL 303.** Ligand exchange and catalysis on thiolate-protected nanoparticles. C.M. Aikens, A. Fernando, B.M. Barngrover

**9:40 COLL 304.** Magic sized gold nanoclusters as supermolecules. C. Zeng, R. Jin

**10:00** Intermission.

**10:30 COLL 305.** Tuning the properties of atomically precise silver nanoclusters. O.M. Bakr

**11:05 COLL 306.** Molecular silver nanoparticles: Chemical, optical, and structural properties. T.P. Bigioni

**11:40 COLL 307.** Structure and properties of nanometals from X-ray absorption spectroscopy. P. Zhang

## Section E

San Diego Convention Center  
Room 10

### Frontier of the Interface of Materials & Biology: Protein Based Nanomaterials

#### Protein Assembly & Materials Development

Q. Wang, *Organizer*

H. Yi, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 COLL 308.** Creation of stable protein films through nanoimprint lithography. V.M. Rotello

**9:05 COLL 309.** Construction of functional nano protein assembly. J. Liu

**9:35 COLL 310.** Design of functional nanostructured materials. E. Paskaleva, K. Mehta, X. Wu, R. Mundra, J.S. Dordick, R.S. Kane

**10:05 COLL 311.** Peptide assembly for nanoparticle fabrication in complex shapes and the shape matters for drug delivery efficiency in cancer cells and MR imaging. H. Matsui, J. Fang, N. Yakob, S. Rampersaud

**10:35 COLL 312.** Building hybrid architectures for optical sensing and protonic devices with solid binding proteins. F. Baneyx

**11:05 COLL 313.** Charge effects on the self-assembly of protein block copolymer nanostructures. B.D. Olsen, C. Lam, D. Chang, M. Kim

**11:35 COLL 314.** Atomistic modeling of biologically active nanoparticles and nanomedicines. P. Kral

## Section F

San Diego Convention Center  
Room 11A

### Colloids for Medical Imaging

#### Nanoparticles as Contrast Agents

J. M. Berlin, P. del Pino, W. Parak, *Organizers, Presiding*

**8:30 COLL 315.** Multifunctional nanoprobe for targeted photoacoustic imaging and photothermal therapy of cancer stem-like cells. D. Cui

**9:00 COLL 316.** Plasmonic ruler: From cells to detection of micrometastasis in patients. L. Geoffrey P., J. Aaron, M. Jeffrey N., A. Gillenwater, S. Emelianov, K.V. Sokolov

**9:30 COLL 317.** <sup>19</sup>F MRI contrast agent based on mesoporous silica nanoparticles. J.L. Steinbacher, J. Rutowski, S. Fitzgerald, J. Binns, J. Kasper

**9:45 COLL 318.** New approach to achieve enhanced MRI signal using <sup>19</sup>F-containing polymeric tracer. O. Munkhbat, S. Thayumanavan

**10:00 COLL 319.** Layer-by-layer assembled theranostics in the second near-infrared window for Non-invasive monitoring of ovarian cancer treatment. L. Gu, X. Dang, P.T. Hammond, A.M. Belcher

**10:15 COLL 320.** Hydrophobic mesoporous silica nanoparticles as fluorocarbon-free nanoscale ultrasound contrast agents. A. Yildirim, R. Chattaraj, N.T. Blum, G.M. Goldscheliter, A.P. Goodwin

**10:30** Intermission.

**11:00 COLL 321.** Magneto-liposomes for magnetic resonance imaging theranostics. P. Ramos-Gabrer

**11:30 COLL 322.** Multifunctional silica nanoparticles for MR imaging and high intensity ultrasound ablation. J. Wang, A. Liberman, R. Viveros, S. Sammet, N. Lu, M. Kim, W.C. Trogler, A. Kummel

**11:45 COLL 323.** Ultrasound activated film for *in vivo* biomedical marker. J. Yang, J. Wang, N. Mendez, C. Barback, E. Ward, C.N. Ta, S. Blair, W.C. Trogler, A. Kummel

**12:00 COLL 324.** Stöber silica nanoparticles can concentrate methylene blue for a charge-tunable photoacoustic imaging agent. J. Wang, F. Chen, J.V. Jokerst

**12:15 COLL 325.** *In vivo*, ppb uranium detection via a porphyrinoid-containing nanoparticle and *in vivo* photoacoustic imaging. I. Ho, J.L. Sessler, J.V. Jokerst

## Section G

San Diego Convention Center  
Room 11B

### Computational & Experimental Advances Towards Design of Energy Efficient Catalysts

K. Challa, C. M. Friend, *Organizers, Presiding*

**8:30 COLL 326.** Multifunctional catalysis for low temperature upgrade of biomass. D.G. Vlachos

**9:00 COLL 327.** Atomic-scale observations of heterogeneous catalyst reactions at up to atmospheric pressure. A.K. Datye, L.F. Allard

**9:30 COLL 328.** Understanding the activity of Pt-Re bimetallic catalysts. D.A. Chen, A. Duke, K. Xie, R.P. Galhenage, G. Seuser

**10:00 COLL 329.** Improving the accuracy of DFT modeling of electrochemistry. M.A. Caro, T. Laurila, O. Lopez-Acevedo

**10:30 COLL 330.** Analyzing the case for bifunctional catalysis. M. Andersen, A.J. Medford, J.K. Norskov, K.U. Reuter

**11:00 COLL 331.** Nickel-gold single and multiple atom alloys; understanding the relationship between atomic geometry and chemical reactivity. E.H. Sykes

**11:30 COLL 332.** Active gold on active oxides. H. Hakkinen

## Section H

San Diego Convention Center  
Room 24B

### Basic Research in Colloids, Surfactants & Nanomaterials

#### Carbon Materials

R. Nagarajan, *Organizer*

H. Liu, *Presiding*

**8:30 COLL 333.** Withdrawn.

**8:50 COLL 334.** Polymer substituted vertically aligned carbon nanotube membranes for protection against aarfare agents. M.B. Herbert, F. Fornasiero, T.M. Swager

**9:10 COLL 335.** Solution processable molecular transport junctions employing carbon nanoelectrodes. J. McMorrow, J. Zhu, R. Crespo-Otore, A. Geyou, M. Zheng, W. Gillin, M. Palma

**9:30 COLL 336.** Photoluminescence quenching of single-walled carbon nanotubes through C<sub>60</sub>: Functionalized flavin helices. M. Mollahosseini, E. Karunaratne, J. Gascon, G. Gibson, F. Papadimitrakopoulos

**9:50 COLL 337.** Keeping graphene clean: Prevention of airborne contamination using water. H. Liu

**10:10 COLL 338.** Synthesis and characterization of meso-graphene oxide roses for cancer applications. S. Sharma, V.H. Pham, J.H. Dickerson, R. Tannenbaum

**10:30 COLL 339.** Crumpling of graphene nanosheets for 3D networks preparation. D. Parviz, M. Plummer, F. Iri, S. Das, M. Green

**10:50 COLL 340.** Withdrawn.

**11:10 COLL 341.** Reversible near-infrared fluorescence quenching of flavin suspended single-walled carbon nanotubes. M. Mollahosseini, F. Papadimitrakopoulos

**11:30 COLL 342.** Characterizing the differences in adsorbed surfactant and hydration layers around single wall carbon nanotubes using analytical ultracentrifugation. S. Lam, J.A. Fagan

## Environmental Interfaces

### Redox Reactions

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### Physical Chemistry of Complex Environmental Interfaces

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## MONDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 7A

**ACS Award in Colloid & Surface Chemistry: Symposium in honor of Nicholas L. Abbott**

**Interactions Between Surfaces & Nanoparticles**

P. Alexandridis, *Organizer*

M. A. Bevan, R. D. Tilton, *Presiding*

**2:00 COLL 343.** Precise chemical, physical, and electronic nanoscale contacts. P.S. Weiss

**2:30 COLL 344.** Nanoparticles interactions. N. Kotov, R.G. Larson, C. Silvera Batista

**3:00 COLL 345.** Responsive polymeric nanoassemblies. S. Thayumanavan

**3:30 COLL 346.** Design rules for thermally reversible bioadhesive thin films. D.E. Leckband, S. Choi, C. Xue

**4:00 COLL 347.** Star polymer adsorption and surface forces. J.K. Riley, R.D. Tilton

**4:30 COLL 348.** Design of new classes of responsive soft matter by embedding nanoparticle structures in Pickering foams and multiphase gels. O.D. Velev

**5:00 COLL 349.** Non-equilibrium colloidal assembly pathways via synergistic dipolar, depletion, and hydrodynamic interactions. M.A. Bevan

## Section B

San Diego Convention Center  
Room 7B

**Biomembrane Synthesis, Structure, Mechanics & Dynamics**

J. Katsaras, S. Muralidharan, M. Nieh, N. Srividya, *Organizers*

A. N. Parikh, *Organizer, Presiding*

**2:00 COLL 350.** Specificity and mechanism of an aminophospholipid flippase. D. Dudek, J. Paterson, D.L. Daleke

**2:30 COLL 351.** Probing cellular mechanosensitivity using cadherin-functionalized polymer-tethered lipid bilayer architectures. C. Naumann, Y. Ge, K. Shilts

**3:00 COLL 352.** Fully automated, parallel lipid bilayer platform for specific nucleic acid detection. E. Schopf, J. Poulos, J. Schmidt

**3:30** Intermission.

**3:40 COLL 353.** Consequences of lipid oxidation on bilayer structural and mechanical properties. N. Malmstadt

**4:10 COLL 354.** Interplay of the physical microenvironment, contact guidance and cell signaling in cell decision making. C.D. Paul, K. Konstantopoulos

**4:40 COLL 355.** Evaluation of drug-mediated changes in cardiomyocytes by AFM. S. Zou, A. Chen

**5:10 COLL 356.** Nanomechanical properties of the stratum corneum and its interaction with a single hair fiber. N. Nordgren, R. Álvarez-Asencio, V. Wallqvist, M. Kjellin, M.W. Rutland, A. Camacho, G.S. Luengo

## Section C

San Diego Convention Center  
Room 8

**Nanomedicines: Targeting & Clearance**

G. Han, J. Xie, J. Zheng, *Organizers*

Z. Gu, Z. Wang, *Organizers, Presiding*

**2:00 COLL 357.** Smart pH-activated nanoparticles for targeting the tumor microenvironments. S. Nie, J. Du

**2:30 COLL 358.** Renally excreted ultrasmall silica nanoparticles as clinically translated multimodal cancer-targeted platforms for nanomedicine. M. Bradbury, P. Mohan, K. Ma, B. Yoo, P. Zanzonico, S. Patel, U.B. Wiesner

**3:00 COLL 359.** Renally cleared contrast agents for tissue-specific targeting. H. Choi

**3:30 COLL 360.** What may happen to hybrid nanoparticles once they are administered *in vitro* or *in vivo*. W. Parak

**4:00 COLL 361.** Near IR nanobiophotonics for nanomedicine: From targeting, to theranostics, to clearance. P.N. Prasad

**4:30 COLL 362.** Surface engineered ferritins for drug delivery and photodynamic therapy. J. Xie

**5:00 COLL 363.** Cell membrane-camouflaged nanomotors for biodetoxification and drug delivery. J. Li, L. Zhang, J. Wang

**5:20 COLL 364.** Stability of gold nanoaggregates affects biological fate. A. Liu, D. Van Haute, J.M. Berlin

## Section D

San Diego Convention Center  
Room 9

**Nanometal: Synthesis, Structure, Property & Application**

**Nanoparticles, Nanowires & 2D Materials**

D. Jiang, *Organizer*

Y. Han, J. Zheng, *Organizers, Presiding*

**2:00 COLL 365.** Molecular mimicking self-assembly: Precise positioning of nanoparticles using non-biological molecules. Z. Nie, C. Yi, S. Zhang

**2:35 COLL 366.** Controlled synthesis of nanostructured metal catalysts. S. Dai

**3:10 COLL 367.** Microscopic insights into the synthesis of discrete and hybrid colloidal metal nanoparticles. R.E. Schaak

**3:45 COLL 368.** Computational design of nanoparticles and nanowires for electrocatalysis. Z. Chen, X. Zhang, G. Lu

**4:20** Intermission.

**4:50 COLL 369.** Designed chemical synthesis and assembly of uniform-sized nanoparticles for medical and energy applications. T. Hyeon

**5:25 COLL 370.** Crystal phase-controlled synthesis of novel noble metal nanomaterials. H. Zhang

**6:00 COLL 371.** Heterostructures of two-dimensional materials and their potential applications. L. Li

## Section E

San Diego Convention Center  
Room 10

**Frontier of the Interface of Materials & Biology: Protein Based Nanomaterials Protein Assembly & Other Nanoparticles**

Q. Wang, *Organizer*

H. Yi, *Organizer, Presiding*

**1:30 COLL 372.** Fluorescent, edible protein nanoparticles for pH sensing, small molecule sensing, and cellular imaging. B. Stromer, C.V. Kumar

**1:50 COLL 373.** Formation of protein fibers around gold nanoparticles: Fiber formation more likely for hydrophilic proteins at low concentrations. M.R. Hartings, D. Fox

**2:10 COLL 374.** Proton conduction in a cephalopod structural protein. D.D. Ordinario, L. Phan, W. Walkup, J. Jocsion, N. Huesken, A.A. Gorodetsky

**2:30 COLL 375.** Crystalline silk nanodiscs: One material many applications. R. Patwa, P. Dhar, A. Kumar, V. Katiyar

**2:50 COLL 376.** Self-assembly of nanodiscs by apolipoprotein C-III. C. Brisbois, J.C. Lee

**3:10 COLL 377.** Profiling the dielectric constant at the membrane-peptide interface of silica-nanoparticle-supported lipid bilayer using ionizable EPR probes. E. Ou, M. Donohue, M. Vovnov, S. Milkislyants, A.I. Smirnov, T. Smirnova

**3:30 COLL 378.** Edible chemistry 101: Direct exfoliation of graphite to graphene in serum. A. Pattammattel, C.V. Kumar

**3:50 COLL 379.** Peptides with selective affinity to polymers for harvesting the cell sheet. S. Lee, K.J. Shea

**4:10 COLL 380.** Stability of proteins in supraparticles. G.D. Silveira, T.D. Nguyen, J. Bahng, S.C. Glotzer, N. Kotov

**4:30 COLL 381.** Protein-nanoparticle conjugate scaffolds for versatile biosensing. S. Unser, L. Litosh

## Section F

San Diego Convention Center  
Room 11A

**Colloids for Medical Imaging Synthesis & Applications**

J. M. Berlin, P. del Pino, W. Parak, *Organizers, Presiding*

**2:00 COLL 382.** Determination of nanocrystal size by analytical ultracentrifugation: Limits of Stokes law. P. Mulvaney

**2:30 COLL 383.** Upconverting nanoparticles as platforms for multimodal imaging and metal-based photochemotherapy. S. Alonso de Castro, E. Ruggiero, L. Salassa

**3:00 COLL 384.** Controlled assembly of biocompatible metallic nanoaggregates using a small molecule crosslinker. J.M. Berlin

**3:30 COLL 385.** Characterization of amphiphilic copolymer micelles for drug delivery. S. Kaur, B. Gupta, X. Xu, J. Nguyen, A. Watterson, M. Ruths

**3:50** Intermission.

**4:20 COLL 386.** Imaging gold nanoparticles in and around cells. C.J. Murphy

**4:50 COLL 387.** PEGylated gold nanoparticles: Impact on cell fitness. B. Pelaz, P. del Pino, W. Parak

**5:20 COLL 388.** Enhanced two-photon photoluminescence with colloidal plasmonic semiconductor nanocrystals. B. Marin, S. Hsu, A.R. Tao

**5:40 COLL 389.** Controlling the morphology: A facile approach to prepare fluorescent nano-objects via polymerization-induced self-assembly. M. Huo, M. Sun, X. Chen, J. Yuan, Y. Wei

## Section G

San Diego Convention Center  
Room 11B

**Computational & Experimental Advances Towards Design of Energy Efficient Catalysts**

K. Challa, C. M. Friend, *Organizers, Presiding*

**2:00 COLL 390.** Synthesis of bulk mesoporous dilute alloy catalysts. J. Biener, J. Ye, T. Egle, M.M. Biener, J. Shan, N. Janvelyan, L. Wang, C. Barroo, M.A. Worsley, M. Stephanopoulos, R.J. Madix, C.M. Friend

**2:30 COLL 391.** Structure and reactivity of AgAu Alloys. M. Montemore, E. Kaziras

**3:00 COLL 392.** Continuous gas phase catalytic production of methyl acrylates by nanoporous gold-mediated cross coupling. R.J. Madix, B. Zugic, S.G. Karakalos, K. Stowers, M. Biener, J. Biener, C.M. Friend

**3:30 COLL 393.** Catalytic reactions on optically excited plasmonic metal nanoparticles. S. Linic

**4:00 COLL 394.** Experimental establishment of scaling relationships for processes on alloy catalysts. A.J. Gellman, J. Liu, C. Yin, X. Yun

**4:30 COLL 395.** Discovery and optimization of catalysts using high-throughput approaches. J. Lauterbach

**5:00 COLL 396.** Modeling energy efficient catalysts from first principles. A. Tkatchenko

## Section H

San Diego Convention Center  
Room 24B

**Basic Research in Colloids, Surfactants & Nanomaterials**

**Biointerfaces**

R. Nagarajan, *Organizer*

G. P. Holland, *Presiding*

**2:00 COLL 397.** Understanding the interactions of conjugated oligoelectrolytes in phospholipid membranes for enhanced cross membrane charge transfer. J. Jahnke, M. Bryan, J. Belanger, L. Ista, G.C. Bazan, J. Sumner

**2:20 COLL 398.** Fixed membranes for the study of wildtype  $\alpha$ -synuclein's binding to lipid bilayers. W. Lin, D. Berthold, C. Rienstra, C.J. Murphy

**2:40 COLL 399.** Interactions of nano-size antibiotics with biomimetic bacterial cell membranes. J. Hoyo, M. Fernandes, T. Tzanov

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

- 3:00 COLL 400.** Interaction between triblock copolymer poly (propylene glycol) – poly (ethylene glycol) – poly (propylene glycol) and model lipid membranes. Y. Xia, H. Jang, C. Yu, N. Tennakoon, M. Nieh
- 3:20 COLL 401.** Molecular mechanisms of peptide and protein binding at nanostructured interfaces. H.L. Swanson, C. Guo, S.K. Davidowski, G.P. Holland
- 3:40 COLL 402.** Semiconductor nanorods functionalization for plasma membrane insertion. J.J. Li, Y. Kuo, S. Weiss
- 4:00 COLL 403.** Transforming liquid crystal interfaces with enzyme-responsive polymers and surfactants. L. Adamiak, D. Ma, D. Miller, X. Wang, N.L. Abbott, N.C. Gianneschi
- 4:20 COLL 404.** Aggregation properties of a short antimicrobial peptide in the presence of model membranes. N. Phambu, A. Sunda-Meya
- 4:40 COLL 405.** Enzymatically-crosslinked multilayer antioxidant/nanoantibiotic coatings for prevention of bacterial biofilms. K. Ivanova, M. Metieva, T. Tzanov
- 5:00 COLL 406.** Antibacterial approaches from materials engineering perspective: Enzymes on work. T. Tzanov, K. Ivanova, P. Petkova, E. Ramon, M. Fernandes, C. Diaz Blanco
- 5:20 COLL 407.** Contrasting the interactions of dental pulp stem cells with 3-D printed vs molded polymer constructs. M. Rafailovich, M. Simon, A. Pinkas-Sarafova, K. Che

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## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

R. Nagarajan, Organizer

#### 8:00 - 10:00

132, 135-139, 141, 143-144, 146-152, 155-156, 159-162, 169-173, 177-180, 183-185, 189, 192, 196, 198, 200-201, 203, 206, 208, 212-216, 219-220, 222, 224, 226-228, 231, 234, 236, 242, 244-245, 250-251, 262, 264-265, 269-270, 279. See previous listings.

456, 465, 578. See subsequent listings.

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## TUESDAY MORNING

### Section A

San Diego Convention Center  
Room 7A

#### ACS Award in Colloid & Surface Chemistry: Symposium in honor of Nicholas L. Abbott

#### Biomolecules & Biointerfaces

P. Alexandridis, Organizer

R. S. Kane, D. B. Weibel, Presiding

**8:30 COLL 408.** DNA from mm to nm length scales. J.J. De Pablo

**9:00 COLL 409.** Programming molecular self-assembly of intrinsically disordered proteins. G. Lopez, J. Simon, N. Carroll, M. Rubinstein, A. Chilkoti

**9:30 COLL 410.** Design and assembly of nanostructured polyvalent materials. C. Varner, T. Rosen, A. Arsiwala, J.T. Martin, M. Arha, R.S. Kane

**10:00 COLL 411.** Tension in phase separated bilayers: From molecular structure to system-scale morphology. M.M. Santore, D. Chen

**10:30 COLL 412.** Molecular structures of biological molecules at abiotic/biotic interfaces. Z. Chen

**11:00 COLL 413.** Electron transfer within microheterogeneous domains: Colloidal Au-nucleated cytochrome c superstructures. D.R. Rolison, A.S. Harper-Leatherman, J.M. Wallace, C.P. Rhodes, J. Long

**11:30 COLL 414.** Self-propelled particles in anisotropic environments: From collective bacterial behavior to urinary tract infections. D.B. Weibel, G. Auer, R. Trivedi, P. Oliver, R. Maeda, S. Spagnolie, N.L. Abbott

### Section B

San Diego Convention Center  
Room 7B

#### Biomembrane Synthesis, Structure, Mechanics & Dynamics

#### Dynamics & Modeling

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, N. Sridivya, Organizers

F. Gai, Presiding

**8:30 COLL 415.** Growth, coarsening, and alignment of compositional lipid domains in supported bilayer membrane systems. M. Haataja

**9:00 COLL 416.** Influence of periodic boundary conditions on lateral diffusion in membranes. F.L. Brown

**9:30 COLL 417.** Evaluating the raftophilicity of rhodopsin photoreceptor in a patterned model membrane. K. Morigaki, Y. Tanimoto, F. Hayashi

**10:00** Intermission.

**10:10 COLL 418.** Short range interactions in model membranes measured by atom recombination and mass spectrometry. S.G. Boxer, F. Moss

**10:40 COLL 419.** Spatiotemporal control of membrane fusion through photolabile PEGylation of liposome membranes. A. Kros

**11:10 COLL 420.** De novo lipid membrane synthesis using chemoselective reactions. N.K. Devaraj

**11:40 COLL 421.** Glycan density controls the phase behavior of lipid membranes. A. Subramaniam

### Section C

San Diego Convention Center  
Room 8

#### Nanomedicines: Targeting & Clearance Theranostics & Imaging Guided Surgery

Z. Gu, J. Xie, J. Zheng, Organizers

G. Han, Z. Wang, Organizers, Presiding

**8:30 COLL 422.** From nano to micro and back: Theranostic porphyrin assemblies and their *in vivo* fate. G. Zheng

**9:00 COLL 423.** Building nanoparticles *in situ* for molecular imaging applications. J. Rao

**9:30 COLL 424.** Application of optical probes in preclinical imaging and translational disease research. K.P. Francis

**10:00 COLL 425.** Super-enhanced nanodrug delivery after photoimmunotherapy (NIR-PIT): Oncologic applications. H. Kobayashi

**10:30 COLL 426.** Rationally designed theranostic nanoparticles for applications of precision oncology for image-guided cancer treatment. L. Yang

**11:00 COLL 427.** Beyond fluorescence: Small and bright upconversion nanoparticles for biological applications. G. Han

**11:30 COLL 428.** Silver deposited in porous silicon nanoparticles as a potent theranostic antibacterial agent. T. Kim, M.J. Sailor

### Section D

San Diego Convention Center  
Room 9

#### Nanometal: Synthesis, Structure, Property & Application

#### Plasmonics & 3D Structures

D. Jiang, Organizer

Y. Han, J. Zheng, Organizers, Presiding

**8:30 COLL 429.** Plasmonic nanoparticles: From fundamental optical properties to applications. S. Link

**9:05 COLL 430.** Dynamically responsive plasmonic nanostructures. Y. Yin

**9:40 COLL 431.** Recent theory studies of vibrations at surfaces: SERS, FSRS. G.C. Schatz

**10:15** Intermission.

**10:45 COLL 432.** Bifunctional Ag@Pd-Ag nanocubes for highly sensitive monitoring of catalytic reactions by surface-enhanced Raman spectroscopy. D. Qin, J. Li, X. Sun

**11:20 COLL 433.** Plasmon-exciton coupling with colloidal metal nanoparticles. A.R. Tao, A. Rodarte, B. Marín

**11:40 COLL 435.** Three-dimensional positions of individual atoms in nanometals revealed by electron tomography. J. Miao

**12:15 COLL 434.** 3D reconstruction of colloidal superstructures at atomic resolution. N. Nonappa, P. Engelhardt

### Section E

San Diego Convention Center  
Room 10

#### Surface Characterization & Manipulation for Electronic Applications

A. Bergren, C. A. Hacker, Organizers, Presiding

**8:30 COLL 436.** Molecular electronics using carbon: A reliable device platform for rock and roll. A. Bergren, R.L. McCreery, L. Zeer-Wanklyn, M. Sempke, N. Pekas, B. Szeto, T. Schwallenberg

**8:50 COLL 437.** Molecular charge rectification. A. Rodriguez, Y. Li, L. Wang, E. Mucciolo, E. del Barco, C. Nijhuis

**9:10 COLL 438.** Interface engineering in future of computing technologies. C.A. Hacker, S. Pookpanratana, H. Jang, C.A. Richter

**9:30 COLL 439.** Engineering of spin injection and spin transport in organic spin valves (OSVs) using  $\pi$ -conjugated polymer brushes. A. Roy, R. Geng, W. Zhao, R. Subedi, J.J. Locklin, T. Nguyen, X. Li

**9:50 COLL 440.** Towards molecular electronics: Using solution-based methods to deposit nano-objects. A. Ellsworth, A.V. Walker

**10:10 COLL 441.** Investigating the assembly and binding of tetrazine to alkenes via scanning tunneling microscopy (STM) for sensing applications. M. Krikorian, J.M. Azzarelli, T.M. Swager

**10:30 COLL 442.** Molecular rectifiers: Role of the Fermi level alignment and new design based on asymmetric anchoring moieties. C. Van Dyck, M.A. Ratner

**10:50 COLL 443.** Functional high-yield molecular electronic devices. T. Lee

**11:10 COLL 444.** Characterization of polymer/epoxy buried interfaces with silane adhesion promoters before and after hydrothermal aging for the elucidation of molecular level details relevant to adhesion. N.W. Ulrich, J. Myers, Z. Chen

**11:30 COLL 445.** Curing behavior & surface characterization of BADGE-based epoxy resins. Z. Zhang, A. Moser, M. Feuchter, F. Stelzer, F. Wiesbrock

**11:50 COLL 446.** Patterning of Au on PMMA using contact printing of chloroform for adhesion promotion. W. Stahl, C. Hughes, B.H. Augustine, H. Hu

### Section F

San Diego Convention Center  
Room 11A

#### Colloids for Medical Imaging

#### Diagnostics

J. M. Berlin, Organizer

P. del Pino, W. Parak, Organizers, Presiding

J. Berlin, Presiding

**8:30 COLL 447.** Array-based profiling for diagnostics and high-throughput screening. V.M. Rotello

**9:00 COLL 448.** Noble metal nanoparticles for rapid diagnostics. C. Yen, H. de Puig, J.O. Tam, C.R. Clavet, J. Gómez-Márquez, I. Bosch, L. Gehrke, K. Hamad-Schifferli

**9:30 COLL 449.** Quantitative multiplexed nanoparticle platform for the identification and imaging of mammalian cells by surface-enhanced Raman spectroscopy based on surface receptor overexpression. A. Pallao, R. Mirsafavi, G.B. Braun, W.T. Culp, C.D. Meinhart, M. Moskovits

**9:50 COLL 450.** Engineering lanthanide-doped multifunctional nanoparticles for biomedical diagnostic and therapeutic applications. **S. He**, N.J. Johnson, E. Cory Burak, R.L. Sah, A. Almutairi

**10:10** Intermission.

**10:40 COLL 451.** SPIONs and the protein corona: Importance for cellular binding and T2 relaxation. **C.K. Payne**

**11:10 COLL 452.** In-solution biosensing via aggregation of nanodroplets containing mutually reactive, fluorogenic hydrocyanine/quinone reporter molecules. **R. Chattaraj**, P. Mohan, C.M. Livingston, J.D. Besmer, K. Kumar, A.P. Goodwin

**11:30 COLL 453.** Sensing membrane potential by inorganic semiconductor nanorods. **K. Park**, **Y. Kuo**, V. Shvadchak, A. Ingarigiola, X. Dai, S. Hsiung, W. Kim, Z. Zhou, P. Zou, A.J. Levine, J. Li, S. Weiss

**11:50 COLL 454.** Self-assembled split-FP/metal nanoclusters as Raman enhancers for molecular and cellular detection. **T. Koker**, T. Chung, F. Pinaud

**12:10 COLL 455.** Fluorescent silica nanoparticles for selective detection of small ovarian tumors during surgery. **T. Haber**, J. Berlin

## Section G

San Diego Convention Center  
Room 11B

### Computational Modeling & Simulations in Colloid & Surface Chemistry

#### Surfaces & Interfaces

R. Nagarajan, *Organizer*

R. Sureshkumar, *Presiding*

**8:30 COLL 456.** Adsorption of CO<sub>2</sub> on clean CaO(001) surfaces: A joint computational-experimental investigation. **B.H. Solis**, Y. Cui, S. Shaikhutdinov, H. Freund, J. Sauer

**8:50 COLL 457.** DFT study of the Mars-van Krevelen mechanism for ammonia synthesis on Co<sub>3</sub>Mo<sub>3</sub>N (111)-surfaces. **C.D. Zeinalipour-Yazdi**, J. Hargreaves, C.A. Catlow

**9:10 COLL 458.** Box effects in nonliving and living polymerization of 2D surface. **A.D. Benedicto**

**9:30 COLL 459.** Effects of surface geometry and surface-interaction potential on water freezing temperature. **D. Slough**, Y. Lin

**9:50 COLL 460.** Charge dynamics at the silica-electrolyte interface. **B. Lowe**, Y. Shibuta, T. Sakata, C. Skylaris, N. Green

**10:10 COLL 461.** Ono-kondo lattice modeling of CO<sub>2</sub> adsorption on various solid adsorbents. **A. Rony**, K. Gasem, M. Fan, Y. Zheng

**10:30 COLL 462.** DFT modeling of zirconium hydroxide. **I. Iordanov**, V.M. Bermudez, C. Knox, W. Gordon, J. Lundin, J.H. Wynne, D. Barlow, R. Balow, C.J. Karwacki, G.W. Peterson, P. Pehrsson

**10:50 COLL 463.** Effect of surface polarity on physisorption of biomolecules: Molecular modeling. **H. Kim**, Y.G. Yingling

**11:10 COLL 464.** Semi-infinite solid model for DFT calculations of surface properties, rather than slab. **S. Smidstrup**, T. Ghosh, E. Jónsson, K. Stokbro, **H. Jonsson**

**11:30 COLL 465.** *Ab initio* thermodynamics of surface properties of ruthenium and rhodium nanoparticles. **L. Cusinato**, I. Del Rosal, R. Poteau

## Section H

San Diego Convention Center  
Room 24B

### Computational & Experimental Advances Towards Design of Energy Efficient Catalysts

K. Challa, C. M. Friend, *Organizers, Presiding*

**8:30 COLL 466.** Thin film oxide systems for electron transfer control. **H. Freund**

**9:00 COLL 467.** Kinetic and surface analysis of active sites in the hydrogenation of phenol using palladium nanoparticles. **A.L. Marsh**, J. Kauffman, N. Ginder, A. Lehman, K. Kelsall

**9:30 COLL 468.** Chemistry in confined environments: Water reaction in MOF-74. **Y.J. Chabal**, K. Tan, E. Fuentes, S. Zuluaga, J. Li, T. Thonhauser

**10:00 COLL 469.** Conversion of small alcohols on ceria surfaces: A DFT study. **A. Beste**, S.H. Overbury

**10:30 COLL 470.** Improved supported metal oxides for the oxidative dehydrogenation of propane. **I. Hermans**

**11:00 COLL 471.** Degree of rate control: A tool for analyzing microkinetic models and high-throughput computational screening of catalyst materials. **C.T. Campbell**

**11:30 COLL 472.** Continuous flow catalytic reactors: Opportunities for *in situ* time-resolved mechanistic investigations. **K. Challa**

### Applications of Polymer Surfaces & Interfaces

#### Energy Conversion

*Sponsored by POLY, Cosponsored by COLL and PMSE*

#### Environmental Interfaces

##### Surface Adsorption

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG†*

##### Physical Chemistry of Complex Environmental Interfaces

*Sponsored by PHYS, Cosponsored by COLL*

##### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

## TUESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 7A

#### ACS Award in Colloid & Surface Chemistry: Symposium in honor of Nicholas L. Abbott

#### Liquid Crystals: Colloidal & Interfacial Phenomena

P. Alexandridis, *Organizer, Presiding*

R. Nagarajan, *Presiding*

**2:00 COLL 473.** Confined liquid crystals: Harnessing director fields to direct colloid assembly. **K.J. Stebe**

**2:30 COLL 474.** Stimuli responsive LC/polymer material combinations. **T.J. Bunning**, T.J. White

**3:00 COLL 475.** Spontaneous emergence of chirality in lyotropic chromonic liquid crystals in cylindrical confinement. **M. Srinivasarao**

**3:30 COLL 476.** Combining theory and experiment for designing liquid crystal-based chemical sensors. **M. Mavrikakis**, L. Rolling, T. Szilvasi, M. Bedolla, S. Choi, N.L. Abbott

**4:00 COLL 477.** **Award Address (ACS Award in Colloid and Surface Chemistry sponsored by the Colgate-Palmolive Company).** Colloidal and interfacial phenomena with liquid crystalline solvents. **N.L. Abbott**

### Applications of Polymer Surfaces & Interfaces

#### Membranes

*Sponsored by POLY, Cosponsored by COLL and PMSE*

#### Environmental Interfaces

##### Complex Surface Reactions

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG†*

##### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

## TUESDAY EVENING

### Applications of Polymer Surfaces & Interfaces

*Sponsored by POLY, Cosponsored by COLL and PMSE*

## WEDNESDAY MORNING

### Section A

San Diego Convention Center  
Room 7A

#### Basic Research in Colloids, Surfactants & Nanomaterials

#### Surfactants, Amphiphiles, Self-Assembly

R. Nagarajan, *Organizer*

K. Sakurai, *Presiding*

**8:30 COLL 478.** Withdrawn.

**8:50 COLL 479.** Diclofenac sodium-induced micelle-to-vesicle transition in ionic liquid based surfactant systems: Relevance to drug delivery. **Z.S. Vaid**, N.I. Malek, O.E. Seoud

**9:10 COLL 480.** Shape persistence micelles having the same aggregation numbers with the platonic solids. **K. Sakurai**

**9:30 COLL 481.** Enhanced solubility and self-assembly of nonionic surfactants in electrolyte solution. **C. Acevedo-Velez**, M. Gao, W. Yu

**9:50 COLL 482.** Interfacial structure of small molecule surfactant, polymeric surfactant and particle stabilised air-in-water foams. **O.T. Mansour**, J. Hurcoom, P. Griffiths

**10:10 COLL 483.** Thermodynamic study of the self-assembly behaviors of the giant amphiphiles (dihydroxy groups functionalized polyhedral oligomeric silsesquioxane-polystyrene) in solution. **B. Zhang**

**10:30 COLL 484.** Structure and stability of reverse micelles with salt additions: Experimental and modeling insights. **R.E. Ridley**, H. Fathi-Kelly, J.P. Kelly, V.R. Vasquez, O. Graeve

**10:50 COLL 485.** Impact of rock wettability on surfactant-enhanced aquifer remediation. **G. Javanbakht**, L. Goual

**11:10 COLL 486.** Expanding applications and structures of modified sophorolipid derivatives. **A. Koh**, R.A. Gross

**11:30 COLL 487.** Controlled self-assembly of dendritic amphiphiles in micromixers. **A. Bertin**, S. Taabache, M. Maskos

**11:50 COLL 488.** Surfactants and polymers in rinse-off cosmetics: Challenges and innovations. **M.S. Vethamuthu**, E. DiAntonio, V.S. Johnson, S. Ozkan, H. Fares

## Section B

San Diego Convention Center  
Room 7B

### Biomembrane Synthesis, Structure, Mechanics & Dynamics

#### Using X-ray & Neutron Scattering & Simulation

S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

J. Katsaras, *Organizer, Presiding*

**9:00 COLL 489.** Development of neutron reflectometry as a probe of biomembrane structure. **C.F. Majkrzak**

**9:30 COLL 490.** Evolution of membrane systems for neutron scattering: From lipid vesicles to living cells. **J. Nickels**, S. Chatterjee, D.A. Myles, R.F. Standaert, J.G. Elkins, J. Katsaras

**10:00 COLL 491.** Investigating the mechanism of electromechanical coupling in voltage-gated ion channels by time-resolved X-ray & neutron interferometry. **A.Y. Tronin**, C.E. Nordgren, J.W. Strzalka, I. Kuzmenko, V. Lauter, J.A. Freitas, D. Tobias, **J.K. Blasie**

**10:30** Intermission.

**10:40 COLL 492.** Using neutron scattering in biology: The case for membrane proteins and lipoprotein particles. **M. Cardenas**

**11:10 COLL 493.** Structure determination of peripheral membrane proteins adopting multiple configuration. **F. Heinrich**

**11:40 COLL 494.** New tools for probing the spatial organization of biomimetic membranes. **F. Heberle**, M. Doktorova, R.A. Dick, D. Marquardt, B. Geier, V.N. Anghel, G. Pabst, J. Katsaras

**12:10 COLL 495.** Frontiers in membrane biophysics. **M. Rheinstadter**

## Section C

San Diego Convention Center  
Room 8

### Nanomedicines: Targeting & Clearance Controlled Delivery

Z. Gu, G. Han, Z. Wang, *Organizers*

J. Xie, J. Zheng, *Organizers, Presiding*

**8:30 COLL 496.** Smart polymeric nanomedicines at work in rational antitumor drug delivery. **X. Chen**, J. Ding, C. Xiao, Z. Tang

**9:00 COLL 497.** Tools for mapping and understanding complex biological systems in normal and disease states. **Y. Zhao**, O. Bucur, P. Valdes Quevedo, N.M. Sobhana, M.S. Viapiano, E. Chioccia, A. Beck, E.S. Boyden

**9:30 COLL 498.** Using elasticity to control biological transport of polymer nanogels. **M. Zhang**, A. Anselmo, M. Nowak, S. Mitragotri, **M.E. Helgeson**

**9:50 COLL 499.** Hemorrhage control using biocompatible polyphosphate bound silica nanoparticles. **C.K. Nguyen**, K. Ploense, D. Kudela, J.H. Morrissey, T. Kippin, G.D. Stucky

**10:10 COLL 500.** Anticancer platelet-mimicking nanovehicles. **Q. Hu, W. Sun, C. Qian, C. Wang, H. Bomba, Z. Gu**

**10:30 COLL 501.** Therapeutic enzyme-responsive nanoparticles for targeted delivery and accumulation in tumors. **C.E. Callmann, N.C. Gianneschi**

**10:50 COLL 502.** Gold nanorod-assisted selective photothermolysis of adipose tissue. **W. Sheng**

**11:10 COLL 503.** Targeted photodynamic therapy with size-controlled nanoscale MOFs. **J. Park, Q. Jiang, D. Feng, L. Mao, H. Zhou**

**11:30 COLL 504.** Withdrawn.

**11:50 COLL 505.** Enzyme-responsive nanoparticles for targeted accumulation and prolonged retention in heart tissue after myocardial infarction. **A.S. Carlini, M.M. Nguyen, M. Chien, S. Sonnenberg, C. Luo, R.L. Braden, K.G. Osborn, Y. Li, K.L. Christman, N.C. Gianneschi**

**12:10 COLL 506.** Neural stem cell/nanoparticle hybrids for targeted cancer therapy and imaging. **J.M. Berlin**

## Section D

San Diego Convention Center  
Room 9

### Nanometal: Synthesis, Structure, Property & Application

**Synthesis & Application**

D. Jiang, J. Zheng, *Organizers*

Y. Han, *Organizer, Presiding*

Q. Wang, *Presiding*

**9:00 COLL 507.** Synthetic tailoring of Pt-based nanowires for enhanced catalysis. **H. Zhu, S. Sun, S. Dai**

**9:15 COLL 508.** Hybrid Fe<sub>3</sub>O<sub>4</sub>-Au nanostructures: Synthesis, properties, and applications. **S. Hunyadi Murph**

**9:30 COLL 509.** Tuning the size and shape of magnetic-plasmonic core-shell nanoparticles. **E. Kwizera, S. Bhana, X. Huang**

**9:45 COLL 510.** Spectroelectrochemistry of halide anion adsorption and dissolution of single gold nanorods. **B. Hoener, C. Byers, S. Indrasekara, S. Link, C.F. Landes**

**10:00 COLL 511.** Understanding interparticle interactions and properties for SPR and SERS. **Z. Skeete, H. Cheng, Q. Minh Ngo, J. Luo, C. Zhong**

**10:15 COLL 512.** Nanoporous metal films and powders formed with soft templates. **D.B. Robinson, P.J. Cappillino, C.G. Jones, G.F. Garcia, M.A. Hekmaty, B.W. Jacobs, L.R. Parent, I. Arslan**

**10:30 COLL 513.** Nanospace-confined solid-state conversion chemistry for morphology-controlled syntheses of metal/metal-oxide hybrid nanocrystals. **J. Choi, D. Lee, I. Lee**

**10:45 Intermission.**

**11:15 COLL 514.** Withdrawn.

**11:30 COLL 515.** Nanometal synthesis, morphogenesis, and colloidal stabilization enabled by amphiphilic polymers. **T. Sakai, P. Alexandridis**

**11:45 COLL 516.** Synthesis of Au nanocages from Pd templates. **A. Shakiba, S. Shah, A.C. Jamison, T. Lee**

**12:00 COLL 517.** Voltage control of magnetization in FePd nanocrystals for the next generation of magnetoelectric memory. **S. Robbenolt, M. Akylol, X. Li, P. Khalili, K. Wang, S.H. Tolbert**

**12:15 COLL 518.** Withdrawn.

**12:30 COLL 519.** Simultaneous reduction of metal ions by multiple reducing agents initiate the asymmetric growth of metallic nanocrystals. **M.A. Mahmoud**

**12:45 COLL 520.** Strong coupling between periodic arrays of gold nanostructures and excitonic states in light-harvesting complexes. **G.J. Leggett, A. Tsargorodskaya, M. Cartron, C. Hunter**

## Section E

San Diego Convention Center  
Room 10

### Surface Characterization & Manipulation for Electronic Applications

A. Bergren, C. A. Hacker, *Organizers, Presiding*

**8:30 COLL 521.** Impedance spectroscopy as useful tool to study molecule-electrode interfaces and the dielectric response of molecular tunnel junctions. **C.A. Nijhuis**

**8:50 COLL 522.** Replacing a solid with a liquid needle for measuring static and advancing contact angles. **R. Sanedrin, M. Jin, D. Frese, C. Scheithauer, T. Willers**

**9:10 COLL 523.** Scanning Kelvin probe microscopy for understanding the causes of electrical disorder in organic semiconductor. **C.D. Frisbie**

**9:30 COLL 524.** Surface modification of gallium liquid metal alloy interfaces. **C. Tabor, N. Ilyas, B. Cumby, M.F. Durstock**

**9:50 COLL 525.** Chemical self-assembly strategies for conductive metal-organic surface structure. **W.T. Tysoe, J. Kestell, M. Garvey, R. Abulhaha, J.A. Boscoboinik**

**10:10 COLL 526.** Insights on molecular junctions through applied density-functional theory: Examining the changes in molecule and substrate properties upon junction formation. **G. DiLabio, J. Gibbs, A. Otero-de-la-Roza**

**10:30 COLL 527.** Law of corresponding states, scaling properties and other related issues for the charge transport in molecular junctions. **I. Baldea**

**10:50 COLL 528.** Characterizing surface chemistry of high-N-content mesoporous carbon oxygen reduction electrocatalysts. **N.P. Zussblatt, N. Fechner, M. Antonietti, B.F. Chmelka**

**11:10 COLL 529.** Epitaxial self-assembly of polymorphic, porous, and host-guest nanostructures on surfaces using monolayer-substrate interactions. **B. Chilukuri, R.N. McDougald, U. Mazur Hipps, M.A. Omary, K. Hipps**

**11:30 COLL 530.** Precious poison: The self-assembly of cyanide on Au(111). **A. Guttenberg, T. Wächter, K. Barr, J.M. Abendroth, T. Song, Y. Yang, D.L. Allara, M. Zharnikov, P.S. Weiss**

**11:50 COLL 531.** X-ray spectroscopic characterization of organic semiconductor nanowires. **A. Mazaheripour, N. Huesken, J. Jocsion, G. Kladnik, A. Cossaro, L. Floreano, A. Verdini, A.M. Burke, K. Miller, A. Marsukar, I. Kymissis, D. Cvetko, A. Morgante, A.A. Gorodetsky**

## Section F

San Diego Convention Center  
Room 11A

### Colloids for Medical Imaging

#### Synthesis & Applications

J. M. Berlin, P. del Pino, W. Parak, *Organizers, Presiding*

**9:00 COLL 532.** Crucial role of lateral size for graphene oxide in activating macrophages and stimulating pro-inflammatory responses in cells and animals. **S. Liu**

**9:30 COLL 533.** Self-assembling peptide nanotubes. Modulation of internal and external properties. **J.R. Granja, J. Montenegro, M. Amorin, N. Rodriguez-Vazquez, L. Ozores, J. Prieguez**

**10:00 COLL 534.** Fluorine labels for 19F-magnetic resonance imaging. **M. Carril**

**10:30 COLL 535.** Anisotropic nanoparticles for multimodal imaging and therapy. **P. Taboada Antelo, S. Barbosa, A. Pardo, M. Blanco-Loimil, R. Martinez-Gonzalez**

**11:00 COLL 536.** Functionalization of metal, metal oxide and semiconductor nanocrystals using a multi-coordinating polymer. **W. Wang, X. Ji, A. Kapur, H.M. Mattoussi**

**11:20 COLL 537.** Effect of morphology and surface chemistry of gold nanoparticles on cellular uptake and cytotoxicity. **M. Bhamidipati, L. Fabris**

**11:40 COLL 538.** In vitro imaging with biodegradable hybrid organic-inorganic bridged silsesquioxane nanoparticles. **Y. Fatiev, J.G. Croissant, K. Julfikyan, L. Deng, D.H. Anjum, A. Gurinov, N.M. Khashab**

**12:00 COLL 539.** Crossing blood-brain-barrier and bio-imaging using carbon dots: A zebrafish model study. **S. Li, Z. Peng, J. Dallman, I. Skromme, R.M. Leblanc**

**12:20 COLL 540.** Exchange-coupled core-shell ferrite nanoparticles for maximal hysteretic loss. **P. del Pino, Q. Zhang, B. Pelaz, W. Parak**

## Section G

San Diego Convention Center  
Room 11B

### Computational Modeling & Simulations in Colloid & Surface Chemistry

#### Polymers & Colloids

R. Nagarajan, *Organizer*

P. Kral, *Presiding*

**9:00 COLL 541.** Hydration repulsion between carbohydrate surfaces mediated by temperature and specific ions. **H. Chen, J. Cox, H. Ow, R. Shi, A. Panagiotopoulos**

**9:20 COLL 542.** Insight on growth mechanism of gold nanorods from molecular dynamics simulations. **S. Meena, S. Celiksoy, P. Schafer, A. Henkel, C. Sonnichsen, M. Sulpizi**

**9:40 COLL 543.** Emergence of a stern layer from the incorporation of hydration interactions into the Gouy-Chapman model of the electrical double layer. **M.A. Brown, G. Bossa, S.E. May**

**10:00 COLL 544.** Molecular dynamics simulations for emerging computational immunology. **A. Golius, L. Gorb, J.R. Leszczynski, O. Isayev**

**10:20 COLL 545.** Sensing power of two nanoparticles at near sub-nanometer, in different orientations. **N. Hooshmand, J.A. Bordley, M.A. El-Sayed**

**10:40 COLL 546.** ReaxFF reactive force field study of oriented attachment of TiO<sub>2</sub> nanocrystals in non-aqueous solvents. **M. Raju, R. Penn, K.A. Fichtorn, M. Ihme**

**11:00 COLL 547.** Beyond DLVO: Solvation structure and effective interactions of nanocolloids in solutions from 3D-RISM-KH molecular theory of solvation. **A. Kovalenko**

## Section H

San Diego Convention Center  
Room 24B

### Basic Research in Colloids, Surfactants & Nanomaterials

#### Colloidal Systems

R. Nagarajan, *Organizer*

O. D. Velev, *Presiding*

**8:30 COLL 548.** Preparation of non-aqueous pickering emulsions using anisotropic block copolymer nanoparticles. **E. Jones, S. Rizzelli, K. Thompson, S.P. Armes**

**8:50 COLL 549.** Highly stable titanate nanowire dispersions as potential nanocarriers. **M. Pavlovic, E. Horvath, L. Forro, I. Szilagy**

**9:10 COLL 550.** Destabilization of non-ionic surfactant stabilized oil-in-water emulsions: Effect of particle wettability. **H. Katepalli, D. Blankschtein, T. Hatton**

**9:30 COLL 551.** Holographic characterization of individual colloids in complex mixtures. **D.B. Ruffner, J.M. Blusewicz, L.A. Philips**

**9:50 COLL 552.** Colloidal dimerization of hard annular sector particles. **P. Wang, T.G. Mason**

**10:10 COLL 553.** Mechano-switchable, luminescent gels derived from salts of a long-chained, fatty acid gelator. **M. Zhang, R.G. Weiss**

**10:30 COLL 554.** Responsive stabilization of nanoparticles for extreme salinity and high-temperature reservoir applications. **M. Ranka, T. Hatton**

**10:50 COLL 555.** Characterization of Norovirus colloidal interactions as means of controlling virus stability and infectivity. **B.S. Mertens, O.D. Velev**

**11:10 COLL 556.** Nanofiber composites containing fumed silica fillers: From controlled wettability to physical characteristics. **M.T. Geiger, M. Dufficy, C.A. Bonino, S. Khan**

**11:30 COLL 557.** Anomalous dispersion of 'hedgehog' particles. **J. Bahng, B. Yeom, Y. Wang, S. Tung, D. Hoff, N. Kotov**

**11:50 COLL 558.** Inorganic chiral nanomaterials: Design strategies and origin of homochirality. **J. Yeom, B. Yeom, H. Chan, J. Bahng, G. Zhao, P. Zhang, P. Kral, N. Kotov**

**12:10 COLL 559.** Withdrawn.

### Applications of Polymer Surfaces & Interfaces

#### New Techniques & Characterization

*Sponsored by PQLY, Cosponsored by COLL and PMSE*

#### Environmental Interfaces

#### Complex Surface Reactions

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG†*

#### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*



## WEDNESDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 7A

Basic Research in Colloids,  
Surfactants & Nanomaterials

## Biomolecular Systems

R. Nagarajan, *Organizer*

J. C. Lee, *Presiding*

**2:00 COLL 560.** Determination of structure and morphology of gold nanoparticle-HSA protein complexes. L. Calzolari

**2:20 COLL 561.** Importance of lipopolysaccharide aggregate disruption for the anti-endotoxic effects of host defense peptides. S. Singh, P. Papareddy, M. Kalle, A. Schmidtchen, M. Malmsten

**2:40 COLL 562.** Observing the dynamics of stimuli-responsive nanomaterials at high resolution by liquid cell transmission electron microscopy (LCTEM). M.A. Touve, J.P. Patterson, N.C. Gianneschi

**3:00 COLL 563.** Chitosan-coated BSA nanoparticles for oral delivery. J. Cunha, R. Lima, H. Sousa, A. Cavaco-Paulo

**3:20 COLL 564.** Single-particle tracking of lipoproteins and lipid vesicles. M. de Messieres, A. Ng, V. Melson, C. Duarte, A. Remaley, J.C. Lee

**3:40 COLL 565.** Facile synthesis of archaea-inspired lipids for the assembly of archaeosomes. S. Nguyen, N.C. Bell, G. Leriche, J.C. Yang, N.C. Gianneschi

**4:00 COLL 566.** Protein adsorption to charged nanospheres. J.M. Dennison, W. Lin, J. Zupancic, C.J. Murphy

**4:20 COLL 567.** Picosecond energy relaxation dynamics of amyloid beta peptide at nanoscale interface. K. Yokoyama

**4:40 COLL 568.** Inhibition of amyloid fibrillation of  $\beta$ -lactoglobulin by hydrolyzed hydrophobic alkoxi- and fluoro-silanes. A. Giasuddin

## Section B

San Diego Convention Center  
Room 7B

Biomembrane Synthesis, Structure,  
Mechanics & DynamicsUsing X-ray & Neutron  
Scattering & Simulation

J. Katsaras, S. Muralidharan, A. N. Parikh, N. Srividya, *Organizers*

M. Nieh, *Organizer, Presiding*

**2:00 COLL 569.** Membrane domain formation on nanostructured scaffolds. C.P. Collier, F. Liu, B. Srijanto

**2:30 COLL 570.** Structure analysis of membrane fusion by X-ray diffraction: From model membranes to organelles. T. Salditt

**3:00 COLL 571.** Stress-free asymmetric lipid vesicles for the study of transverse lipid motion. D. Marquardt, F. Heberle, M. Doktorova, B. Geier, J. Katsaras, G. Pabst

**3:30 Intermission.**

**3:40 COLL 572.** Computational and experimental study on the 2D self-assembly of the carboxysome's shell proteins. J. Mahalik, G.K. Vestal, X. Cheng, D. Garcia, M. Doktycz, M. Fuentes-Cabrera

**4:10 COLL 573.** Observation of nanoscale structure in the liquid ordered phase by molecular simulation and small angle neutron scattering. E. Lyman, M. Dorrell, F. Heberle, J. Katsaras

**4:40 COLL 574.** Lateral organization and inter-leaflet coupling of biological membranes. X. Cheng

**5:10 COLL 575.** Hydrophobic mismatch tunes lipid bilayer dynamics. M. Nagao, R. Ashkar, E.G. Kelley, R. Bradbury, P. Butler

## Section C

San Diego Convention Center  
Room 8

## Nanomedicines: Targeting &amp; Clearance

## Basic Research

G. Han, Z. Wang, J. Xie, *Organizers*

Z. Gu, J. Zheng, *Organizers, Presiding*

**2:00 COLL 576.** Controlled synthesis of Au-CuS heterodimers with tunable light absorption for photothermal therapy in the second NIR window. J. Jiang

**2:20 COLL 577.** Carbon nanoparticles as a platform therapeutic for oxidative stress. W.K. Sikkema, L.G. Nilewski, K. Mendoza, J.M. Tour

**2:40 COLL 578.** Controlled assembly of biocompatible metallic nanoaggregates using a small molecule crosslinker. D. Van Haute, J.M. Berlin

**3:00 COLL 579.** Tumor targeted ferritin nanocages for efficient photodynamic therapy. W. Tang, Z. Zhen, J. Xie

**3:20 COLL 580.** Plasma membrane-derived vesicles with engineered transmembrane protein ligands: A new system for cellular targeting. C. Zhao, D. Busch, C. Vershel, J. Stachowiak

**3:40 COLL 581.** Characterizing polymeric micelles employed for DDS combining SAXS and FFF. K. Sakurai

**4:00 COLL 582.** Filomicelles self-assembled from degradable di-block copolymers delay clearance *in vivo*, and deliver retinoids & chemotherapeutics in irreversible control of carcinoma cell fate. P. Nair, K. Spinler, M. Vakili, A. Lavasanifar, D.E. Discher

**4:20 COLL 583.** Immunomodulatory activity of colloidal supramolecular particles made from guanosine derivatives. M. Acosta Santiago, J.M. Rivera

**4:40 COLL 584.** Carbon nanotube-based immunotherapeutic both enhances immune stimulation and inhibits tumor migration. E. White, D. Alizadeh, T. Sanchez, B. Badie, J.M. Berlin

**5:00 COLL 585.** Selective photothermal killing of tumor cells by SELEX-derived DNA aptamer-targeted gold nanorods. R. Chandrasekaran, A. Sheng Wei Lee, L. Wei Yap, D. A. Jans, K. M. Wagstaff, W. Cheng

**5:20 COLL 586.** Withdrawn.

## Section D

San Diego Convention Center  
Room 9

Nanometal: Synthesis, Structure,  
Property & Application

## Biomedical Applications

Y. Han, D. Jiang, *Organizers*

J. Zheng, *Organizer, Presiding*

W. Wang, *Presiding*

**2:00 COLL 587.** Deliberate design of optical properties in DNA-programmed nanoparticle superlattices. M.B. Ross, C.A. Mirkin, G.C. Schatz

**2:15 COLL 588.** Directed movement of magnetic nanoparticle-loaded immune cells using a compact 3D printed chamber. P. Cao, A. Pai, M. Wang, E. White, A. Hajmiri, B. Badie, J.M. Berlin

**2:30 COLL 589.** *In vivo* renewable persistent luminescence nanoparticles. G. Han

**2:45 COLL 590.** Mechanistic investigation into the effect of DNA in shape control of metal nanoparticles. N. Satyavolu, L. Tan, Y. Lu

**3:00 COLL 591.** Bimetallic nanostructures as artificial peroxidases for sensitive colorimetric detection of cancer biomarkers. X. Xia

**3:15 COLL 592.** Selective colorimetric detection of *Staphylococcus aureus* using oligonucleotide-functionalized gold nanoparticles. P. Tiet, J.O. McNamara, J.M. Berlin

**3:30 Intermission.**

**4:00 COLL 593.** Novel method based on photothermal cleavage of thermolabile molecules on Au nanoparticles for controlled release. E. Goren, H. Causoglu, E. Yavuz, H. Usta, M. Citir, M. Yavuz

**4:15 COLL 594.** Plasmonic modulation of fluorescence in gold nanostar-NaYF<sub>4</sub>: Yb/Er for multimodal imaging, photothermal, and photodynamic therapy. L. He, C. Mao, S. Cho, K. Ma, A. Yildirim, A.P. Goodwin, W. Park, J. Cha

**4:30 COLL 595.** Layer-by-layer assembled gold nanoring-photosensitizer complex for enhanced photodynamic therapy in the near infrared. Y. Hu, Y. Yang, H. Wang, H. Du

**4:45 COLL 596.** Biogenic silver metal nanoparticle enhanced bioassays. S. Rajput, M.T. McDermott

**5:00 COLL 597.** Transparent flexible electrodes based on copper and silver nanowires integration into devices and stability study. J. Simonato, A. Cabos, T. Sanniccolo, C. Celle, A. Carella

**5:15 COLL 598.** Understanding the properties of electroactive poly(amic) acid membranes, their interaction with nanoparticles and applications. V.M. Kariuki

**5:30 COLL 599.** Organic surface functionalization technique for colloidal silver nanoparticles designed to inhibit precipitation caused by hydrogen sulfide gas. J.M. Snitker, S. David, M.O. Montes

## Section E

San Diego Convention Center  
Room 10

Surface Characterization &  
Manipulation for Electronic  
Applications

A. Bergren, C. A. Hacker, *Organizers, Presiding*

**2:00 COLL 600.** Surface engineering of two-dimensional nanoelectronic heterostructures. M. Hersam

**2:20 COLL 601.** Directed assembly of 1D nanostructures on lithographically patterned surfaces. R. Wang, E. Penzo, M. Palma, S. Wind

**2:40 COLL 602.** Constructing molecular electronic devices incorporating organic molecules: From simple alkanes to conjugated polymers. R.C. Bruce, T. LaJolie, J. Yablonski, W. You

**3:00 COLL 603.** Lead sulfide quantum dot/lead halide perovskite heterostructures from a single colloidal suspension. T. Hull, O. Semonin, J.S. Owen

**3:20 COLL 604.** Colloidal precursors to ultra-thin-film photovoltaics. D.R. Radu, K. Dobson, P. Hwang, C. Lai

**3:40 COLL 605.** Making connections between molecules and silicon. J.M. Buriak, F. Liu

**4:00 COLL 606.** Hydrogenated graphene for surface engineering and transfer. K.E. Whitener, W.K. Lee, R. Stine, J. Robinson, N. Bassim, R. Stroud, P. Sheehan

**4:20 COLL 607.** Organometallic molecular compound integrated into a memory device by "click" chemistry. S. Pookpanratana, H. Zhu, E. Bittle, S.N. Natoli, T. Ren, C.A. Richter, Q. Li, C.A. Hacker

**4:40 COLL 608.** Processing colloidal-synthesized 2D tin chalcogenide semiconductors for application in electronic devices. A.J. Biacchi, S.T. Le, S. Pookpanratana, J.A. Hagmann, C.A. Richter, A.R. Hight Walker

**5:00 COLL 609.** Conversion of surface silanol to silicon hydride on solid silicon oxide surfaces. S. Darmakolla, H. Tran, A. Gupta, J.M. Blackwell, S.B. Kananavare

## Section F

San Diego Convention Center  
Room 11A

Basic Research in Colloids,  
Surfactants & Nanomaterials

## Colloidal Assembly

R. Nagarajan, *Organizer*

D. Tsai, *Presiding*

**2:00 COLL 610.** Withdrawn.

**2:20 COLL 611.** Shape control of supraparticles on the three-dimensional slippery surfaces. S. Wooh, Y. Lee, H. Huesmann, D. Vollmer, W. Tremel, K. Char, P. Papadopoulos, H. Butt

**2:40 COLL 612.** Acoustic radiation forces for the rapid and programmable assembly of microparticles and nanoparticles. W. Shields, C. Owens, P. Austin Suthanthiraraj, C. Reyes, D. Cruz, L. Fu, B. Wiley, P. Charbonneau, G. Lopez

**3:00 COLL 613.** Electrostatic assembly of functional nanoparticles for biomedical applications. D. Tsai, H. Wang, T. Nguyen, C. Zhou, F. Lee, T. Tang, Y. Lai

**3:20 COLL 614.** Size-controlled and redox-responsive supramolecular nanoparticles. R. Weinhart-Mejia, G.A. Kronig, J. Huskens

**3:40 COLL 615.** Evaporation controlled pattern formation in a polymer droplet. C. Zhang, P. Akcora

**4:00 COLL 616.** Kinetics of nanocrystal superlattice self-assembly revealed by real-time *in situ* X-ray scattering. M.C. Weidman, D. Smilgies, W.A. Tisdale

**4:20 COLL 617.** Dendrimer induced organization and self-assembly of colloidal nanoparticles. D. Jishkariani, B. Diroll, M. Cargnello, C.B. Murray, B. Donnio, D. Klein, L. Hough

**4:40 COLL 618.** Active colloidal polymer. J. Zhang, S. Granick

**5:00 COLL 619.** Understanding local and long-range 3-dimensional arrangements of components in colloidal nanocrystal frameworks using STEM tomography. T.E. Williams, P. Ercius, B. Helms

**5:20 COLL 620.** Formation of semifaceted, oriented thin calcite films by aggregation of nanoparticles. M.H. Schmidt, K. Ullé, S. Callinan

## Section G

San Diego Convention Center  
Room 11B

**Computational Modeling & Simulations in Colloid & Surface Chemistry**
**Surfactants & Self-Assembled Systems**

R. Nagarajan, *Organizer*

M. Dutt, *Presiding*

**2:00 COLL 621.** Double-tailed surfactants simulated on single-walled carbon nanotubes: A molecular dynamics simulation study. **M. Suttipong**, A. Striolo

**2:20 COLL 622.** Interactions between peptide-mimetic nanoparticles and synthetic cells. **X. Chu**, F. Aydin, **M. Dutt**

**2:50 COLL 623.** Multiscale modeling of self-assembled colloidal nanoparticles. **P. Kral**

**3:20 COLL 624.** Confined disordered jammed sphere packings in three dimensions. **D. Chen**, S. Torquato

**3:40 COLL 625.** Integrating molecular-dynamics simulations with molecular-thermodynamics to predict the interfacial tensions of non-ionic surfactants. **V. Sresht**, D. Blankschtein

**4:00 COLL 626.** Molecular dynamics simulations of NAPL removal from contaminated rocks using surfactants. **E. Lowry**, M. Sedghi, L. Goual

**4:20 COLL 627.** Molecular dynamics simulations of micelle and micelle-nanoparticle solutions: Structure, dynamics, and rheology. **S. Dhakal**, A. Sambasivam, **R. Sureshkumar**

**4:50 COLL 628.** Modeling of dynamically self-assembling nanoflasks. **S. Sen**, P. Kral

**5:10 COLL 629.** Molecular dynamics simulations together with experimental studies reveal strong membrane activity of a small peptide. **E. Antunes**, N.G. Azoia, A. Cavaco-Paulo

## Section H

San Diego Convention Center  
Room 24B

**Basic Research in Colloids, Surfactants & Nanomaterials Semiconductors & Quantum Dots**

R. Nagarajan, *Organizer*

D. A. Rider, *Presiding*

**2:00 COLL 630.** Photoinduced electron transfer as a means to modulate the plasmon resonance of  $Cu_2-xS$  quantum dots. **R. Alam**, P.V. Kamat

**2:20 COLL 631.** Vibrational spectroscopy of single quantum dots. **C.O. Topal**, J. Bao, A. Kalkan

**2:40 COLL 632.** Size- and surface ligand-dependent photocatalytic performance of  $CuInSe_2$  nanocrystals in water. **R. Sardar**, K.N. Lawrence

**3:00 COLL 633.** Non-spectroscopically dependent study of neutral amine ligand binding interactions with  $CdSe$  quantum dots. **M.Y. Gee**, R. Tan, Y. Shen, A.B. Greytak

**3:20 COLL 634.** Mechanism of energy transfer between molecules and  $PbS$  nanocrystals during upconversion. **M. Mahboub**, M. Tang

**3:40 COLL 635.** Size dependent ligand layer dynamics in semiconductor nanocrystals probed by anisotropy measurements. **I. Hadar**, T. Abir, S. Halilni, A. Faust, U. Banin

**4:00 COLL 636.** Homochiral semiconductor nanohelices. **W. Feng**, J. Kim, X. Wang, H. Calcaterra, N. Kotov

**4:20 COLL 637.** Optical and electrical properties of a tube-in-a-tube semiconductor. **A.L. Ng**, **Y. Wang**

**4:40 COLL 638.** Counterion-mediated ligand exchange for  $PbS$  colloidal quantum dot superlattices. **D.M. Balazs**, D.N. Dirin, H. Fang, L. Protesescu, G.H. ten Brink, B.J. Koo, M. Kovalenko, M. Loi

**5:00 COLL 639.** Colloidal synthesis of monodisperse semiconductor nanocrystals through the saturated atomic layer adsorption reaction. **M. Zamkov**, N. Razgoniaeva, L. Carrillo

**5:20 COLL 640.** Investigating the doping of nanocrystals with hydrazine. **M. Mahboub**, M. Tang

## Environmental Interfaces

## Complex Surface Reactions

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## Applications of Polymer Surfaces &amp; Interfaces

## Anti-fouling

*Sponsored by POLY, Cosponsored by COLL and PMSE*

## Elucidation of Mechanisms &amp; Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

## Physical Chemistry of Complex Environmental Interfaces

*Sponsored by PHYS, Cosponsored by COLL*

## WEDNESDAY EVENING

## Environmental Interfaces

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## THURSDAY MORNING

## Section A

San Diego Convention Center  
Room 7A

**Basic Research in Colloids, Surfactants & Nanomaterials**
**Polymers, Gels, Polyelectrolytes**

R. Nagarajan, *Organizer*

K. Sakurai, *Presiding*

**8:30 COLL 641.** Effect of polyelectrolyte multilayers shell on thermal properties of *n*-octadecane phase change material nanocapsules. **Y. Lamphaojeen**, P. Siriphannon

**8:50 COLL 642.** Structural control of self-assembled porous polyelectrolyte films by interaction with specific metal ions. **Y. Tsuge**, S. Shiratori

**9:10 COLL 643.** Microwave welding/reinforcing approach at the interface of thermoplastic materials. **X. Zhang**, S. Poyraz, L. Zhang

**9:30 COLL 644.** Two faces of a polyelectrolyte multilayer: Tailoring the structure and the properties. **Y. Ghousseoub**, J.B. Schlenoff

**9:50 COLL 645.** Electrochemically-triggered microgel size modulation. **O. Mergel**, P. Wünnemann, A. Böker, U. Simon, F. Plamper

**10:10 COLL 646.** Tuning the properties of oligo ethylene glycol and poly (*N*-isopropylacrylamide) microgel for future biomedical applications. **M. Islam**, N. Welsch, L.A. Lyon

**10:30 COLL 647.** Spiky hedgehog particles with conformal layer-by-layer coatings. **D. Montjoy**, J. Bahng, Y. Kim, X. Wang, N. Kotov

**10:50 COLL 648.** Strong and tunable wet adhesion with rationally designed layer-by-layer assembled triblock copolymer films. **A. Traeger**, S.A. Pendergraph, T. Pettersson, A.E. Carlmark, L. Wågberg

**11:10 COLL 649.** Cellulose nanocrystals as additive and reinforcing agent in melt-spinning of polypropylene. **X. Lu**, O.J. Rojas, J. Genzer, K. Efimenko, B. Pourdeyimi

**11:30 COLL 650.** Stimuli responsive polymer capsules with multiple concentric shells. **B.C. Zarket**, S. Antozewski, T. Coyne, J. Heckelman, S.R. Raghavan

**11:50 COLL 651.** *N*-halamines: Antimicrobial surface functionalization of polymers & nanomaterials. **K. Rashwan**, L. Stael, G. Sereda, D. Engebretson, G. Bertsch

## Section B

San Diego Convention Center  
Room 7B

**Biomembrane Synthesis, Structure, Mechanics & Dynamics**
**Synthesis, Mechanics & Characterization**

J. Katsaras, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

S. Muralidharan, *Organizer, Presiding*

**9:00 COLL 652.** Interlayer coupling and compositional domain growth in stacked lipid bilayer membrane systems. **Y. Xu**, J. Berry, M. Haataja

**9:20 COLL 653.** Engineered nanostructures of lipopolysaccharide triggers rapid morphogenesis among dendritic cells. **Y. Liu**, K. Wang, M. Zhang, H. Chen, J. Li, R.S. Shailise, T. Laurence, F. Liu, G. Liu

**9:40 COLL 654.** Effects of cationic and anionic surfactant concentrations on adsorbed self-assembled micellar structure at graphite surfaces. **B. Micklavzina**, M.L. Longo

**10:00 COLL 655.** Stability of giant vesicles in salinity gradients. **V.N. Ngassam**, N. Wang-Tomic, Y. Deng, Z. Yang, A.N. Parikh

**10:20** Intermission.

**10:30 COLL 656.** Using infrared measurements to probe the structure and local environment of membrane proteins. **B.N. Markiewicz**, W. Zhang, H. Jo, W.F. Degrado, F. Gai

**10:50 COLL 657.** Cholesterol-enriched microdomain formation induced by viral-encoded, membrane active amphipathic peptide. **D.L. Gettel**, J.M. Hanson, A.N. Parikh

**11:10 COLL 658.** Multivalent presentation enhances the evolution of membrane structure and actin assembly. **V. Tran**, A. Karsai, M. Fong, E. Ogorodnik, J. Yip, D. Haudenschild, **G. Liu**

**11:30 COLL 659.** Configurable lipid membrane gradients quantify diffusion, phase separations, and binding densities. **K.N. Liu**, C.S. Hung, M.A. Swift, K.A. Muñoz, J.L. Cortez, B. Sanii

## Section C

San Diego Convention Center  
Room 8

**Basic Research in Colloids, Surfactants & Nanomaterials**
**Nanomedicine**

R. Nagarajan, *Organizer*

P. C. Ray, *Presiding*

**8:30 COLL 660.** Stimuli-responsive hydrogels for treatment of severe limb trauma and controlled drug delivery. **B. Streifel**, J. Lundin, J. Duncan, J.H. Wynne

**8:50 COLL 661.** Cellulose nanocrystals and closite- $Na^+$  clay micro-nano complex formation and its application in drug delivery studies. **P. Dhar**, S. Singh Gaur, A. Kumar, V. Katiyar

**9:10 COLL 662.** Titanium dioxide nanoparticles induce oxidative stress. **S. Runa**, C.K. Payne

**9:30 COLL 663.** Mesostuctured silica nanorod based fluorescent sensor for highly sensitive and visual detection of dopamine. **P. Beyazklic**, M. Bayindir

**9:50 COLL 664.** Profiling heterogeneity of circulating tumor cells using multifunctional nanoplatform. **P.C. Ray**

**10:10 COLL 665.** Lateral phase separation in superheated perfluorocarbon nanodroplet monolayers leading to enhanced ultrasound contrast imaging. **R. Chattaraj**, G.M. Goldscheitter, A. Yildirim, A.P. Goodwin

**10:30 COLL 666.** Controlled local chemotherapeutic drug delivery through self-assembled peptide amphiphile hydrogels. **G. Gunay**

**10:50 COLL 667.** Probing polymeric nanoparticles with solid perfluorocarbon for *in vivo* imaging. **O. Koshkina**, I. Tirotta, E. Swider, C. Figdor, J. de Vries, G. Resnati, F. Baldelli Bombelli, P. Metrangolo, M. Srinivas

**11:10 COLL 668.** Mixed micelles of chemically modified Pluronic as drug delivery system. **T. Pettersson**, Z. Feng, S. Hassanzadeh, M. Hakkarainen

**11:30 COLL 669.** Pulsed laser generated gold nanoparticles allow optimization of surface tri-functionalization for their targeted delivery into cancer cell nuclei. **W.D. Qian**

**11:50 COLL 670.** Impact of amphiphile packing parameter on the drug loading and delivery properties of an anticancer liposomal delivery system. **M.A. Ilies**, A.M. Shabana, S. Akocak

## Section D

San Diego Convention Center  
Room 9

### Basic Research in Colloids, Surfactants & Nanomaterials

#### Novel Materials

R. Nagarajan, *Organizer*

J. L. Liu, *Presiding*

**8:30 COLL 671.** Surfactant effect on synthesis of silica hollow particles by encapsulation of water droplet with perhydropoly-silazane in octane/dibutylether mixtures. **R. Saito**, T. Kanahara, K. Kuramochi

**8:50 COLL 672.** Solid-state reactivity of nanoparticulate ZnO in templated ZIF synthesis. **I. Brekalo**, C. Kane, J.R. Ramirez, K.T. Holman

**9:10 COLL 673.** Feasible colloidal approach to produce nanostructured composites to inactivate pathogenic bacteria under visible light conditions. **B. Ancha**, S. Bashir, J.L. Liu

**9:30 COLL 674.** Designed mussel-inspired boat for smart crude oil cleanup. **Z. Wang**, L. Shao

**9:50 COLL 675.** Magneto-acoustic hybrid nanomotor: Dynamic actuation and assembly of nanomaterials under complex external stimuli. **J. Li**, J. Wang

**10:10 COLL 676.** Tuning localized surface plasmon resonance wavelengths of nanoparticles by mechanical deformation. **F. Ameer**, J.N. Anker, M. Kennedy, G. Chumanov, S. Varahagiri, D. Benza, D. Willett

**10:30 COLL 677.** WSe<sub>2</sub> nanoflower synthesis and application for catalysis. **O. Lenz**, D. Henckel, K. Krishnan, B.M. Cossairt

**10:50 COLL 678.** Microwave synthesis of colloidal nanozeolite and polymorphism mechanism. **B. Wang**, P. Dutta

**11:10 COLL 679.** Facile immobilization of nano-TiO<sub>2</sub> on cotton fabrics. **P. Siriphannon**

**11:30 COLL 680.** Hydrophobic aluminosilicate aerogel and their composites. **H. Guo**, F.I. Hurwitz

**11:50 COLL 681.** Polymer templated mesoporous frameworks for strain-coupled magnetoelectric composites. **A.N. Buditama**, D. Chien, L. Schelhas, J. Chang, S.H. Tolbert

## Section E

San Diego Convention Center  
Room 10

### Surface Characterization & Manipulation for Electronic Applications

A. Bergren, C. A. Hacker, *Organizers, Presiding*

**8:30 COLL 682.** Transport across 5–25 nm in carbon based molecular junctions. **O. Ivashenko**, A. Bayat, A. Morteza-Najaran, A. Bergren, **R.L. McCreery**

**8:50 COLL 683.** Phenyl ring as an electronic design motif: Orientation and coupling. **A. Vilan**

**9:10 COLL 684.** What is in a contact? Understanding basic interfacial properties of self-assembled monolayers by engineering substrate roughness. **J. Chen**, Z. Wang, **M. Thuo**

**9:30 COLL 685.** Intersection of metals and organics on the properties of molecular-based devices. **R.C. Bruce**, R. Wang, M.J. Therien, W. You, C.A. Hacker

**9:50 COLL 686.** Environmental gating of single-molecule circuits. **L. Venkataraman**

**10:10 COLL 687.** Stereo-electronic effects on charge transport across large area tunneling junction. **J. Chen**, Z. Wang, M. Thuo

**10:30 COLL 688.** Controlling charge transport mechanisms in nanoscaled porphyrin assemblies on Au surfaces. **A. Pawlicki**, E. Avery, M.J. Jurov, A. Vilan, C.M. Drain, **J.D. Batteas**

**10:50 COLL 689.** Size-dependent measurements with spatially confined nano-clusters of porphyrins using conductive probe atomic force microscopy. **X. Zhai**, N. Kuruppu Arachchige, J.C. Garno

**11:10 COLL 690.** Interfacial electron-transfer processes at diamond-aqueous interfaces. **R.J. Hamers**

## Section F

San Diego Convention Center  
Room 11A

### Basic Research in Colloids, Surfactants & Nanomaterials

#### Patterning, Functionalization & Applications

R. Nagarajan, *Organizer*

S. Bashir, *Presiding*

**8:30 COLL 691.** Chemical fabrication of patterned transparent gold-coated polydimethylsiloxane. **L. Slaughter**, H. Cao, Q. Yang, T.D. Young, C.M. Kevin, A.C. Serino, D. Zosso, J. An, J.R. Stevick, N. Takaki, M. Weiss, A. Bertozzi, A.M. Andrews, P.S. Weiss

**8:50 COLL 692.** Directed autonomic flow: Functional motility fluids. **P. Kuhn**, B.S. de Miranda, P. van Rijn

**9:10 COLL 693.** Supramolecular engineering: Applications to molecular recognition and biocatalysis. **P. Shahgaldian**, M.R. Corroero, N. Moridi, S. Sykora, P.F. Corvini

**9:30 COLL 694.** Shear banding in drying films of colloidal nanoparticles. **B. Yang**, J.S. Sharp, M. Smith

**9:50 COLL 695.** Biomolecule triggered shape transformation of hybrid hydrogels. **J. Athas**, C.P. Nguyen, B.C. Zarkat, Z. Nie, S.R. Raghavan

**10:10 COLL 696.** Block copolymer template-directed synthesis of mono- and bimetallic nanoparticle catalysts. **D.A. Rider**

**10:30 COLL 697.** Cytotoxicity of metal-organic frameworks derived from wet-chemistry approach. **B. Martinez**, Y. Chen, S. Koppaka, J.L. Liu, **S. Bashir**

**10:50 COLL 698.** Application of reactive amphiphilic clay nanogels for removal of toxic cationic dye and heavy metals water pollutants. **A.M. Atta**, H.A. Al-Lohedan

**11:10 COLL 699.** Enhancing chemical adsorption and biodegradation using bioactive phenyl-functionalized silica gels. **A. Radian**

**11:30 COLL 700.** Morphic atomic switch networks for beyond: Moore computing architectures. **R. Aguilera**, J. Gimzewski, A. Stieg

**11:50 COLL 701.** Dioid fluid flow rectification with low surface energy fluids. **J.E. Mates**, R. Campos, J.R. Alston, J.M. Mabry

**12:10 COLL 702.** Adsorption properties of novel silica gel sorbents surface-functionalized with salicylhydroxamic acid-attached polystyrenes for quercetin. **R. Wang**

## Section G

San Diego Convention Center  
Room 11B

### Basic Research in Colloids, Surfactants & Nanomaterials

#### Surface Chemistry & Surface Science

R. Nagarajan, *Organizer*

M. Ruths, *Presiding*

**8:30 COLL 703.** Lowering the barrier to C-H activation using Pt/Cu single atom alloys. **M. Marcinkowski**, M. El Soda, F.R. Lucci, E.H. Sykes

**8:50 COLL 704.** Surface modification of basic sites on MgO by varying surfactant and precipitating agent concentrations. **N.F. Dummer**, Y. Jiang, L. Joyce

**9:10 COLL 705.** Photoinduced actuation of aqueous solutions containing a photoresponsive surfactant. **Y. Takahashi**, Y. Ayako, Y. Kondo

**9:30 COLL 706.** Nanotribology of a catechol-functionalized alkane with terminal chain branching. **M. Ruths**, K. Persson

**9:50 COLL 707.** Use of chemical kinetics to examine spreading sessile drop behavior on solid surfaces. **J.R. Moffatt**

**10:10 COLL 708.** Probing interfacial chemical reaction and surface interactions of electrochemically active galena mineral surface using atomic force microscope. **L. Xie**, J. Wang, C. Shi, Q. Lu, J. Huang, H. Zeng

**10:30 COLL 709.** Specific ion effects at the silica nanoparticle-electrolyte interface: Quantifying the structure of the electrical double layer. **M.A. Brown**

**10:50 COLL 710.** Structure of zirconium(IV) hydroxide materials for chemical warfare agent decomposition. **D. Barlow**, R. Balow, J. Lunding, J.H. Wynne, A. Ng, R. Stroud, V.M. Bermudez, W. Gordon, I. Iordanov, C. Knox, C.J. Karwacki, G.W. Wagner, G.W. Peterson, P. Pehrsson

**11:10 COLL 711.** Surface profile exploration of thin film auto-stratification with atomic force microscopy. **X. Liu**, A.F. Routh, S. Bhatia

**11:30 COLL 712.** Adsorption of Cu<sup>2+</sup> from aqueous solution on Irvingia gabonensis biomass: Kinetics and thermodynamics studies. **A. Inyinbor**, F. Adekola, G. Olatunji

**11:50 COLL 713.** Reactions in Individual droplets on a superhydrophobic surface: Effect of convection. **Y. Liu**, X. Chen, Q. Xu, A. Greer, Y. Zhao, **A.M. Lyons**

### Applications of Polymer Surfaces & Interfaces

#### Low Energy Surfaces & De-Icing

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### Elucidation of Mechanisms & Kinetics on Surfaces

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### Physical Chemistry of Complex Environmental Interfaces

Sponsored by PHYS, Cosponsored by COLL

## THURSDAY AFTERNOON

### Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

### Physical Chemistry of Complex Environmental Interfaces

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## COMP

## Division of Computers in Chemistry

H. L. Woodcock, *Program Chair*

### BUSINESS MEETINGS:

**Business Meeting**, 3:00 PM: Sat

## SUNDAY MORNING

### Section A

San Diego Convention Center  
Room 28A

#### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

#### Protein-Ligand Binding & Dynamics

Cosponsored by PHYS

H. Nguyen, J. Shen, *Organizers*

M. Feig, *Organizer, Presiding*

**8:30 COMP 1.** Multi-site  $\lambda$ -dynamics as a tool for large-scale exploration of chemical space in protein-ligand free energy based optimization. **C.L. Brooks**

**9:10 COMP 2.** Enhanced sampling of ligand binding: Pathways and kinetics. **A. Dickson**

**9:40 COMP 3.** Virtual screening and biophysical characterization of GRK2 and GRK5 inhibitors. **R. Armen**

**10:10** Intermission.

**10:25 COMP 4.** Atomic-resolution dynamics and thermodynamics of protein-carbohydrate interactions: CD44-hyaluronan binding. **O. Guvench**

**10:55 COMP 5.** Insights into the pH-dependent activity and inhibition of BACE1. **J. Shen**

**11:25 COMP 6.** Comprehensive prediction of drug-protein interactions and side effects for the human proteome. **J. Skolnick**

### Section B

San Diego Convention Center  
Room 26B

#### Computational Materials Chemistry

#### Discovery from Prediction & Screening

D. Jiang, *Organizer, Presiding*

Y. Ma, *Presiding*

**8:30** Introductory Remarks.

**8:35 COMP 7.** Discovering new materials and new phenomena with evolution. **A. Oganov**

**9:10 COMP 8.** CALYPSO: A structure design method for materials discovery. **Y. Ma**

**9:45 COMP 9.** Chemical bonding (in solids) from local orbitals and plane waves. **R.V. Dronskowski**

- 10:20 COMP 10.** Structural information: How knowledge of crystal structures can improve our understanding of materials. **S. Vyas**, A. Sarjeant, N. Feeder, C. Groom, S. Ward
- 10:35** Intermission.
- 11:05 COMP 11.** Quantum chemistry-based screening of battery electrolyte components. **O. Borodin**, M. Olquin, F. Wu, G. Yushin, K. Leiter, C. Eisner, J. Knap
- 11:40 COMP 12.** Scalable models of ion transport for electrolyte materials discovery. **B.M. Savoie**, T.F. Miller
- 12:05 COMP 13.** Withdrawn.

### Section C

San Diego Convention Center  
Room 25C

#### Drug Discovery

##### Ligand-Based Drug Design

M. R. Landon, Y. Tseng, *Organizers*  
R. P. Pemberton, *Presiding*

- 8:30 COMP 14.** Exploring and exploiting natural products for computational drug design. **G. Schneider**
- 8:50 COMP 15.** Pitfalls in the assessment of ligand-based virtual screening accuracy. **A. Heifets**, I. Wallach, M. Dzamba
- 9:10 COMP 16.** Virtual substitution scan. **Y. Chiang**, Y. Wang
- 9:30 COMP 17.** Using the open source project, DataWarrior, for analyzing the performance of sub-pharmacophore models as seeds in drug discovery. **M. von Korff**, J. Freyss, T.L. Sander
- 9:50 COMP 18.** Combining ligand-based and structure-based ligand design towards the development of potent and selective antagonists for the adenosine receptors. **H. Gutierrez de Teran**, E. Sotelo
- 10:10** Intermission.
- 10:25 COMP 19.** Improving lead-hopping using electrostatic similarity. **P.C. Hawkins**
- 10:45 COMP 20.** Application of virtual screening to the discovery of novel, nicotinamide phosphoribosyltransferase (NAMPT) inhibitors with potential for the treatment of axonopathies. **D. Clark**, B. Waskowycz, M. Wong, P. Lockey, J. Clark, M. Coleman
- 11:05 COMP 21.** Physical property-scaled virtual screening of fragments. **M. Verdonk**
- 11:25 COMP 22.** Rapid, ligand-receptor binding affinity prediction via petascale computing. **W. Jiang**, S. Yang

### Section D

San Diego Convention Center  
Room 26A

#### From Synthesis to Design: Modeling Tools for Medicinal Chemists

*Cosponsored by CINF and MEDI*

M. R. Landon, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 COMP 23.** Advancing compound design with structure-liability models. **S. Posy**, M.E. Davis, B.L. Claus
- 9:05 COMP 24.** Closing the loop between synthesis and design: Helping chemists to use all the information in compound optimization. **T.E. Mansley**, E.J. Champness, P.A. Hunt, J.A. Chisholm, C.J. Leeding, A. Elliott, S.J. Dowling, F. Ahmed, M.D. Segall
- 9:35 COMP 25.** Shifting medchem tasks in 21st century drug discovery: The importance of syncing 2D and 3D. **C. Detering**

- 10:05** Intermission.
- 10:20 COMP 26.** Putting modeling in the non-modelers' hands using LiveDesign. **M.L. Hall**
- 10:50 COMP 27.** From structural chemistry to medicinal chemistry. **J. Cole**, C. Groom, E. Davis
- 11:20 COMP 28.** Structure- and knowledge-driven interactive design. **M. Rarey**
- 11:50** Discussion.

### Section E

San Diego Convention Center  
Room 28B

#### Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications

*Cosponsored by CATL and PHYS*

V. Glezakou, R. Rousseau, *Organizers*  
M. Salvalaglio, *Presiding*

- 8:30** Introductory Remarks.
- 8:40 COMP 29.** Computational characterization of solar interfaces: Coupling *ab initio* molecular dynamics and first-principles spectroscopy. **G.A. Galli**
- 9:25 COMP 30.** Reactive nanosystems: Billion atom reactive and quantum molecular dynamics simulations. **P. Vashishta**
- 10:10** Intermission.
- 10:40 COMP 31.** Path integral metadynamics. **M. Parrinello**
- 11:40** Discussion.

### Multiscales Chemistry

#### Energy

*Sponsored by MPPG, Cosponsored by ANYL, BIOL, COMP and PHYS*

#### Computational Chemistry Across Catalysis

#### Modeling Complex Reaction Networks in Catalysis

*Sponsored by CATL, Cosponsored by COMP, ENFL and WCC*

## SUNDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 28A

#### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

#### Protein Folding, Surfaces & Membranes

*Cosponsored by PHYS*

M. Feig, H. Nguyen, J. Shen, *Organizers*  
J. Chen, *Presiding*

- 1:30 COMP 32.** *In-situ* data analysis of protein-folding trajectories. **M. Taufer**, T. Johnston, B. Zhang, A. Liwo, S. Crivelli
- 2:00 COMP 33.** Simulation and experiment: The power of a combined approach to protein folding and dynamics. **C.R. Matthews**
- 2:30 COMP 34.** Effect of surfaces in modulating peptide folding mechanisms. **J.E. Shea**
- 3:00 COMP 35.** Encoding of structural information in protein sequences by physical properties. **Y. He**, S. Rackovsky, H.A. Scheraga

- 3:30** Intermission.
- 3:45 COMP 36.** Mechanism of transmembrane voltage-sensing in voltage-dependent potassium and proton channels. **D. Tobias**
- 4:15 COMP 37.** Structure and dynamics of viral lytic peptides in membrane environments. **S. Nangia**, E.R. May
- 4:45 COMP 38.** Progress in coarse grain modeling of lipid-protein interactions. **R.D. Hills**

### Section B

San Diego Convention Center  
Room 26B

#### Computational Materials Chemistry

#### Organic, Polymeric & 2D Materials

D. Jiang, *Organizer, Presiding*  
Z. Shuai, *Presiding*

- 1:30 COMP 39.** Multiscale simulation of proton transport in proton exchange membranes. **G.A. Voth**
- 2:05 COMP 40.** First-principles evaluations of thermoelectric figure of merits for organic and polymeric materials. **Z. Shuai**, W. Shi, D. Wang
- 2:40 COMP 41.** Theoretical design of hydrogen-evolving molecular electrocatalysts. **S. Hammes-Schiffer**
- 3:15** Intermission.
- 3:45 COMP 42.** First-principles study of 2D van der Waals heterojunctions. **J. Yang**
- 4:20 COMP 43.** Electronic/spinronic transport, spectroscopy, and dynamics. **K.S. Kim**
- 4:55 COMP 44.** Theoretical design of 2-dimensional organic frameworks for CO<sub>2</sub> capture. **Z. Tian**, D. Jiang
- 5:10 COMP 45.** Mechanism of strength reduction along the graphenization pathway of polycrystalline graphene. **A. Gamboa**, B. Farbos, P. Aurel, G. Vignoles, J. Leyssale

### Section C

San Diego Convention Center  
Room 25C

#### Drug Discovery

#### Binding, Docking & Scoring

M. R. Landon, Y. Tseng, *Organizers*  
R. Malmstrom, *Presiding*

- 1:30 COMP 46.** Design rules for lipidoids as intracellular protein delivery vectors: Insights from computational studies of RNase A-lipidoid assembly. **D. Slough**, H. Yu, Y. Lin
- 1:50 COMP 47.** Absolute free energy of binding for drug molecules: Application to bromodomains. **M. Aldeghi**, A. Heifetz, M. Boddin, S. Knapp, P. Biggin
- 2:10 COMP 48.** Exploring physics-based methods for predicting protein-ligand binding. **K. Roos**, R.A. Friesner
- 2:30 COMP 49.** Thinking outside the box: Allosteric fragments targeting coxsackievirus 3C protease. **R. Schulz**, G. Wolber
- 2:50 COMP 50.** Energy decomposition analysis for linear-scaling DFT calculations in drug design. **M. Phipps**, T.S. Fox, C. Tautermann, C. Skylaris
- 3:10** Intermission.
- 3:25 COMP 51.** Diverse applications of free energy calculations in drug discovery. **W. Sherman**

- 3:45 COMP 52.** Improving both scoring and docking powers of protein-ligand scoring functions with random forest. **C. Wang**, Y. Zhang
- 4:05 COMP 53.** Grand canonical solute sampling in combination with the site identification by ligand competitive saturation (SILCS) ligand design methodology. **S.K. Lakkaraju**, E.P. Raman, W. Yu, A.D. Mackerell
- 4:25 COMP 54.** Toward predictive structural polypharmacology via flexible docking of ligands to the organismal pocketomes. **R. Abagyan**, A. Ilatovskiy, I. Kufareva, P. Lam, Y. Chen, M. Totrov

### Section D

San Diego Convention Center  
Room 26A

#### COMP Undergraduate Research & National Meeting Roundtable

E. C. Sherer, *Organizer*  
M. C. Nagan, *Organizer, Presiding*

- 1:30 COMP 55.** Introduction to computational chemistry and career panel in COMP. **M.C. Nagan**, E.C. Sherer
- 3:45** Intermission.
- 4:00** Panel Discussion.
- 5:00** Concluding Remarks.

### Section E

San Diego Convention Center  
Room 28B

#### Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications

*Cosponsored by CATL and PHYS*

V. Glezakou, R. Rousseau, *Organizers*  
J. P. Greeley, *Presiding*

- 1:30 COMP 56.** Electrons and holes at TiO<sub>2</sub> anatase surfaces and aqueous interfaces. **A. Selloni**
- 2:15 COMP 57.** First-principles investigation of the role of pyridinium and adsorbed dihydropyridine in pyridine-catalyzed CO<sub>2</sub> reduction on p-GaP photoelectrodes. **M. Lessio**, E.A. Carter
- 2:40 COMP 58.** Classical, molecular-dynamic simulations on water/phenol speciation at the surface-liquid interface. **Y. Wang**, D.C. Cantu, V. Glezakou, R. Rousseau
- 3:05** Intermission.
- 3:30 COMP 59.** Simulations of water-solid interfaces. **H.H. Kristoffersen**, R. Liu, J.E. Shea, **H. Metiu**
- 4:15 COMP 60.** Towards the aldol condensation mechanism of biomass derivatives. **E. Miliordos**, S. Caratzoulas, D.G. Vlachos
- 4:40 COMP 61.** Electron transfer and proton-coupled electron transfer at electrode-molecule interfaces: Calculation of properties relevant to rate constants. **S. Ghosh**, A. Soudackov, S. Hammes-Schiffer

### Multiscales Chemistry

#### Mini-Platform

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

#### Trends in Computational Chemistry: Biophysical to Materials Chemistry

*Sponsored by SOCED, Cosponsored by COMP*

## Global Initiatives in Research Data Management & Discovery

### Global Landscape

Sponsored by *CINF*, Cosponsored by *ANYL*, *COMP*, *MEDI* and *PHYS*

### Data Mining: Searching Non-covalent Interactions in Chemical Databases

Sponsored by *CINF*, Cosponsored by *COMP*

### Computational Chemistry Across Catalysis

### QMMM & Reaction Pathway Sampling

Sponsored by *CATL*, Cosponsored by *COMP*, *ENFL* and *WCC*

## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 28A

### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

### Pushing the Envelope, Polarizability & Quantum Effects

Cosponsored by *PHYS*

M. Feig, H. Nguyen, *Organizers*

J. Shen, *Organizer, Presiding*

**8:30 COMP 62.** Milestones in simulation of plant cell-wall carbohydrates and biofuel-related enzymes. M.F. Crowley, A. Hynninen, G. Beckham, B. Knott, L. Bu

**9:00 COMP 63.** Biomolecular simulations are more physically realistic than they used to be. D.A. Case

**9:30 COMP 64.** Polarizable force field for RNA based on the classical Drude oscillator. J.A. Lemkul, A.D. Mackerell

**10:00 COMP 65.** Charge equilibration force fields for molecular modeling. S.A. Patel

**10:30** Intermission.

**10:45 COMP 66.** Computing protein circular dichroism spectroscopy in the near-ultraviolet. J.D. Hirst, Z. Li

**11:15 COMP 67.** Simulation of the structure and spectroscopy of blue copper proteins. N.A. Besley

**11:45 COMP 68.** Novel sampling and reweighting approaches for computing accurate QM/MM free energies: Solvation free energy, pKa, reaction paths, and more. P.S. Hudson, F.L. Kearns, S. Boresch, H.L. Woodcock

### Section B

San Diego Convention Center  
Room 26B

### Computational Materials Chemistry

### Quantum Fundamentals

D. Jiang, *Organizer*

A. D. Becke, M. Pederson, *Presiding*

**8:30 COMP 69.** B13 strongly-correlated density functional and multi-reference states. A.D. Becke

**9:05 COMP 70.** Exchange-correlation and excitation energies from pairing matrix fluctuations and the particle-particle random phase approximation. W. Yang

**9:40 COMP 71.** Removing most self-interaction errors from density functional calculations. M. Kim, E. Sim, K. Burke

**10:15** Intermission.

**10:45 COMP 72.** Self-interaction corrected density-functional theory with unitary invariance: Applications to molecules. M.R. Pederson, H. Torsten, T. Baruah, D. Kao, L. Simon, K. Jens

**11:20 COMP 73.** Density functionals for electronic excitations. B. Krull, S. Balasubramani, S.M. Parker, F.U. Furche

**11:55 COMP 74.** Benchmarking molecular crystal lattice polymorph- and solvation free energies using effective field coupled-cluster theory. J.N. Byrd, R.W. Molt, B.A. Sanders, R.J. Bartlett

### Section C

San Diego Convention Center  
Room 25C

### Drug Discovery

### Structure-Based Drug Design

M. R. Landon, Y. Tseng, *Organizers*

K. Armacost, *Presiding*

**8:30 COMP 75.** pMD-membrane: A tool to determine allosteric binding pockets in membrane-bound biomolecules. P. Srivastava, A. Sayyed-Ahmad, A. Gorfe Abebe

**8:50 COMP 76.** Recent algorithmic developments for prediction and dynamics of ligands in protein binding sites. D. Janezic, J. Konc

**9:10 COMP 77.** Integrating genetic and structural data on human kinase in network-based modeling of kinase sensitivities and resistance to targeted anticancer drugs. G. Verkhivker

**9:30 COMP 78.** New insight into the catalytic and inhibition mechanism of the human acyl protein thioesterase. M. Audagnotto, S. Ho, P. Sandoz, G. van der Goot, M. Dal Peraro

**9:50 COMP 79.** Web portal for structure-based drug discovery: DrugDiscovery@TACC. W.J. Allen, S.A. Mock, J.M. Fonner, R. Dooley, M.W. Vaughn, S.J. Watowich

**10:10 COMP 80.** Structural database of small molecule-transcription factor (SM-TF) complexes with application to drug design. X. Xu, Z. Ma, H. Sun, X. Zou

**10:30** Intermission.

**10:45 COMP 81.** Structural solvent detection and placement and scoring functions for protein-ligand docking based on the 3D-RISM-KH molecular theory of solvation. A. Kovalenko, N. Blinov

**11:05 COMP 82.** Forgotten value of small molecule crystal structures in molecular design. E. Davis, C. Groom

**11:25 COMP 83.** Withdrawn.

**11:45 COMP 84.** Polyphony: Superposition independent methods for ensemble-based drug discovery. W. Pitt

### Section D

San Diego Convention Center  
Room 26A

### Molecular Mechanics

### Force Fields, Parameterization & Validation

M. Feig, *Organizer*

C. R. Allen, *Presiding*

**8:00 COMP 85.** Further along the road less traveled: A truly *ab-initio* approach to force field design. K.T. Debic, D.S. Cerutti, A.M. Gronenborn, D.A. Case, L.T. Chong

**8:25 COMP 86.** Efficient, analytic algorithms for induced dipoles. A.C. Simmonett, F.C. Pickard, B. Brooks

**8:50 COMP 87.** Systematic improvement of intramolecular parameters for protein force fields from quantum chemistry data. L. Wang, K. Beauchamp, W.C. Swope, J.E. Rice, T.L. Head-Gordon, T.J. Martinez, V.S. Pande

**9:15 COMP 88.** Electric fields in biomolecular systems using the AMOEBA polarizable force field. R.T. Bradshaw, J.W. Essex

**9:40 COMP 89.** Biomolecular force field parameterization via atoms-in-molecule electron density partitioning. D. Cole, J.Z. Vilseck, J. Tirado-Rives, M.C. Payne, W.L. Jorgensen

**10:05 COMP 90.** Two tales of molecular dynamics parameters: Fluorescent protein chromophores and aqueous ions. J. Dood, D.L. Blood, A. Rosnik, B.P. Krueger

**10:30 COMP 91.** Quantum chemical approach for evaluating molecular mechanics force fields based on comparison of computed and observed NMR chemical shifts. D. Koes, J. Vries

**10:55 COMP 92.** Statistical distance between thermodynamic systems as a theoretical basis for force field development. L. Vıcek, A.A. Chialvo

**11:20 COMP 93.** Benchmarking adaptive steered molecular dynamics (ASMD) across the family of CHARMM potentials. C.R. Allen, H. Bureau, R. Hernandez

**11:45 COMP 94.** Optimizing molecular models through force-field parameterization. K. Kirschner, M. Hülsmann, A. Krämer, O. Krämer-Fuhrmann, D. Reith

### Section E

San Diego Convention Center  
Room 28B

### Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications

Cosponsored by *CATL* and *PHYS*

V. Glezakou, R. Rousseau, *Organizers*

C. Skylaris, *Presiding*

**8:30 COMP 95.** Relative propensity of the hydrated excess proton and hydroxide anion for the air-water interface. G.A. Voth

**9:15 COMP 96.** Molecular simulation of mechanisms CO<sub>2</sub>, N<sub>2</sub> adsorption, and diffusion inside hydrated NaX (Si/Al=1.0). S. Chakraborty, P. Dutta, S.J. Singer

**9:40 COMP 97.** Determinants of membrane protein integration mediated by the Sec translocon. R. Van Lehn, B. Zhang, M. Niesen, C. Wang, T.F. Miller

**10:05** Intermission.

**10:30 COMP 98.** Many-body molecular dynamics: A spectroscopically accurate approach to vibrational spectroscopy of water at complex interfaces. F. Paesani

**11:15 COMP 99.** High temperature properties and anharmonic effects from *ab initio* molecular dynamics simulations. M. Lee, R. Rousseau, V. Glezakou

**11:40 COMP 100.** Quantum chemical insight into a single-site nickel hydrogenation catalyst produced via atomic layer deposition on a metal-organic framework. A.B. League, V. Bernales, Z. Li, C.J. Cramer, L. Gagliardi

## Global Initiatives in Research Data Management & Discovery

### Role of Community & Standards

Sponsored by *CINF*, Cosponsored by *ANYL*, *COMP*, *MEDI* and *PHYS*

### Multiscales Chemistry

### Bio

Sponsored by *MPPG*, Cosponsored by *BIOL*, *COMP* and *PHYS*

### WCC 2016 Rising Stars Awards Symposium

Sponsored by *WCC*, Cosponsored by *CATL*, *CEI*, *COMP*, *ENFL* and *PMSE*

### Preparing for the Real World: Challenges Faced by Young Investigators

### Choosing Grad Research Advisors & a Career in Academia or Industry

Sponsored by *MPPG*, Cosponsored by *CHED*, *CINF*, *COMP*, *PHYS* and *YCC*

### Computational Chemistry Across Towards Chemical Accuracy

Sponsored by *CATL*, Cosponsored by *COMP*, *ENFL* and *WCC*

### Computational Design of Advanced Materials

Sponsored by *COMSCI*, Cosponsored by *COMP* and *PHYS*

## MONDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 28A

### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

### Evolution, Extremes & Mechanisms

Cosponsored by *PHYS*

M. Feig, J. Shen, *Organizers*

H. Nguyen, *Organizer, Presiding*

**1:30 COMP 101.** Characterizing biomolecular evolution through molecular dynamics simulations. B.N. Dominy, Z. Jia, Y. Liu, T. Han, V. Agrawal, R. Overstreet

**2:00 COMP 102.** How did simple and complex life originate? A protein perspective. R. Mannige

**2:30 COMP 103.** Extreme biology and molecular dynamics simulations: Proteins under pressure. T. Ichiye

**3:00 COMP 104.** Uncovering a hidden pH-triggered catalytic pathway of the hairpin ribozyme using constant pH molecular dynamics. G. Goh, K. Sripathi, A. Dickson, N.G. Walter, C.L. Brooks

**3:30 COMP 105.** Hybrid approaches to characterize structure and dynamics of biomolecular systems from single molecule experiments. F. Tama

**4:00 COMP 106.** Implications of the interaction between myosin heads in relaxed *Lethocerus* asynchronous flight muscle for stretch activation. K. Taylor

## Section B

San Diego Convention Center  
Room 26B

## Computational Materials Chemistry

## Surface Chemistry &amp; Processes

D. Jiang, *Organizer, Presiding*

A. Selloni, *Presiding*

**1:30 COMP 107.** Sub-nano, surface-deposited Pt cluster catalysts: Realistic modeling and tuning through the electronic structure insights. E. Jimenez-Izal, M. Ha, H. Zhai, A. Alexandrova

**1:55 COMP 108.** Water adsorption and oxidation on anatase TiO<sub>2</sub>. A. Selloni

**2:30 COMP 109.** Density functional theory investigation of carboranethiolboranethiolboranethiol self-assembled monolayers on Au(111). M. Danisman, E. Mete, G. Güney, A. Yilmaz

**2:45 COMP 110.** Optical spectra of nano-ferro- and antiferro-magnets. Y. Dahnovsky, V. Proshchenko

**3:00** Intermission.

**3:30 COMP 111.** Role of charge-transfer excitations in Au-Fe alloys for heterogeneous N<sub>2</sub> dissociation catalysis. J. Martirez, E.A. Carter

**3:55 COMP 112.** Linker rectifiers for covalent attachment of catalysts to semiconductor surfaces. V.S. Batista

**4:30 COMP 113.** Examining the role of morphology on proton transport in PFSA membranes. C. Arntsen, J. Savage, G.A. Voth

**4:45 COMP 114.** Dendrimers for water purification and oil dispersion: Atomistic and coarse-grained molecular dynamics investigations of dendrimer-hydrocarbon interactions. R. DeFeaver, D. Jacobs, S. Sarupria, D. Barton

**5:00 COMP 115.** Solvent and pH responsive polymers. S.W. Rick, A. Sharma

**5:15** Concluding Remarks.

## Section C

San Diego Convention Center  
Room 25C

## Drug Discovery

## Structure-Based Drug Design

M. R. Landon, Y. Tseng, *Organizers*

R. P. Pemberton, *Presiding*

**1:30 COMP 116.** Withdrawn.

**1:50 COMP 117.** Comparing protein electrostatics to ligand SAR: Double the fun? T. Cheeseright, G. Tedesco, S. Tomasio, P. Tosco, M. Mackey

**2:10 COMP 118.** FolditDD: Crowdsourcing drug discovery. S. Combs, S. Kothiwale, J. Meiler, M. Vieth

**2:30 COMP 119.** Reactivating the p53 Y220C mutant by targeting a cryptic druggable pocket. O. Demir, J.D. Durrant, R. Mathur, G. Durairaj, P. Kaiser, R.E. Amaro

**2:50 COMP 120.** Addressing the elephant in the room: The impact of experimental protein structural quality on our ability to model protein function. O. Borbulevych, R.I. Martin, L.M. Westerhoff

**3:10 COMP 121.** Phospholipases A<sub>2</sub>: A pharmaceutical target to diminish inflammation. V.D. Mouchlis, J. McCammon, E.A. Dennis

**3:30** Intermission.

**3:45 COMP 122.** Exploring the allosteric regulatory mechanism triggered by inhibitor binding at the myristoylation pocket of BCR-ABL1. N.A. Vellore, M. Zabriskie, M. Deininger, T. O'Hare

**4:05 COMP 123.** Molecular modeling of OXA-405, a new member of the OXA-48 carbapenemase family. B. Jorga, P. Retailleau, L. Marchini, S. Oueslati, L. Dortet, T. Naas

**4:25 COMP 124.** Modeling, synthesis, and biological activities of thioguanine derivatives for Dengue-2 NS2B/NS3 protease. E.E. Kamarulzaman, H. Wahab, M. Hariono

**4:45 COMP 125.** Withdrawn.

## Section D

San Diego Convention Center  
Room 26A

## Molecular Mechanics

## Interacting Biomolecules

M. Feig, *Organizer*

K. E. Hauser, *Presiding*

**1:30 COMP 126.** Improved prediction of protein-ligand binding affinity on not-so-big data. R. Wang

**1:55 COMP 127.** Protein-ligand interactions through the computational microscope: Allosterism in a canonical signaling domain. R. Malmstrom, A.P. Kornev, S.S. Taylor, R.E. Amaro

**2:20 COMP 128.** Dynamics-based drug design: The discovery and development of protein functional activators. G. Colombo

**2:45 COMP 129.** Novel *in silico* approach for modeling the dynamic nature of proteins. A. Hogner, K. Edman, V. Guallar, C. Grebner

**3:10 COMP 130.** Structure and thermodynamics of peptide crystals from simulations with a polarizable force field. I. Nessler, M.J. Schnieders

**3:35** Intermission.

**3:50 COMP 131.** Dynamics, stability, and interactions of biomolecules in bacterial cytoplasm: Microscopic understanding with atomistic simulation. I. Yu, T. Mori, T. Ando, R. Harada, J. Jung, M. Feig, Y. Sugita

**4:15 COMP 132.** Impact of the intracellular environment on NF- $\kappa$ B signaling. M.R. Jones, A.K. Wilson

**4:40 COMP 133.** Mechanistic insights into the activation mechanism of cellular signaling proteins. D. Shukla

**5:05 COMP 134.** Interactions of insulin with calcium alginate from molecular dynamics simulations. D. Nadvorniy, J.L. Soares, G.M. Seabra

## Section E

San Diego Convention Center  
Room 28B

## Structure, Dynamics &amp; Reactivity at Complex Interfaces with Relevance in Renewable Energy &amp; Environmental Applications

*Cosponsored by CATL and PHYS*

V. Glezakou, R. Rousseau, *Organizers*

R. Van Lehn, *Presiding*

**1:30 COMP 135.** Large-scale DFT simulations of O adsorption on Pt nanoparticles. C. Skylaris, J. Aarons, D. Thompsett, M. Sarwar

**2:15 COMP 136.** Molecular oxygen reactivity at graphene-metal interfaces: New insights from first-principles calculations. M. Pavone, E. Schiavo, A.B. Muñoz-García

**2:40 COMP 137.** First-principles studies of electrocatalysis at three-phase boundaries. J.P. Greeley, Z. Zeng, J. Kubal, H. Chun

**3:05 COMP 138.** Computational modeling of electrochemical bio-oil upgrading. D.C. Cantu, Y. Wang, Y. Yoon, A. Padmaperuma, M.A. Lilja, V. Glezakou, R. Rousseau

**3:30** Intermission.

**3:55 COMP 139.** Towards a mechanistic understanding of molecular crystals nucleation: Insights from enhanced sampling simulations. M. Salvagallo

**4:40 COMP 140.** Pegylated ionic liquid for solvation of biomass: *In-silico* insights into solvation, conformation effects, and energetics. T. Schutt, C.M. Maupin

**5:05 COMP 141.** Interactions of biogenic organic molecules with soil minerals and ionic species: An atomistic view. A. Andersen, P. Reardon, S. Chacon, N. Qafoku, N. Washton, M. Kleber

**5:30 COMP 142.** Influence of humidity on adsorption/desorption structure and dynamics in enhanced gas recovery. M.D. Kilmer, L. Tribe

## Multiscales Chemistry

## Mini-Platform

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

## WCC 2016 Rising Stars Awards Symposium

*Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE*

## Global Initiatives in Research Data Management &amp; Discovery

## Technical Infrastructures: Enabling Cultural Shifts

*Sponsored by CINF, Cosponsored by ANYL, COMP, MEDI and PHYS*

## Preparing for the Real World: Challenges Faced by Young Investigators

## Research at PUI's

*Sponsored by MPPG, Cosponsored by CHED, CINF, COMP, PHYS and YCC*

## Computational Chemistry Across Catalysis

## Oxide Catalysts &amp; Key Industrial Reactions

*Sponsored by CATL, Cosponsored by COMP, ENFL and WCC*

## Undergraduate Research Posters

## Computational Chemistry

*Sponsored by CHED, Cosponsored by COMP and SOCED*

## MONDAY EVENING

## Section A

San Diego Convention Center  
Halls D/E

## Sci-Mix

H. L. Woodcock, *Organizer*

**8:00 - 10:00**

26, 85. See previous listings.

150, 232, 248, 257, 268, 327, 406, 413, 448-449, 452, 513, 599. See subsequent listings.

## TUESDAY MORNING

## Section A

San Diego Convention Center  
Room 28A

## ACS Award for Computers in Chemical &amp; Pharmaceutical Research: Symposium in honor of Warren J. Hehre

A. J. Shusterman, *Organizer*

J. P. Bowen, *Organizer, Presiding*

**8:30 COMP 143.** Combinatorial design of density functionals: Survival of the most transferable, applied to the design of range-separated, hybrid meta GGAs. N. Mardirossian, M.P. Head-Gordon

**9:00 COMP 144.** Bringing computational chemistry into an undergraduate physical chemistry course. T. Engel, L.E. Johnson

**9:30 COMP 145.** Electronic structure methods for small-gap systems. F.U. Furche, V. Voora, S. Balasubramani, G. Chen, A. Le, M. Muuronen

**10:00** Intermission.

**10:15 COMP 146.** CHARMM interface and graphics: A flexible web-user interface for education and application in molecular simulation and multiscale modeling. V. Schalk, Y. Pevzner, B.T. Miller, H.L. Woodcock

**10:45 COMP 147.** Dr. Warren Hehre: Theoretician turned catalyst. S. Profeta

**11:15 COMP 148.** Quantum pharmacology, pharmacophores, and more: Approaches for the identification of novel lead compounds. J.P. Bowen, O.F. Güner, J. Shim, K. Murnane, R.S. Phillips

## Section B

San Diego Convention Center  
Room 26B

## Materials Science

M. Haranczyk, *Organizer*

R. C. Remsing, *Presiding*

**8:30 COMP 149.** Computational screening for compatibility between organic solvents and photovoltaic materials. A. Goldberg, M. Halls, T.J. Mustard, D. Lupyan, J. Gavartin, S. Kwak, D. Giesen, T. Hughes, Y. Cao

**9:00 COMP 150.** Importance of polarization in simulations of H<sub>2</sub> sorption in *rht*-MOF-1. T. Pham, K. Forrest, B. Space

**9:30 COMP 151.** Molecular dynamics simulations of a light-harvesting molecular triad in explicit tetrahydrofuran solvent using polarizable force field. O.N. Starovoytov, M.S. Cheung

**10:00 COMP 152.** Three-body interactions of solid helium calculated within the Einstein model. D. D'Andrea, R.J. Hinde

**10:20** Intermission.

**10:35 COMP 153.** Core-softened potentials for modelling the anomalous properties of silica. S. Izvekov, B. Rice

**11:05 COMP 154.** Sustainable cyberinfrastructure for computational chemistry. S.V. Pamidighantam, N. Doshi, S. Nakandala, S. Maru, M. Pierce

**11:35 COMP 155.** Structure and dynamics of electrostatic striped colloidal assemblies. G. Chong, N. Sarda, R. Hernandez

**11:55 COMP 156.** Computational exploration of how hydroxamate groups bind to TiO<sub>2</sub> surfaces. B. Rudsteyn, J. Chen, B.J. Brennan, C.F. Negre, S. Chaudhuri, B.Q. Mercado, R.D. Silva, A. Monti, L.G. Rego, G.W. Brudvig, R.H. Crabtree, V.S. Batista

## Section C

San Diego Convention Center  
Room 25C

## Drug Discovery

## ADMET Modeling &amp; Informatics

M. R. Landon, Y. Tseng, *Organizers*  
D. Janezic, *Presiding*

**8:30 COMP 157.** Scaffold analysis of Ames mutagenicity. Y. Tseng

**8:50 COMP 158.** Study and prediction of the toxicity of high-energy molecules. C. Alliod, J. Chemelle, G. Jacob, R. Terreux

**9:10 COMP 159.** Which P450: Predicting which cytochrome P450 isoforms are involved in the metabolism of a xenobiotic. P. Hunt, J. Tyzak, M.D. Segall

**9:30 COMP 160.** *In silico* methods for quantitative structure-phenotype relationships. M.L. Hall

**9:50 COMP 161.** Molecular diagnostic system: A step toward virtual pharmaceutical company. H. Sun

**10:10** Intermission.

**10:25 COMP 162.** *De novo* design in the synthetically accessible compounds universe. C. Lemmen

**10:45 COMP 163.** Computational drug discovery using deep learning approaches. O. Isayev, R. Politi, A. Tropsha

**11:05 COMP 164.** BCL::EvoGen: A reaction-based, evolutionary algorithm for *de-novo* molecular design. A. Geanes, J. Meiler

**11:25 COMP 165.** Pharmit: Interactive exploration of chemical space. D. Koes

**11:45 COMP 166.** AtomNet: A deep, convolutional neural network for bioactivity prediction in structure-based drug discovery. I. Wallach, M. Dzamba, A. Heifets

## Section D

San Diego Convention Center  
Room 26A

## Molecular Mechanics

## Nucleic Acids

M. Feig, *Organizer*

C. R. Allen, *Presiding*

**8:30 COMP 167.** Molecular dynamics studies targeting the DNA-binding process of ERG focusing on autoinhibition and sequence recognition. I.R. Gould

**8:55 COMP 168.** Hybrid modeling of ubiquitin- and SUMO-modified PCNA complexes: Implications for DNA damage responses. C. Yan, S. Tsutakawa, X. Xu, Z. Zhuang, M. Washington, J.A. Tainer, I.N. Ivanov

**9:20 COMP 169.** Clues for fidelity and overall efficiency of human DNA polymerase  $\eta$ . M.N. Ucisik, S. Hammes-Schiffer

**9:45 COMP 170.** Human transcription factor in search mode. K.E. Hauser, B. Esuman, Y. He, E.A. Coutasias, M. Garcia-Diaz, C.L. Simmerling

**10:10 COMP 171.** Cyclic, nucleotide modulation of structure and dynamics of the cytoplasmic domain of the HCN2 ion channel. F. Tofoleanu, B. Brooks

**10:35** Intermission.

**10:50 COMP 172.** QM/MM approach to the phosphate cleavage of non-reactive RNA nucleotides. V. Mlynsky, G. Bussi

**11:15 COMP 173.** Mg<sup>2+</sup>/RNA binding: Insights from atomistic molecular dynamics with enhanced sampling. R.A. Cunha, G. Bussi

**11:40 COMP 174.** BI/BII backbone substate dynamics in protein-bound DNA. J.C. Robertson, T.E. Cheatham

**12:05 COMP 175.** DNA strand length differences and their impact on hybridization in model DNA microarrays: A Monte Carlo molecular simulation study. J.M. Stubbs, S. Cooper, B.R. Rivard, L. Pelletier

## Section E

San Diego Convention Center  
Room 28B

## Quantum Mechanics

*Cosponsored by PHY5*

S. E. Wheeler, *Organizer*

A. Saha, *Presiding*

**8:30 COMP 176.** Black-box, highly accurate approach to dynamic and static electron correlation based on spin projection. T. Tsuchimochi, S. Ten-no

**9:00 COMP 177.** Approximate coupled-cluster methods: Addition by subtraction? V. Rishi, A. Perera, R.J. Bartlett

**9:20 COMP 178.** New index for dynamic electron correlation. E. Ramos-Cordoba, P. Salvador, E. Matito

**9:50** Intermission.

**10:05 COMP 179.** cc-pv5Z-F12 basis set: Reaching the basis set limit in explicitly correlated calculations. J.M. Martin, K.A. Peterson, M.K. Kesharwani

**10:35 COMP 180.** Making and breaking bonds with absolutely localized molecular orbitals: An energy-decomposition analysis for bonded interactions. D.S. Levine, M.P. Head-Gordon

**10:55 COMP 181.** Orbital, optimized, random-phase approximation and intermolecular interactions. V.K. Voora, S. Balasubramani, F.U. Furche

**11:25 COMP 182.** QM/MM protocol for direct molecular dynamics of chemical reactions in solution: The water-accelerated Diels-Alder reaction and rebound oxidation reactions. Z. Yang, C. Doubleday, K.N. Houk

**11:45 COMP 183.** Polarizable QM/MM based on the AMOEBA force field and linear-scaling DFT. J. Dziedzic, M.P. Head-Gordon, T.L. Head-Gordon, C. Skylaris

## Computational Chemistry Across Catalysis

## Electrocatalysis &amp; Photocatalysis

*Sponsored by CATL, Cosponsored by COMP, ENFL and WCC*

## Multiscales Chemistry

## Soft Matter

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

## Computer-Aided Drug Design

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MED1 and PHYS*

## TUESDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 28A

## ACS Award for Computers in Chemical &amp; Pharmaceutical Research: Symposium in honor of Warren J. Hehre

J. P. Bowen, *Organizer*

A. J. Shusterman, *Organizer, Presiding*

**1:30 COMP 184.** Dynamic criteria of mechanisms of organic reactions. K.N. Houk

**2:00 COMP 185.** Computational approaches to identifying biological dark matter, exemplified by "hidden genes" in HIV-1 and Ebola. E.W. Taylor, L. Premadasa, M.E. Morgan, J.A. Ruzicka

**2:30 COMP 186.** Molecular models for the organic chemistry classroom: A look back and a look forward. A.J. Shusterman

**3:00** Intermission.

**3:15 COMP 187.** Molecular interactions from first principles. M.S. Gordon, S.R. Pruitt, K. Brorson

**3:45 COMP 188.** Exploring flexibility and molecular recognition in the human cytochrome 3A4. M. Kontoyianni, B. Lacy, C. Hayes, D. Ansbro

**4:15 COMP 189.** Award Address (ACS Award for Computers in Chemical and Pharmaceutical Research sponsored by the ACS Division of Computers in Chemistry). Bringing quantum chemistry into the mainstream. W.J. Hehre

## Section B

San Diego Convention Center  
Room 26B

## Materials Science

M. Haranczyk, *Organizer*

B. RudshTEYN, *Presiding*

**1:30 COMP 190.** Assessing zeolite frameworks for noble gas separations through a joint experimental and computational approach. K.V. Lawler, A. Sharma, B. Alagappan, P. Forster

**1:55 COMP 191.** Tuning the electronic and optical properties of complex oxides for efficient light harvesting. I. Nayyar, S.E. Chamberlin, T. Kaspar, N. Govind, S. Chambers, P.V. Sushko

**2:20 COMP 192.** Insights into the interfacial interactions controlling the liquid phase exfoliation of phosphorene from molecular dynamics. V. Sresht, A. Pádua, D. Blankschtein

**2:40** Intermission.

**2:55 COMP 193.** Rapid screening to identify new proton-conducting electrolytes. P. Wisesa, T. Mueller

**3:25 COMP 194.** Electronic frustration-driven ionic conductivity in a superionic solid electrolyte: Simulating dynamic disordering of polar covalent bonds. N. Adelstein, B. Wood

**3:55 COMP 195.** Predictive design and validation of novel ion-selective membranes for energy storage devices. B. Helms, C. Li, A. Ward, S. Doris, T. Pascal, D. Prendergast, X. Qu, K. Persson

**4:25 COMP 196.** Tuning the electronic properties of ZnO nonpolar surfaces for solar energy conversion devices: New insights from a first-principles study. A. Rodríguez García, A.B. Muñoz-García, R. Di Girolamo, F. Auremma, C. De Rosa, M. Pavone

## Section C

San Diego Convention Center  
Room 25C

## Drug Discovery

## Molecular Dynamics Simulation

M. R. Landon, Y. Tseng, *Organizers*  
R. Malmstrom, *Presiding*

**1:30 COMP 197.** Molecular dynamics-generated ensemble structures improve virtual screening performance. S. Jusoh, R.V. Swift, T.L. Offutt, J.D. Durrant, R.E. Amaro

**1:50 COMP 198.** Prediction of protein-ligand binding using QM/MM-based methods. C. Zheng, A. Marion, I. Antes

**2:10 COMP 199.** Withdrawn.

**2:30 COMP 200.** Drug-membrane interactions at different pH values: Molecular dynamics simulations in combination with experimental techniques. S. Jakobtorweihen, D. Lopes, C. Nunes, S. Reis, I. Smirnova

**2:50 COMP 201.** Withdrawn.

**3:10 COMP 202.** Investigation of binding affinity in bio-molecular complexes. G. Calabro

**3:30** Intermission.

**3:45 COMP 203.** Structural effects of post-translational modifications of polytheonamide B revealed by molecular dynamics simulations. A. Renevey, S. Riniker

**4:05 COMP 204.** Detection and evolution of allosteric pockets and their networks from MD simulations. G. La Sala, S. Decherchi, W. Rocchia, M. De Vivo

**4:25 COMP 205.** Synergistic use of QM/MM x-ray crystallography and time-averaged MD analysis: Protonation-state modeling. O. Borbulevych, C. Velez Vega, L.M. Westerhoff, D. Mckay, J. Duca

**4:45 COMP 206.** Targeted approach to automating the discovery of transition state geometries with minimal input in order to predict reactivity. L.D. Jacobson, A. Bochevarov

**5:05 COMP 207.** Can we turn the histidine switch off? Molecular dynamics simulations of flavivirus envelope proteins. D.I. Osolodkin, E.V. Dueva, V.A. Palyulin, N.S. Zefirov

## Section D

San Diego Convention Center  
Room 26A

## Molecular Mechanics

## Solvation, pH &amp; Ions

M. Feig, *Organizer*

K. E. Hauser, *Presiding*

**1:30 COMP 208.** Coarse grained description of electronic structure yields water's unique properties from ice to the supercritical phase. G.J. Martyna

**1:55 COMP 209.** Water solvation under pH and temperature variations in type III antifreeze protein: A molecular dynamics computational analysis. A. Peramo

**2:20 COMP 210.** Origin of pKa shifts of SNase internal ionizable residues via VMMS simulation in explicit water. X. Wu, A. Damjanovic, B. Brooks

**2:45 COMP 211.** Advances in constant pH molecular simulation with the EDS-HREM and 2D-EDS-HREM methods. B.T. Miller, J. Lee, A. Damjanovic, B. Brooks

**3:10 COMP 212.** Further step to the understanding of the solvation behavior of alcohols in ionic liquids. A. Appelhagen, D. Kerle

3:35 Intermission.

3:50 **COMP 213.** Truth and lies of MM/GBSA. Z. Jia, V. Agrawal, Y. Liu, T. Han, B.N. Dominy

4:15 **COMP 214.** Solute-solvent energetics based on proximal radial distribution functions. S. Ou, B.M. Pettitt

4:40 **COMP 215.** Fluctuation solution theory investigation of the Kirkwood superposition approximation for pure water. G. Pallewela, E.A. Ploetz, P.E. Smith

5:05 **COMP 216.** Modeling the nucleation of organic molecules. E.E. Santiso

## Section E

San Diego Convention Center  
Room 28B

### Quantum Mechanics

*Cosponsored by PHYS*

S. E. Wheeler, *Organizer*

P. S. Hudson, *Presiding*

1:30 **COMP 217.** Multiscale modeling with no loss of accuracy: Dynamics of embedded ground and excited states. M. Pavanello

2:00 **COMP 218.** Accurate, fragment-based quantum chemistry methods for large molecular systems. A. Saha, K. Raghavachari

2:20 **COMP 219.** Libra: An open-source, "methodology discovery" library for quantum and classical dynamics simulations. A.V. Akimov

2:50 **COMP 220.** Electronic couplings in complex molecular systems: A computational implementation. D. Kosenkov, Y. Kholod

3:20 Intermission.

3:35 **COMP 221.** Non-equilibrium ring-polymer molecular dynamics. R. Welsch, S. Althorpe, T.F. Miller

4:05 **COMP 222.** Quantum Andersen thermostat. D. Rogers

4:35 **COMP 223.** Electron trajectories in molecular orbitals. I. Sumner, H. Anthony

### Computational Chemistry Across Catalysis

#### From Metallic Nanoparticles to Isolated Metal Active Site

*Sponsored by CATL, Cosponsored by COMP, ENFL and WCC*

### Multiscales Chemistry

#### Liquids

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

### Computer-Aided Drug Design

#### Computational Biophysics

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

### Opportunities & Progress in Computational Prediction of Contaminant Toxicity, Fate & Transport Properties

*Sponsored by ENVR, Cosponsored by COMP*

## TUESDAY EVENING

### Section A

San Diego Convention Center  
Hall E

#### Chemical Computing Group Excellence Award for Graduate Students

C. L. Simmerling, *Organizer*

6:00 - 8:00

**COMP 224.** High-order diagrammatic vibrational coupled-cluster theory. J. Fauchaux, S. Hirata

**COMP 225.** Towards a real-time description of magnetic systems with applications to magnetic circular dichroism spectroscopy. J.J. Goings, X. Li

**COMP 226.** Modeling reactivity to soft, hard, and biological targets with a deep learning network. T. Hughes, N. Dang, G.P. Miller, S. Swamidass

**COMP 227.** Insights on TET2 activity for DNA demethylation from MD simulations. H. Torabifard, M. Yan Liu, R.M. Kohli, G.A. Cisneros

**COMP 228.** Chemically specific dynamic bond percolation model for computational screening of polymer electrolytes. M. Webb, B.M. Savoie, Z. Wang, T.F. Miller

### Section B

San Diego Convention Center  
Hall E

#### NVIDIA GPU Award

M. E. Berger, *Organizer*

6:00 - 8:00

**COMP 229.** Automated code engine for generation and optimization of electronic integrals on graphics processing hardware. C. Song, L. Wang, T.J. Martinez

**COMP 230.** Constant pH-replica exchange on graphics processors applied to beta-secretase 1 inhibitor design. D. Mermelstein, J. McCammon, R. Walker

**COMP 231.** Predicting binding-free energies in a combinatorial chemical space using a GPU implementation of multisite lambda dynamics. K. Armacost, G. Goh, C.L. Brooks

**COMP 232.** GPU implementation of energy minimization for virtual screening. J. Sunseri, D. Koes

**COMP 233.** Routinely tracing long-timescale protein motions via GPU-based orthogonal space sampling molecular dynamics. E. Aitchison, D. Wu, W. Yang

### Section C

San Diego Convention Center  
Hall E

#### OpenEye Outstanding Junior Faculty Award in Computational Chemistry

C. L. Simmerling, *Organizer*

6:00 - 8:00

**COMP 234.** Enabling transport across the blood brain barrier. S. Nangia

**COMP 235.** Density-functional theory electron density errors in ionization and dynamics. C. Isborn

**COMP 236.** Accelerating *ab initio* simulations of molecular motion. R. Steele

**COMP 237.** High-throughput prediction of minor groove electrostatic potential in studies of protein-DNA recognition. T. Chiu, R. Rohs

### Section D

San Diego Convention Center  
Hall E

#### Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:00

**COMP 238.** Withdrawn.

**COMP 239.** Comparison of the structure and bonding in the aliphatic boronic R-B(OH)<sub>2</sub> and borinic R-BH(OH) acids (R = H; NH<sub>2</sub>, OH, and F): A computational investigation. N.Z. Rao, J.D. Larkin, C.W. Bock

**COMP 240.** Protein deamidation prediction with machine learning and molecular dynamics. L. Jia, Y. Sun

**COMP 241.** First-principles molecular dynamics studies of mercury solvation in a deep eutectic solvent. E.O. Fetisov, D. Harwood, I.W. Kuo, C.J. Peters, J.I. Siepmann

**COMP 242.** In-silico design of drug-like molecules by a fragment-based molecular evolutionary approach. K. Kawai, N. Nagata

**COMP 243.** Accurate, on-the-fly interpolation of quantum mechanical energy and forces of large systems incorporated into an adaptive multi-level QM/MM simulation tool. M.R. Salazar

**COMP 244.** Ground state stabilization of non-enzymatic  $\beta$ -keto acid decarboxylation in aqueous solution. A. Tamez, J.D. Evansck

**COMP 245.** Effect of bulky substituents with varying electronic characteristics on the stereoselective synthesis of substituted pyrrolidines. D. Jones, M. Milletti

**COMP 246.** Light-harvesting in heterogeneous environments. C. Steinmann, J. Kongsted

**COMP 247.** Benchmarking computational protein design methodologies: Transaminases as a case study. A. Crespo, A. Rodriguez-Granillo, K. Lexa, J.C. Moore, N. Marshall, K. Hiraga, E.C. Sherer, B. Sherborne, K. Canada, M. Truppo

**COMP 248.** New approaches to the chemical synthesis of acetylanosterol and its computer approaches to MNDO calculation. E.J. Parish, Y. Lo, W. Huang, H. Honda, T. Wei

**COMP 249.** Improving the scoring of protein-ligand binding affinity by including the desolvation energy. Y. Li, R. Wang, M.K. Holloway, Y. Gao

**COMP 250.** Stochastic simulation algorithm applied to electrochemical systems. O. Beruski, E.G. Machado, H. Varela

**COMP 251.** Normal mode analysis of alpha-beta tubulin dimers. A. Manandhar, M. Kang, S. Loverde

**COMP 252.** Development of force field for diorganopolysilanes: Silicon, carbon, and hydrogen system. N. Suzuki, N. Nakayama, M. Fujiki, H. Goto

**COMP 253.** Predicting partition coefficients and solvation using alchemical free energy calculations. C.C. Bannan, D.Y. Kyu, D.L. Mobley

**COMP 254.** Elucidating an intrinsic role of glycosylation on protein secondary structure. J. Rogers, S. McHugh, Y. Lin

**COMP 255.** Withdrawn.

**COMP 256.** Binding free-energy analysis of alanine mutations of the interface residues in blood coagulation factor VIIIa: Functional implications for thermo-stable co-factor variant. S.M. Shearin, D. Venkateswarlu

**COMP 257.** Interfacial adsorption of patchy nanoparticles onto hairy vesicles. M. Dutt, F. Aydin, G. Uppaladadiam

**COMP 258.** Development of extended force field for Ru-carbene complex and conformational energy profiles of Ru=C rotation. N. Nakayama, Y. Nakagawa, H. Gotoh, S. Iwasa

**COMP 259.** Treatment of sulfur electrostatic anisotropy in the OPLS-AA force field. X. Yan, W.L. Jorgensen

**COMP 260.** Effect of single nucleotide polymorphisms on drug responses in erythrocyte metabolism. N. Mih, E.C. Brunk, A. Bordbar, B.O. Palsson

**COMP 261.** Systematized procedure for the theoretical study of a diatomic substance. C. Cronic, G.G. Hoffman

**COMP 262.** Molecular dynamics study of the selective encapsulation of galactose by arylamide foldamers. A. Lai, Z. Liu, A. Abramyan, V. Pophristic

**COMP 263.** Sensitivity in predicted relative binding free energies from incremental ligand changes within a model binding site. N. Lim, L. Wang, D.L. Mobley, R. Abel

**COMP 264.** High-performance calculation of HF exchange using GPUs. S. Nagashiro, Y. Furukawa, R. Koga, K. Yasuda

**COMP 265.** Structural basis of partial agonism at the dopamine D<sub>3</sub> receptor. M. Michino, C.A. Boateng, P. Donthamsetti, O.M. Bakare, A. Bonifazi, M. Ellenberger, T.M. Keck, C. Zhu, J.A. Javitch, A.H. Newman, L. Shi

**COMP 266.** Molecular dynamics of single-chain hydrophobic polymers in water. M. Drewnsko, S. Loverde

**COMP 267.** Stochastic model of Ca<sup>2+</sup> sparks in cardiomyocytes: Using MCell to investigate the fundamental sub-cellular processes of the heartbeat. S.P. Hrakis, T. Bartol, T. Sejnowski, R.E. Amaro

**COMP 268.** Comparison between Darcy's law and Darcy-Brinkman formulation for reactant transport in PEFC porous media. O. Beruski, T. Lopes, A.R. Kucernak, J. Perez

**COMP 269.** Implicit solvent coarse-grained model of polyamidoamine dendrimers: Role of generation and pH. L. Chong, F. Aydin, M. Dutt

**COMP 270.** Advanced multi-modal scanning tunneling microscopy and spectroscopic imaging analyses. M. Corneliu

**COMP 271.** Convolutional neural networks for protein-ligand scoring. M. Ragoza, J. Collins, D. Koes

**COMP 272.** How many sulphur(S) can be in a row? B. Fiser, B. Jójart, B. Viskolcz, I.G. Csizmadia, E. Gomez-Bengoa

**COMP 273.** DFT analysis of water clusters, dopaminergic derivatives, and their desolvation energies. M. Morris, A.K. Hatstat, L.W. Peterson, M.L. Cafiero

**COMP 274.** Oncogenic mutations hijack Bax toward an off-pathway nonproductive state. M. Zhang, R. Hu, R. Nussinov, B. Ma, J. Zheng

**COMP 275.** How structural and thermodynamic properties scale with the length of a model, disordered polypeptide. J. Drake, B.M. Pettitt

**COMP 276.** Effect of electronic couplings on charge transfer rates in Cd<sub>33</sub>Se<sub>33</sub> quantum dots functionalized by Ru(II) complexes. P. Cui, S. Kilina



- COMP 277.** DFT design of inhibitors of the LPXC enzyme. C. Dishuck, A.J. Dewar, L.W. Peterson, M.L. Cafiero
- COMP 278.** DFT analysis of the selectivity of known bioactive ligands in the sulfotransferase and catechol-O-methyltransferase enzymes. C. Pinckney, L.W. Peterson, M.L. Cafiero
- COMP 279.** *Ab initio* design of novel inhibitors for catechol-O-methyltransferase. A.K. Hatstat, M.L. Cafiero, M. Morris, L.W. Peterson
- COMP 280.** Computational determination of pK<sub>a</sub>s on pH-responsive and luminescent dimetallic lanthanide complexes. J.S. O'Brien, L.E. Hopper, M. Bailey, M.J. Allen, G.A. Cisneros
- COMP 281.** Scalable, fragment-based ensemble generator for docking studies, structure prediction, and condensed-phase simulations. D.S. Cerutti, Z. Zheng, N. Bansal, K.M. Merz
- COMP 282.** Fragment based energetic analysis of conformers with linear-scaled CCSD method. Y. Jin, R.J. Bartlett
- COMP 283.** Development of algorithms advancing all-atom lipid bilayer simulations. C. Lin, R. Walker
- COMP 284.** Computational insights into the optimization of anti-HIV alternating copolymers. L.R. Hollingsworth, R. Fuchs, C. Werle, A. Brown, D.R. Bevan, R.D. Gandour
- COMP 285.** Molecular dynamics simulation of C<sub>60</sub> fullerenes encapsulation into graphene trench. E. Lee, S. Kim, K. Kim, J. Kang
- COMP 286.** Binding free energy study of a small molecule to a target by metadynamics and alchemical transformation. Y. Tanida, A. Matsuura
- COMP 287.** Kinetics of proton transfer for ligands in the SULT1A1 active site. D. Wilson, A. Weems, L.W. Peterson, M.L. Cafiero
- COMP 288.** DFT study of the selectivity of DOPA-decarboxylase. A. Ritter, E. Harrison, L.W. Peterson, M.L. Cafiero
- COMP 289.** *Ab-initio* potential energy surfaces for bond dissociation through coupled-cluster methods: The case of triple bond-dissociation in nitrogen molecule. V. Rishi, A. Perera, R.J. Bartlett
- COMP 290.** Computing aqueous absorption spectra: The effect of solute polarity and basis set on convergence with respect to the amount of explicit solvent. J. Milanese, C. Isborn
- COMP 291.** Prediction of the molecular weight distribution in ATRP techniques using the RSQSSA methodology. I. Zapata, R. Hutchinson, E. Saldivar, K. Payne, A. Licea-Claverie
- COMP 292.** Molecular-field-based design and analysis of thiophene sulfonamide derivatives as inhibitors of *trans*-2-enoyl-acyl carrier protein reductase, InhA. P.M. Imran, S. Varghese, N.A. Vellore
- COMP 293.** Computational modeling of the conformational dynamics of the activation process of MAPK-interacting kinases (Mnks). M. Kumarasiri, T. Teo, W. Shudong
- COMP 294.** Hydration structure in the active site of human coagulation factor Xa. H. Sato, A. Matsuura
- COMP 295.** Computers and chromatography: From atoms to columns. R.K. Lindsey, M.R. Schure, P. Carr, J.I. Siepmann
- COMP 296.** Investigation of the structure and dynamics of the type IV pilus retraction motor PilT using molecular dynamics simulation. A. Andrews, J.L. Baker
- COMP 297.** Role of side alkyl chains in interactions between conjugated polymers and carbon nanotubes. B.J. Gifford, S. Kilina
- COMP 298.** Development of ionic liquid OPLS-AA force field parameters for use in molecular dynamics and Monte Carlo simulations. O. Acevedo, B. Doherty
- COMP 299.** Investigating molecular recognition in FMN aptamer through molecular dynamics simulations. P. Gasper, A.A. Chen
- COMP 300.** Microwave-assisted synthesis of a MK2 inhibitor by Suzuki-Miyaura coupling for study in Werner syndrome cells. M.A. Baashen
- COMP 301.** Prediction of new thermodynamically stable aluminum oxides. S. Wang, A. Oganov, Q. Zhu
- COMP 302.** Kinetic analysis of the aza-Cope/Mannich reaction of substituted oxazolidines: Effect of an electron-withdrawing group. A.S. Durden, M. Milletti
- COMP 303.** New approach to calculate the complexation-induced <sup>1</sup>H NMR chemical shift changes in proteins. Z. Yu, P. Li, K.M. Merz
- COMP 304.** MT<sub>Rec-His</sub>: A novel method for incorporating flexibility in the receptor's binding pocket. N. Bansal, Z. Zheng, K.M. Merz
- COMP 305.** Withdrawn.
- COMP 306.** Conventional strain energies and relative stabilities of the isomers of dimethyl and dinitrocylobutadiene. B. Peyton, Q. Cheng, S. Smith, D.H. Magers
- COMP 307.** Superconductivity of novel tin hydrides (Sn<sub>n</sub>H<sub>m</sub>) under high pressure. M. Davari Esfahani, A. Oganov, Q. Zhu, S. Wang, X. Zhou, M. Rakinin, H. Dong, Z. Wang
- COMP 308.** Computational methods for the elucidation of polymerase function. T. Coulther, R. Parasuram, P.J. Beuning, M.J. Ondrechen
- COMP 309.** *Ab initio* investigation of the aqueous solvation of the nitrate ion. S.R. Pruitt, K. Brorsen, M.S. Gordon
- COMP 310.** Computational analysis of electrostatic interaction between chronic myeloid leukemia drugs and the target, BCR-ABL kinase. F. Nyaisonga, L. Hiller, L. Liu, M. Radhakrishnan
- COMP 311.** Free energy calculations in enzymes using the paradynamics approach. M. Feliks, A. Warshel
- COMP 312.** Coarse-grained simulations of a coherently dynamic, two-dimensional protein crystal. R. Alberstein, F.A. Tezcan, F. Paesani
- COMP 313.** Electronic excitations in Reichardt's and Brooker's solvatochromic dyes in solvents of varying polarity. J. Zuczek, J. Shaw, D. Kosenkov
- COMP 314.** Investigations into the mechanism of the nucleophilic substitution reaction using M06-2X. P. Vo
- COMP 315.** Quantum chemical study of mechanism and stereoselectivity of zinc- and NADP-dependent secondary alcohol dehydrogenase. S. Moa, F. Himmo
- COMP 316.** Efficient characterization of local millisecond dynamics: Dihedral entropy from accelerated MD. A.S. Kamenik, J. Fuchs, K. Liedl
- COMP 317.** Molecular dynamics investigation of ice nucleation and growth in supercooled water in the presence of an electric field. A. Webb, K. Leong, F. Wang, A.L. Williams
- COMP 318.** QM/MM analysis of the mechanism of the ubiquitin conjugating enzyme UBC13. W.M. Jones, A. Davis, I. Sumner
- COMP 319.** Modeling 10000 antibodies in about an hour: Leveraging the power of the Amazon cloud. E. Metwally
- COMP 320.** Molecular simulations of type IV pilin subunits from three organisms in a lipid bilayer. T. Brier, J.L. Baker
- COMP 321.** Complete basis set limits for the Hartree-Fock and second-order Møller-Plesset energies for DMPO, EMPO, and their hydroxyl radical adducts. H.B. Short, C.E. Warden, S.J. Kirkby
- COMP 322.** Reduction potential studies of respiratory complex I. K. Tran, T. Ichiye
- COMP 323.** Expansion of the Amber Lipid14 force field: Enabling complex membrane molecular dynamics. B. Madej, C. Dickson, A. Skjevik, L. Yang, I.R. Gould, R. Walker
- COMP 324.** Modelling solvation of micelles. O.A. Hull, A. Mishra, D.S. English, K. Mitchell-Koch
- COMP 325.** Exploring the interplay of dynamics and catalysis in *Escherichia coli* prolyl-tRNA synthetase using quantum mechanical/molecular mechanical simulations. T.T. Huynh, C. Reinhardt, A.N. Hodac, L.M. Adams, S. Hati, S. Bhattacharyay
- COMP 326.** Extension of the Amber Lipid14 force field to glycolipids: Parameterization and validation. L. Yang, B. Madej, Å.A. Skjevik, C. Dickson, H. Wang, I.R. Gould, R.C. Walker
- COMP 327.** Monte Carlo studies of vapor-liquid equilibria for a Langmuir monolayer of pentadecanoic acid. M.S. Minkara, R.K. Lindsey, J.I. Siepmann
- COMP 328.** First-principles molecular dynamics study of mercury solvation in an imidazolium ionic liquid. R. Hembree, E. Fetisov, C.J. Peters, J. VandeVondele, J.I. Siepmann
- COMP 329.** Computational approach for performing medicinal chemistry transformations within a 3D active site. R. Alvarez, A. Deschenes, N. Thorsteinson
- COMP 330.** Effects of size, charge, and ligands on photophysical properties of small silver clusters. M.A. Javed, N.K. Dandu, S. Kilina
- COMP 331.** Probing electrostatic interactions between amino acids and urea using *ab initio* calculations. M.S. Minkara, D. Urul, M.N. Weaver, K.M. Merz
- COMP 332.** Enhancing virtual screening performance of protein kinases by incorporating molecular dynamics simulations. T.L. Offutt, R. Swift, S. Jusoh, R.E. Amaro
- COMP 333.** Gauging the performance of density functionals for lanthanide-containing molecules. G. Schoendorf, S. Grimmel, A.K. Wilson
- COMP 334.** Free-energy calculations for ligand/phosphopeptide and BRCT domain binding. W. You, C. Chang
- COMP 335.** Activation barriers for alkylation of nucleotides in aqueous solutions by dimethyl sulfate, diethyl sulfate, and related compounds. G.A. Papadantonakis, D.R. Eichler, H.A. Hamann, K.A. Harte
- COMP 336.** Role of free energy in effectively computing carbohydrate NMR chemical shifts. P.S. Hudson, B. Pollard, M.T. Kemp, M.F. Crowley, H.L. Woodcock
- COMP 337.** Continuous evaluation of ligand pose prediction (CELPP): An automated workflow for weekly cross-docking blinded challenges. S. Liu, C. Chrus, J. Grethe, R.V. Swift, R.E. Amaro, V. Feher, M.K. Gilson
- COMP 338.** Virtual screening of organic dyes based on pseudospectral time dependent density functional theory. A. Bochevarov, Y. Cao, M. Halls, A. Goldberg
- COMP 339.** Shift/collapse algorithm based on neighbor list: Toward fast and scalable dynamic many-body molecular dynamics simulation. M. Kunaseth, A. Nakano, S. Hannongbua
- COMP 340.** Use on implicit solvation in the prediction of sorption free energies of cationic amines on montmorillonite: A linear interaction energy method. A. Villaseñor, M.A. Samaraweera, J. Gascon, W. Jolin, D. Vasudevan, A. MacKay
- COMP 341.** Molecular dynamics study of triptycene rotors in metal organic frameworks: Structure-enforced gearing. S. Yang, X. Jiang, M.A. Garcia-Garibay, K.N. Houk
- COMP 342.** Assigning acetol: Simulated IR spectra using high level *ab-initio* methods. N. Tipton, S.D. Williams
- COMP 343.** Withdrawn.
- COMP 344.** Investigation of ligand binding pathways to neuraminidase using MM/GBSA free energy analysis. P.F. Marriss, L.M. Krause, J. Sorensen, A.W. Van Wynsberghe
- COMP 345.** Effects of roaming on reaction kinetics. M. Zekarias, I. Ulusoy, R. Hernandez
- COMP 346.** Examination of the complete binding pathways of ligands to H274Y and wild-type neuraminidase via multiscale sampling and MM/GBSA analysis. A.W. Van Wynsberghe, R.W. Wenner, E.M. Lewis, D.F. Dacres
- COMP 347.** Human health and the environment: Predicting plasma protein binding and metabolic clearance rates of environmentally relevant chemicals. B.L. Ingle, B.C. Veber, J.W. Nichols, R. Tornero-Velez
- COMP 348.** Steered-molecular dynamics simulations and mutational studies to explore the interplay of coupled-domain dynamics and substrate binding in prolyl-tRNA synthetases. M. Matthew, A.N. Hodac, T.T. Huynh, L.M. Adams, S. Hati, S. Bhattacharyay
- COMP 349.** Computational study examining the stability of 3' overhangs in the RNAi mechanism. S. Telehany, M.C. Nagan
- COMP 350.** Molecular basis of sliding clamp diffusion along DNA. E.K. Carter, I.N. Ivanov
- COMP 351.** Cation-π interactions of curved π surfaces: Corannulene and tweezers. A. Mirchi, T. C. Dinadayalane, J. Leszczynski

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- COMP 352.** Noble gas adsorption on the TiO<sub>2</sub>(110) surface: An *ab-initio*-assisted venture in van der Waals-corrected DFT. **A. Abbaspour Tamijani, A. Salam, M. de Lara-Castells**
- COMP 353.** Characterization of the HLTV-1 rex peptide bound to an RNA aptamer. **Z. Fallon, M.C. Nagan**
- COMP 354.** Virtual screening for inhibitor to monomethyltransferase PR-Set7. **T. Sakano, T. Kawamura, H. Fujitani**
- COMP 355.** Withdrawn.
- COMP 356.** Effects of viscosity and macromolecular crowding on the diffusion-controlled rate constant of ferredoxin with ferredoxin NADP<sup>+</sup> reductase. **S. Sweger, J.D. Madura**
- COMP 357.** Examination of the LCST and hydration properties of PNIPAM and its substituents from molecular dynamics simulations. **M. Galbraith, J.D. Madura**
- COMP 358.** Nucleoid macromolecular crowding effect on protein diffusion. **A. Yildirim, T. Ando, Y. Sugita, M. Feig**
- COMP 359.** Developing monovalent ion parameters for the optimal point charge (OPC) water model. **J. Dood, B.P. Krueger**
- COMP 360.** Computational design of metabotropic glutamate receptors with non-natural ligands. **B. Mueller, J. Meiler**
- COMP 361.** Determining the mechanism of the ubiquitin-conjugating enzyme UBC13 with QM/MM and metadynamics. **A. Davis, W.M. Jones, S. Zamfir, I. Sumner**
- COMP 362.** Picture tells a thousand words: Summarizing SAR for medicinal chemists. **R. Lawrence, G. Tedesco, P. Tosco, T. Cheeseright**
- COMP 363.** Phase diagram prediction using multistate reweighting combined with iterative sampling. **N.P. Schieber, E. Dybeck, M.R. Shirts**
- COMP 364.** Elucidating the isomerization relaxation mechanism of fluorinated azobenzene using transition path sampling with QM/MM molecular dynamics. **A. Muzdalo, P. Saalfrank, M. Santer**
- COMP 365.** Dipole moment and binding energy of water in proteins from crystallographic analysis. **A. Morozenko**
- COMP 366.** Supercomputing technology for chemistry at Radford University. **B. Amofah, T.J. Fuhrer**
- COMP 367.** Global similarity network of flexible ligand-binding sites for predicting ligand toxicity and polypharmacology. **A.V. Ilatovskiy, I. Kufareva, R. Abagyan**
- COMP 368.** Role of electrostatic networks in the stability and function of protein kinase A's regulatory subunit. **E. Pecora de Barros, R. Malmstrom, A.P. Kornev, S.S. Taylor, R.E. Amaro**
- COMP 369.** ENRI: Enriching virtual screening through machine learning. **R. Akbar, S. Jusoh, R.E. Amaro, V. Helms**
- COMP 370.** N-S vs.  $\pi$ -S interactions: A computational study. **V. Nzuwah Nziko, S. Scheiner**
- COMP 371.** Parameterizing fluorescent protein chromophores for molecular dynamics simulations. **D.L. Blood, A. Rosnik, B.P. Krueger**
- COMP 372.** Computational investigation of domain registration of membrane rafts. **N. Chen, P.B. Moore**
- COMP 373.** Identifying hotspot residues for rational enzyme design in haloalkane dehalogenase. **G. Jindal, A. Warshel**
- COMP 374.** Benchmarking computational methods for binding free-energy estimation. **J. Sunseri, D. Koes**
- COMP 375.** Top-down vs. bottom-up formation mechanism for fullerenes and endohedral metallofullerenes. **H. Bell, A. Lambert, T.J. Fuhrer**
- COMP 376.** Computational analysis of proposed tetrafluoromacrolide. **E. Kaufman, J.L. Duffy-Matzner, A. Viste**
- COMP 377.** Fragment oriented molecular shape (FOMS) search: A novel shape-based virtual screening method. **E.R. Hain, D. Koes**
- COMP 378.** Electronic structure calculations of catalyzed lignin decomposition. **J. Hicks, M.R. Hoffmann**
- COMP 379.** Development of the transferable potentials for phase equilibria force field for carbon monoxide. **D. Harwood, J. Grindstaff, J.I. Siepmann**
- COMP 380.** Mechanism of diastereoselective encapsulation of tartaric acid by arylamide foldamers: A computational investigation. **M. Wujcik, Z. Liu, V. Pophristic**
- COMP 381.** Exploration of electronic structures of nitrogen-radical precursors for use in amination. **S. Calderon, E.J. Menke, R.D. Baxter, H.P. Hratchian**
- COMP 382.** Leveraging quantitative structure-activity relationships (QSARs) for small molecule docking into G-protein coupled receptors (GPCRs). **D.Y. Fu, J. Meiler**
- COMP 383.** Determining the structure for Amot 80, 130, and L2. **C. Peck, A.C. Kimble Hill**
- COMP 384.** Constrained<sup>2</sup> density-functional theory. **P. Ramos, M. Pavanello**
- COMP 385.** Thermochemical analysis of intermolecular vs. intramolecular reactions in iridium complexes. **A. Bienvenu, L. Perez, M.B. Hall**
- COMP 386.** Accelerated piezoelectric evaluation (APE). **M.E. Boca, K. Werling, D. Lambrecht**
- COMP 387.** Withdrawn.
- COMP 388.** Probing the function of different regions of a pH-dependent, viral, lytic peptide. **M. Ward, E.R. May**
- COMP 389.** Extension and validation of the GROMOS force field for the simulation of peptides. **K.C. Cunha, R. Lins**
- COMP 390.** Computational investigations into the structure and correlated dynamics of PDE6 and its inhibition by PDE6- $\gamma$ . **S. Kamal, E.R. May**
- COMP 391.** Utilizing temperature gradients to direct peptide translocation in *Pristina leidy* as a model for targeted drug delivery. **S.F. Urfano, M. Oh, K. Slowinska**
- COMP 392.** Non-covalent interactions using orbital optimized random-phase approximation. **V. Voora, S. Balasubramani, F.U. Furche**
- COMP 393.** Computationally engineering a stable, symmetric membrane-protein scaffold. **A.M. Duran, J. Meiler**
- COMP 394.** Towards an understanding of combined ligand/reducing-agent effects on nickel-catalyzed coupling reactions using density functional theory. **L.M. Gong, H.P. Hratchian**
- COMP 395.** Computer-assisted drug design: Towards the discovery of new antibiotics for LpxC. **V.K. Thilakarathne, R. Ishawu**
- COMP 396.** Computationally guided repurposing of approved, multi-targeted therapeutics for smoothened-dependent cancers. **K. Kandhwal, M. Parle, R. Abagyan, I. Kufareva**
- COMP 397.** Conserved hydration sites in Pin1 with a unique water localization motif. **A. Barman, D. Hamelberg**
- COMP 398.** Impact of geometry optimization on base-base stacking interactions: An energy decomposition analysis. **R. Altman, A. Ringer McDonald**
- COMP 399.** Analysis of small molecule ligands with DNA aptamers: Conformational sampling and interaction energy determinations. **C.J. Byrd, Z. Petrek, E. Denning, A. Ringer McDonald**
- COMP 400.** Computational approaches to aid the design of small-molecule HIV gp41 inhibitors. **T. McGee, R.C. Rizzo**
- COMP 401.** Restricted excitation window orthogonality constrained density functional theory: Application to the near-edge x-ray absorption spectra of chemisorbed and solvated molecules. **W. Derricotte, F.A. Evangelista**
- COMP 402.** Polymorphism in pharmaceutical drugs. **A. Margo, C. Desgranges, J. Delhomelle**
- COMP 403.** UV-Vis molecular absorption spectra: Benchmarking *ab initio* computational methods for the quantitative prediction of sunlight-driven pollutant degradation in aquatic environments. **K. Trerayapiwat, S.N. Eustis**
- COMP 404.** Influence of computer-assisted instruction (CAI) in chemistry. **A.E. Folorunso**
- COMP 405.** Modeling interprotein interactions in concentrated solutions of wild-type and cataract-related variants of  $\gamma$ D- and  $\gamma$ S-crystallins. **V. Pрыtkova, M. Heyden, E. Wong, J.A. Freitas, D. Tobias**
- COMP 406.** Computer applications in today's chemistry. **A.E. Folorunso**
- COMP 407.** SHSF: A new and improved scoring function for AutoDock Vina, addressing sigma-hole interactions. **M. Koebel, A. Cooper, G. Schmadeke, S. Sirimulla**
- COMP 408.** LK-peptide structural and behavioral changes in ionic liquid solvents. **K. Palunas, J. Pfaendtner**
- COMP 409.** Origin of distinct, ion-pair dissociation kinetics revealed by the solvent-coordinate, free-energy landscape analysis. **Y. Yonetani**
- COMP 410.** Applying extended Hückel theory to pharmacophore modeling. **A. Ajamian**
- COMP 411.** Hydration and dewetting of graphene plates in course-grained water-like solvents: A molecular dynamics simulation study. **F. Sanoj**
- COMP 412.** ChemDB: Web-accessible database for the automation of computation simulations, curation, and analysis of large materials libraries. **T.J. Mustard, A. Goldberg, B. Robbason, M. Halls**
- COMP 413.** Identification of novel, uncompetitive inhibitors of bacterial MTA/SAH nucleosidase. **D. Xu, A. Tao, P. Erstad, M. Caylor, K. Cornell**
- COMP 414.** Molecular identification and characterization of a novel extracellular metalloproteinase produced by *Clostridium sordellii*. **D. Xu, A. Tao, P. Erstad, M. Aldape**
- COMP 415.** Novel approaches to the application of chemical information with data mining and chemical data warehousing. **E.J. Parish, S. Lee, W. Huang, H. Honda, T. Wei**
- COMP 416.** Novel development to the mathematical model to simulate biosensor kinetic for cholesterol determination. **Y. Lo, W. Huang, H. Honda, T. Wei**
- COMP 417.** New approaches to the computer-assisted informatics of oxysterols. **E.J. Parish, Y. Lo, H. Honda, T. Wei**
- COMP 418.** Fluorescence spectra of substituted 3(2H) furanones: A DFT and experimental investigation. **M. Nolan, H. Moloney, M. Moloney, N. Kirwan, N. Prakash, K. Acheson, D.S. Venables, D.G. McCarthy**
- COMP 419.** Fully *ab initio*, vibrational analysis of Ar-H<sub>2</sub>O van der Waals complex by the finite element method. **D. Xu, P. Zajac, A.L. Cooksy**
- COMP 420.** Harnessing GPU acceleration for analysis of molecular dynamics trajectories. **T. Gokey, A.B. Guliaev**
- COMP 421.** Novel approaches to the network-based development target for chemical-compound identification. **Y. Lo, W. Huang, H. Honda, T. Wei**
- COMP 422.** Krypton oxides under pressure. **P. Lata, P. Zaleski-Ejgierd**
- COMP 423.** Pharmacophore modeling of non-nucleoside DNA methyltransferase inhibitors based on a chemoinformatic analysis. **E. Fernandez, J.L. Medina-Franco**
- COMP 424.** Electron and nuclear dynamics of thiolated protected gold nanoclusters (Au<sub>10</sub>SH<sub>14</sub>, Au<sub>25</sub>SH<sub>18</sub><sup>-1</sup>): A theoretical investigation. **R. Senanayake, C.M. Aikens**
- COMP 425.** Structure, energetics, and chemistry of metal-organic species at surfaces/interfaces: How good is DFT? **B. Chilukuri, U. Mazur Hippias, K. Hippias**
- COMP 426.** Benchmarking the random-phase approximation. **M. Agee, A. Burov, B. Nguyen, F.U. Furche**
- COMP 427.** Quasidynamics of biomolecules steered with 3D-RISM-KH mean solvation forces. **A. Kovalenko, I.P. Omelyan**
- COMP 428.** Long-timescale simulation on the Anton supercomputer reveals the "invisible" excited state of the L99A mutant of T4 lysozyme. **J. Schiffer, R. Sida, R. Malmstrom, V. Feher, R.E. Amaro**
- COMP 429.** QSAR models for CDK/cyclin inhibitors: A comparison between QM and classical descriptors. **S. Dhail**
- COMP 430.** Study of carboxylic ester hydrolases: Structural classification, database, and applications. **Y. Chen, P.J. Reilly**
- COMP 431.** Developing molecular guideless for chemicals with reduced oxidative stress potential through systems analysis of ToxCast. **F. Melnikov, L. Shen, J. Kostal, A. Voutchkova-Kostal, J.B. Zimmerman, P.T. Anastas**
- COMP 432.** Optimal point charge approximation: From the water molecule to the chromatine fiber. **S. Izadi, R. Anandakrishnan, A.V. Onufriev**
- COMP 433.** Systematic parameterization of an accurate nonbonded model for ions. **P. Li, L.F. Song, B.P. Roberts, D. Chakravorty, K.M. Merz**
- COMP 434.** Withdrawn.
- COMP 435.** COSMO-based approach to computer-aided mixture design. **N.D. Austin, N.V. Sahinidis, D.W. Trahan**

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- COMP 436.** Generating novel knowledge based scoring function utilizing Hirshfeld surface analysis of protein-ligand complexes. **P. Saha, N. Sukumar**
- COMP 437.** Withdrawn.
- COMP 438.** Reparameterizing and validating the OPLS-AA force field for proteins and protein-ligand systems. **M.J. Robertson, J. Tirado-Rives, W.L. Jorgensen**
- COMP 439.** Insights into lead optimization of the protein kinase RNA-like endoplasmic reticulum kinase (PERK) inhibitors. **M. Nael, R.J. Doerksen**
- COMP 440.** Stereoelectronic effects are in control: From the anomalous stability of bis-peroxides to radical cascade cyclizations. **G. Gomes, I. Alabugin**
- COMP 441.** DNA backbone BI/BII sub-state distribution and dynamics in protein-bound environment determined by molecular dynamics simulations. **J.C. Robertson, T.E. Cheatham**
- COMP 442.** Design of tailored amphiphilic unimolecular polymeric micelles via molecular dynamics simulations. **A. Sharma, S.W. Rick**
- COMP 443.** Multi-resolution model for biomolecular application. **L. Xiao, Q. Cai, Z. Li, H. Zhao, R. Luo**
- COMP 444.** Molecular modeling of dielectric constant of acetonitrile as a function of salt concentration. **I. Daniels, B. Laird, Z. Wang**
- COMP 445.** Utilizing computational chemistry to characterize the functions of structural genomics proteins. **C.L. Mills, P.J. Beuning, M.J. Ondrechen**
- COMP 446.** Withdrawn.
- COMP 447.** Dopamine transporter conformations induced by cocaine and atypical DAT inhibitors. **B. Jean, J.D. Madura, C.K. Surratt**
- COMP 448.** C-H bond activation of hydrocarbons at exposed iron sites in metal-organic frameworks designed to improve catalytic efficiency. **P. Verma, B. Wang, D.G. Truhlar, B. Keitz, D.J. Xiao, J.R. Long**
- COMP 449.** RNA conformational ensembles: Narrowing the gap between experiments and simulations with metadynamics. **A. Gil-Ley, S. Bottaro, G. Bussi**
- COMP 450.** Withdrawn.
- COMP 451.** Withdrawn.
- COMP 452.** Probing the energetics of  $\beta$ -hairpins using adaptive steered molecular dynamics. **H. Bureau, S. Quirk, R. Hernandez**
- COMP 453.** Multiconfiguration pair-density functional theory: A promising new tool for excited-state chemistry. **C. Hoyer, S. Ghosh, A. Sonnenberger, D. Ma, J. Olsen, D.G. Truhlar, L. Gagliardi**
- COMP 454.** Evaluating free energies of dimerization of short polyglutamine peptides with molecular dynamics simulations. **R.J. Workman, J.D. Madura**
- COMP 455.** Computational investigation of the transport mechanism of neurotransmitter sodium symporters using a physiological ion gradient. **E.M. Benner, J.D. Madura**
- COMP 456.** Sequestration of organophosphorus nerve agents by molecular baskets: A theoretical investigation. **S. Polen, C.M. Hadad, J. Badjic**
- COMP 457.** Evolution of electride behaviour under pressure. **S.G. Dale, A. Otero-de-la-Roza, E.R. Johnson**
- COMP 458.** Computational design of peptide-based self-assemblies. **H. Zhang, F. Polzer, M. Haider, C. MacDermid, D.J. Pochan, J.G. Saven**
- COMP 459.** Elucidating the lower critical solution temperature transition of poly(N-vinylcaprolactam). **X. Sun, X. Qian**
- COMP 460.** Predictive sampling of long-timescale protein functional motions in explicit solvent. **X. Li, C. Lv, K. Corbett, L. Zheng, D. Wu, W. Yang**
- COMP 461.** Withdrawn.
- COMP 462.** Efficient and accurate nonadiabatic quantum dynamics in atomistic condensed phase systems using the generalized quantum master equation. **W.C. Pfalzgraff, A. Kelly, T. Markland**
- COMP 463.** Understanding DNA: From structure and dynamics to physical adsorption on surfaces with surfactants. **H. Kim, Y.G. Yingling**
- COMP 464.** Fragment based drug design as a means of identifying novel dopamine D3 antagonists. **K. Pellegrine, C.K. Surratt, J.D. Madura**
- COMP 465.** Serotonin transporter homology construction utilizing a eukaryotic template for fragment-based compound development. **M. Wasko, C.K. Surratt, J.D. Madura**
- COMP 466.** Deeper understanding of surface chemistry of particles interactions in the formation of nanoplates and nanocrystal aggregate. **N.K. Dandu, K. Velizhanin, D. Klin, S.W. Kilina**
- COMP 467.** Acid-base dissociation mechanisms at the silica-water interface: A DFT study. **B. Lowe, C. Sklyaris, N. Green**
- COMP 468.** Pressure induced novel compounds in the Hf-O system from first-principles calculations. **J. Zhang**
- COMP 469.** Substituent effects on the binding of halides by neutral and dicationic bis-triazolium receptors. **B. Nepal**
- COMP 470.** Average condensed phase model for simulating complex environments. **D. Nocito, G.J. Beran**
- COMP 471.** Withdrawn.
- COMP 472.** Solution structure of the monomeric Lassa virus nucleoprotein and insights into its RNA binding mechanism. **J.G. Pattis, E.R. May**
- COMP 473.** Utility of HomoSAR for mapping activity elements of protegrin antimicrobial peptides. **M. Borkar, E. Coutinho**
- COMP 474.** Epidermal growth factor receptor (EGFR) inhibitors as novel anti-cancer agents to combat triple-negative breast cancer. **E. Yawson, D.H. Lee, R.V. Rajnarayanan**
- COMP 475.** Impacts of native defects on the stability, electronic structure, and optical absorption of BIVO<sub>4</sub> material: A screened coulomb hybrid DFT investigation. **S. Lardhi, M. Harb, L. Cavallo**
- COMP 476.** Time-dependent atomistic reconstruction approach to imaging radiation damage propagation in graphite under high electron dose. **B. Farbos, H. Freeman, J. Da Costa, P. Weisbecker, A.J. Scott, G. Vignoles, J. Leyssale**
- COMP 477.** Elastic network models for RNA: A comparative assessment with molecular dynamics and SHAPE experiments. **G. Pinamonti, S. Bottaro, C. Micheletti, G. Bussi**
- COMP 478.** Electron localization and delocalization in mixed-valent Fe<sub>2</sub>(m-O)<sub>2</sub> cores. **K. Al-Ameeed, J.E. McGrady, R.G. Raptis, Y. Sanakis, R. Herchfeld**
- COMP 479.** Enhanced conformational sampling using replica exchange with collective-variable tempering. **A. Gil-Ley, G. Bussi**
- COMP 480.** Quantifying differences in energetics of peptide secondary structure motifs using adaptive steered molecular dynamics. **H. Bureau, S. Quirk, R. Hernandez**
- COMP 481.** Understanding the effects of dimensionality: Spherocylinder diffusion in two and three dimensions. **B.D. Mahala, R. Hernandez**
- COMP 482.** Trigonal prismatic metal complexes: A not-so-rare coordination geometry? **L. Alcock, G. Cavigliasso, A. Willis, R. Stranger, S. Ralph**
- COMP 483.** Kirkwood-Buff-derived force field for polyols. **N. Kariyawasam Manachchige, P.E. Smith**
- COMP 484.** MD simulations of lipids interaction with ion channels. **T.H. Nguyen, Z. Liu, P.B. Moore**
- COMP 485.** Computer modeling and atomistic, molecular-dynamics simulations of alpha and keto mycolic acids from *Mycobacterium tuberculosis*. **P.Y. Leung, Y. Wang**
- COMP 486.** Determination of the reaction coordinate for a key conformational fluctuation in human carbonic anhydrase II. **S. Paul**
- COMP 487.** Kirkwood-Buff derived force field for aqueous alkali earth metal halides. **N. Naleem, N. Benteinitis, P.E. Smith**
- COMP 488.** Inter-molecular interactions between the monomers in A $\beta$ <sub>17-42</sub> oligomers: A comparative molecular dynamics study. **P. Khatua**
- COMP 489.** Crack-cocaine cutting agents in Brazil: Why phenacetin? **A.G. Castro, R.O. Silva, B.S. Santos, G.M. Seabra**
- COMP 490.** Molecular dynamics study of ALK2 kinase mutations in fibrodysplasia ossificans progressiva disorder. **Y.L. Luo, A. Alsamarah, J. Hao**
- COMP 491.** Probing the influence of the ionic liquid [C<sub>4</sub>mpy][Tf<sub>2</sub>N] on the structure of the miniprotein Trp-cage. **J.L. Baker, G.E. Lindberg**
- COMP 492.** Ligand-dependent selectivity of conformational pathways in CCR7. **Z. Gaieb, D.D. Lo, D. Morikis**
- COMP 493.** Influence of environment and temperature on the structure of the thermophilic intrinsically disordered protein FigM. **E.E. Carter, J.L. Baker, C.J. Hartzell, G. Lindberg**
- COMP 494.** Understanding the mechanism and product specificity of PRMT1 using theory and experiment. **O. Acevedo, S. Gathiaka, B. Boykin, B. Caceres, J. Hevel**
- COMP 495.** Understanding and predicting structures of cyclic peptides. **S. McHugh, J. Rogers, Y. Lin**
- COMP 496.** Hydration dynamics of lanthanide ions from polarizable force field. **Y. Tu, G.A. Cisneros**
- COMP 497.** Transferability of GEM distributed multipoles in AMOEBA for ionic liquids. **H. Torabifard, Y. Tu, G.A. Cisneros**
- COMP 498.** Molecular level interactions in membrane proteins. **R.D. Hills**
- COMP 499.** Molecular modeling self-assembly of anticancer drug amphiphiles. **M. Kang, Z. Pengcheng, H. Cui, S. Loverde**
- COMP 500.** Revealing the pH-controlled release mechanism of lytic peptides from non-enveloped virus capsids. **A.R. Brice, E.R. May**
- COMP 501.** Toward quantitative understanding of ATPase mechanism in ABC-transporter: Development and application of reaction path force matching QM/MM method. **J. Pu**
- COMP 502.** Multiscale molecular dynamics for drug discovery targeting metalloenzymes that process DNA and RNA. **M. De Vivo**
- COMP 503.** Understanding the fidelity and specificity of DNA polymerase I. **B. Miller, C.A. Parish, E.Y. Wu**
- COMP 504.** Free-energy computational protocol for the prediction of the effect of single-point mutations on ligand binding affinities. **H. Gutierrez de Teran, H. Keränen, J. Aqvist**
- COMP 505.** Withdrawn.
- COMP 506.** Large-scale complete active space self-consistent-field methods. **A.E. DePrince**
- COMP 507.** Topological excitations in organic/inorganic nanostructures. **J. Yuen Zhou**
- COMP 508.** Molecular fragment affinity concept from an MO perspective. **Z. Boughlala, C. Fonseca Guerra, F. Bickelhaupt**
- COMP 509.** Increasing the accuracy of excited states calculations with optimized density functional theory. **Y. Jin, R.J. Bartlett**
- COMP 510.** Geometry dependence of exchange coupling parameters in binuclear transition metal complexes: Improving density functional theory with approximate projection. **X. Sheng, L.M. Thompson, H.P. Hratchian**
- COMP 511.** Size-dependent error of the density-functional theory ionization potential in vacuum and solution. **X.A. Sosa Vazquez, C. Isborn**
- COMP 512.** Performance of density functionals for mono-nuclear Cu standard reduction potentials. **B. Dereli, M. Ortuño, C.J. Cramer**
- COMP 513.** *Ab initio* and semi-empirical computational studies of radical intermediates formed during the oxidation of melatonin. **C.E. Warden, S.J. Kirkby**
- COMP 514.** Computational studies of spin trapping of biologically relevant radicals by new heteroaryl nitrones. **E. Asempa, S.J. Kirkby**
- COMP 515.** Adiabatic alignment thresholds of molecules. **J.E. Szekely, T. Seideman**
- COMP 516.** Exploring the linear water-dimer, potential-energy curve using quantum Monte Carlo. **S. Upadhyay, J.D. Madura**

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- COMP 517.** Investigation of copper catalyzed triazole synthesis: A computational exploration. **S. Bidwell**, J. Hein, H.P. Hratchian
- COMP 518.** Transition-state analysis of the uracil DNA glycosylase. **Y. Liu**, T. Han, **Z. Jia**, V. Agrawal, **B.N. Domy**
- COMP 519.** Accurate *ab initio* absorption intensities for HNO: Beyond the double harmonic approximation. **H. Dhadh**, R.J. Hinde
- COMP 520.** Density functional-based studies of inhomogeneous, superfluid helium systems: Supported films and doped droplets. **M. Dutra**, R.J. Hinde
- COMP 521.** Computational study on oxetane formation in taxol biosynthesis. **S. Nandi**
- COMP 522.** Cubic-scaling, random-phase approximation for molecular systems. **G. Chen**, F.U. Furché
- COMP 523.** Non-adiabatic molecular dynamics with spin-symmetry breaking for describing photochemistry of small organic molecules. **J. Vincent**, F.U. Furché
- COMP 524.** Interaction of gold nanoparticles with protein studied by atomistic simulations. **A. Wei**, C. Deng
- COMP 525.** Calculation of nanoparticle surface charge density from experimental zeta potential measurement. **Z. Ge**, Y. Wang
- COMP 526.** Detonation kinetics of isopropanol and oxygen mixtures. **K.N. Struk**, S. Bastea, J.I. Siepmann, I.W. Kuo
- COMP 527.** Withdrawn.
- COMP 528.** Hair keratin molecular dynamics models. **E. Antunes**, N.G. Azoia, A. Cavaco-Paulo
- COMP 529.** Developing an automated QM/MM docking suite for quinone reductases. **C. Reinhardt**, T.T. Huynh, S. Bhattacharyay
- COMP 530.** Predictive modeling of the UV-VIS spectra for a series of short-chained polyenes. **R. Fair**, J.B. Foresman, M.J. Brittain
- COMP 531.** Substitution effects in rhodium-catalyzed intramolecular hydroacylation. **E. Schneider**, J. Scanlon
- COMP 532.** Heuristic of predicting protein flexibility and motions along specific nodes. **S.C. Ojinnaka**, D.A. Snyder
- COMP 533.** Determining proteins structure using NMR: More inclusive cores identified by FindCore2 and Cyrange in MR calculations. **A. Kalds**, D.A. Snyder
- COMP 534.** Withdrawn.
- COMP 535.** Identification of a novel class of BRD4 inhibitors by high-throughput computational structural biology. **B.K. Allen**, S. Mehta, N. Ayad, S. Schuerer
- COMP 536.** Computational analysis of small molecule rescue of p53 cancer mutant. **E. Lambros**, B. Wallentine, H. Luecke, R. Luo

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

- COMP 537.** Dissecting allosteric regulatory mechanisms of the Hsp90 chaperone interactions with the protein kinase clients: Integrating structural bioinformatics with multiscale atomistic simulations and biophysical experiments. **G. Verkhivker**, K. Blacklock, J. Buchner
- COMP 538.** Design of PDE2 inhibitors with free-energy perturbation. **G. Tresadern**, Y. van Roosbroeck, I. Velter, P. Buijnsters
- COMP 539.** GPU-enabled binding free energy calculations of potential ligands for pancreatic cancer imaging. **A. Walker**, G.A. Cisneros
- COMP 540.** Impact of ionic liquids on solvation and hydrolysis of cellulose oligomers. **T. Schutt**, V.S. Bharadwaj, C. Kinsinger, C.M. Maupin
- COMP 541.** Free energy and hidden barriers: The  $\beta$ -sheet structure of the prion protein. **A.A. Paz**, C.F. Abrams
- COMP 542.** Information-driven, fully flexible HADDOCKing: Performance on a benchmark of protein-ligand complexes. **J. Grinstead**, A. Thureau, J. Rodrigues, A.F. Rinsing, T.L. Wormwood, M. Bonvin
- COMP 543.** Molecular mechanism of chromatin targeting by potent rutenium-arene anticancer agents acting at the nucleosome core particle. **G. Palermo**, Z. Ma, B.S. Murray, P. Dyson, C.A. Davey, U. Roethlisberger
- COMP 544.** Molecular dynamics simulations in drug discovery: Structure-based design of allosteric HCV NS5B polymerase inhibitors with picomolar replicon potency. **O. Hucke**, R. Coulombe, P. Bonneau, M. Bertrand-Laperle, C. Brochu, J. Gillard, M. Joly, S. Landry, O. Lepage, M. Llinas-Brunet, M. Poirier, M. Poirier, M. Pesant, G. McKercher, M. Marquis, G. Kukolj, P.L. Beaulieu, T. Stammers
- COMP 545.** Molecular mechanism of the Dengue virus NS3/NS2b protease. **M.P. Lima**, G.M. Seabarb
- COMP 546.** Time-dependent density-functional calculations for hypervelocity physics. **R.J. Magyar**, M.A. Gallis
- COMP 547.** Withdrawn.
- COMP 548.** Withdrawn.

## WEDNESDAY MORNING

### Section A

San Diego Convention Center  
Room 28A

#### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

#### Landscapes, Disorder & Enhanced Sampling

*Cosponsored by PHYS*

M. Feig, H. Nguyen, J. Shen, *Organizers*  
J. E. Shea, *Presiding*

- 8:30 COMP 549.** Protein dynamics studied by generalized-ensemble simulations. **Y. Okamoto**
- 9:00 COMP 550.** Replica exchange with dynamic temperatures. **M.S. Lee**, M.A. Olson
- 9:30 COMP 551.** Recent development of replica-exchange molecular dynamics simulation methods. **Y. Sugita**
- 10:00 COMP 552.** All-atom simulation approaches to probe dynamics in proteins. **H. Vashisth**
- 10:30** Intermission.

- 10:45 COMP 553.** Touring the landscape: The view depends on how you look. **S. Marqusee**
- 11:15 COMP 554.** Multi-scale modeling of IDP structure and interaction. **J. Chen**
- 11:45 COMP 555.** Computational methods and models for intrinsically disordered peptides. **T.L. Head-Gordon**

### Section B

San Diego Convention Center  
Room 26B

#### Materials Science

- M. Haranczyk, *Organizer*  
**A. Saha**, *Presiding*
- 8:30 COMP 556.** DFT+U: Is a general parameterization useful? **P. Verma**, H. Yu, K. Duanmu, D.G. Truhlar
- 8:50 COMP 557.** Non-linear properties with EOM-CCSD: Expectation-value vs. full-response approach. **K. Nanda**, A. Krylov
- 9:15 COMP 558.** Extensive first-principles study of the energy landscape of hybrid organometallic halide perovskites. **L. Tan**, F. Zheng, A.M. Rappe
- 9:40 COMP 559.** Accurate materials properties from an efficient density functional. **R.C. Remsing**, J. Sun, J.P. Perdew, M.L. Klein
- 10:05** Intermission.
- 10:20 COMP 560.** Breaking badly: DFT-D2 gives sizeable errors for tensile strengths in bulk solids. **B.M. Wong**, N. Ilawe
- 10:50 COMP 561.** Self-interaction-corrected DFT calculations of defect states and band gaps of oxides. **H. Jonsson**
- 11:20 COMP 562.** Diffusion in nanoporous materials: Assessing the long time scale from short molecular dynamics trajectories. **A. Ghysels**
- 11:50 COMP 563.** Many-body effects on the thermodynamics of fluids, mixtures, and nanoconfined fluids. **J. Delhomelle**, C. Desgranges

### Section C

San Diego Convention Center  
Room 25C

#### Know Your Unknowns: Estimating the Reliability of Individual Activity & Property Predictions

*Cosponsored by MPPG*  
*Financially supported by Simulations Plus*

R. D. Clark, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:40 COMP 564.** Gaussian processes: We demand rigorously defined areas of uncertainty and doubt. **M.D. Segall**, P. Hunt, E. Champness
- 9:10 COMP 565.** Error models, ensemble models, and goodness models. **D. Honeycutt**
- 9:40 COMP 566.** Reliably estimating classification uncertainty for toxicological models. **V. Gombar**, M.S. Lawless, M. Waldman, R.D. Clark
- 10:10** Intermission.
- 10:30 COMP 567.** Assessing the reliability of individual regression predictions. **M. Waldman**, R.D. Clark
- 11:00 COMP 568.** Error model approach to domain applicability: Is there an activity cliff paradox? **R.P. Sheridan**
- 11:30** Panel Discussion.
- 11:50** Concluding Remarks.

### Section D

San Diego Convention Center  
Room 26A

#### Molecular Mechanics

#### Free Energies & QM/MM

M. Feig, *Organizer*  
K. Armacost, *Presiding*

- 8:30 COMP 569.** Software pipelines for high throughput alchemical binding free energy calculations. **A. Mey**, J. Juarez, J. Michel
- 8:55 COMP 570.** Robust protocols for high-throughput alchemical free energy calculations. **S. Bosisio**, J. Michel
- 9:20 COMP 571.** Improving free energy calculations with non-Boltzmann Bennett reweighting using QM and MM. **F.C. Pickard**, G. Koenig, A.C. Simmonett, Y. Shao, B. Brooks
- 9:45 COMP 572.** Gaussian accelerated molecular dynamics: Unconstrained enhanced sampling and free energy calculation of biomolecules. **Y. Miao**, J. McCammon
- 10:10 COMP 573.** Free energy simulations with the confinement method. **A. Van Der Vaart**
- 10:35** Intermission.
- 10:50 COMP 574.** Comparison of industry-standard QM and MM methods for estimating strain in drug-like molecules. **B.D. Sellers**, N. James, A. Gobbi
- 11:15 COMP 575.** Equilibrium free energy differences between high and low levels of theory via non-equilibrium work approaches. **P.S. Hudson**, H.L. Woodcock, S. Boresch
- 11:40 COMP 576.** QM/MM studies of rhodopsin thermal decay. **H.P. Hendrickson**, J. Ho, Y. Guo, E.C. Yan, J.C. Tully, V.S. Batista
- 12:05 COMP 577.** Modeling chemical reactions in ionic liquids using QM/MM calculations. **O. Acevedo**

### Section E

San Diego Convention Center  
Room 28B

#### Quantum Mechanics

*Cosponsored by PHYS*

S. E. Wheeler, *Organizer*  
**A. Saha**, *Presiding*

- 8:30 COMP 578.** Toward relatively general and accurate quantum chemical predictions of solid-state  $^{17}\text{O}$  NMR chemical shifts in various biologically relevant oxygen-containing compounds. **A. Rorick**, M.A. Michael, L. Yang, **Y. Zhang**
- 9:00 COMP 579.** Role of the protein environment for the  $\text{O}_2$  binding in the active site of histone demethylase JMJ2A. **W. Cortopassi**, R. Simion, C. E. Hornsby, T. Franca, R.S. Paton
- 9:20 COMP 580.** Using first-principle calculations to tune the superoxide production by 1,2-H-atom shift. **D.J. Van Hoomissen**, **S. Vyas**
- 9:50** Intermission.
- 10:05 COMP 581.** Mapping charge transfer pathways in wild-type and mutant photosystem II using time dependent density functional theory. **I.R. Gould**
- 10:35 COMP 582.** Computational study of the dehydration of bortezomib from common antioxidants. **J. Larkin**
- 11:05 COMP 583.** Photosynthesis of cytosine. **J.E. Rice**, T.J. Lee, P.P. Bera

**11:35 COMP 584.** Theoeceptors for lactate dehydrogenase A: A purely quantum mechanical approach to computing binding affinity. **I. Lukac, A. Leach, J. Madden**

## Section F

San Diego Convention Center  
Room 25A

### Advances in Computer-Aided Biologics Design

#### Design & Optimization of Biologics

D. Pearlman, *Organizer*

M. R. Landon, S. Vajda, *Organizers, Presiding*

#### 8:30 Introductory Remarks.

**8:35 COMP 585.** Free energy perturbations for the accurate prediction of protein-protein binding affinity and protein stability. **F. McRobb, J. Sanders, T. Steinbrecher, C. Zhu, L. Wang, T. Lin, B. Kim, R. Abel, W. Sherman**

**9:05 COMP 586.** Analysis of protein aggregation by docking. **C. Yueh, D. Kozakov, S. Vajda**

**9:35 COMP 587.** Computationally-driven deimmunization of biotherapeutics. **C. Bailey-Kellogg**

**10:05 COMP 588.** Computational assessment of pharmaceutical properties for protein therapeutics. **S.R. Krystek, A. Nayeem, A. Yamniuk**

#### 10:35 Intermission.

**10:50 COMP 589.** Modeling interactions of predicted proteins. **I. Anishchenko, T. Dauzhenka, S. Belkin, P. Kundrotas, I. Vakser**

**11:20 COMP 590.** Efficient global peptide docking using motif-derived fragments. **K. Porter, B. Xia, D. Beglov, O. Furman, D. Kozakov**

**11:50 COMP 591.** Computational design of orthogonal antiparallel homodimers. **C. Negron, A.E. Keating**

## The History of Chemistry & Computing

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### Computational Chemistry Across Catalysis

#### From Heterogeneous to Homogeneous Catalysis

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### Computer-Aided Drug Design

#### Real World Dynamics

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## WEDNESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 28A

#### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

#### Interactions at Small & Large Scales

Cosponsored by PHYS

M. Feig, H. Nguyen, J. Shen, *Organizers*

S. A. Patel, *Presiding*

**1:30 COMP 592.** Triplex forming oligonucleotides and gene therapy. **L. Nilsson, A. Villa**

**2:00 COMP 593.** Multiple SH2 domains: Binding and dynamics. **C.B. Post**

**2:30 COMP 594.** Solubility determining protein structure and aggregation. **B.M. Pettitt**

#### 3:00 Intermission.

**3:15 COMP 595.** Connecting structural biology to cellular scales: Atomistic simulations of cytoplasmic environments. **M. Feig**

**3:45 COMP 596.** Chemical tools to modulate p53 folding in cells. **K. Khar, A. Ranjan, J. Niu, W. Lea, M. Fisher, T. Iwakuma, J. Karanicolas**

**4:15 COMP 597.** Rational design of peptide-based functional biomaterials via multiscale modeling. **H. Nguyen**

## Section B

San Diego Convention Center  
Room 26B

### Time-Dependent Dynamics & Electronic Excited States

B. M. Wong, *Organizer, Presiding*

**1:30 COMP 598.** Proceed with caution: Electron dynamics with real-time TDDFT. **C. Isborn**

**2:05 COMP 599.** Non-adiabatic molecular dynamics simulations. **S.M. Parker, M. Muuronen, J. Vincent, S. Roy, B. Krull, J. Yu, B. Nguyen, F.U. Furche**

**2:40 COMP 600.** Nonadiabatic molecular dynamics with time-domain density functional theory. **O.V. Prezhdo**

#### 3:15 Intermission.

**3:30 COMP 601.** *Ab initio* design of organic catalysts and photocatalysts. **C. Lim, J. Theriot, G. Miyake, C. Musgrave, A. Holder, H. Yang, J.T. Hynes**

**4:05 COMP 602.** *Ab initio* spin-dynamics using time-dependent two-component formalism. **X. Li, J.J. Goings**

**4:40 COMP 603.** Node development and evolution in free wave packet propagation. **B.A. Rowland, J. Ficut, C. Lechak**

## Section C

San Diego Convention Center  
Room 25C

### Peptide Modeling

Cosponsored by MPPG

S. N. Ha, *Organizer*

H. L. Woodcock, *Presiding*

**1:30 COMP 604.** Peptide drug hunter: Exploring macrocycle chemical space and design. **T.K. Sawyer**

**2:00 COMP 605.** Probing the origin of structural stability of single- and double-stapled p53 peptide analogs bound to MDM2. **U. Mohanty**

**2:30 COMP 606.** Modeling protein-protein interactions for interaction targets. **R. Nussinov**

#### 3:00 Intermission.

**3:15 COMP 607.** Predicting electrostatics and related biophysical properties for proteins. **L. Yan**

**3:45 COMP 608.** Modeling peptide-protein binding with information accelerated molecular dynamics simulation. **J.A. Morrone, A. Perez, K.A. Dill**

**4:15 COMP 609.** Sub-angstrom accurate computations of macrocycles. **E. Coutsiias**

**4:45 COMP 610.** Predicting permeability of diverse cyclic peptides. **K.W. Lexa, M.P. Jacobson**

## 5:15 Concluding Remarks.

## Section D

San Diego Convention Center  
Room 26A

### Molecular Mechanics

#### Biomolecular Modeling, Prediction & Folding

M. Feig, *Organizer*

P. S. Hudson, *Presiding*

**1:30 COMP 611.** Docking-based symmetry prediction for homotetramers. **L. Qiu, X. Xu, X. Zou**

**1:55 COMP 612.** Integrated structural modeling of protein-protein complexes assisted by comprehensive, conformational sampling. **W. Huang, K. Ravikumar, M. Parisien, S. Yang**

**2:20 COMP 613.** CryoEM-guided iterative molecular dynamics: Rosetta protein structure refinement protocol improves protein model quality. **M. Marlett, S. Lindert**

**2:45 COMP 614.** Protein flexibility and NMR: How can we predict and deal with it? **D.A. Snyder**

**3:10 COMP 615.** Application of rigidity theory to the thermostabilization of proteins. **P. Rath, A. Fulton, K. Jaeger, H. Gohlke**

#### 3:35 Intermission.

**3:50 COMP 616.** Structural determinants of misfolding in multidomain proteins. **P. Tian, R.B. Best**

**4:15 COMP 617.** Helix handedness inversion and induction in arylamide foldamers: Elucidation and free energy profile of the folding/unfolding mechanism. **V. Pophristic, Z. Liu, A. Abramyan**

**4:40 COMP 618.** Dissecting energetic and entropic contributions to protein folding. **D.J. Huggins**

**5:05 COMP 619.** Accelerating metal-directed protein folding and molecular recognition with enhanced sampling techniques. **F. Feixas, M. Swart**

## Section E

San Diego Convention Center  
Room 28B

### Quantum Mechanics

Cosponsored by PHYS

S. E. Wheeler, *Organizer*

B. Rudshteyn, *Presiding*

**1:30 COMP 620.** Evaluation of a perturbative treatment of three-body interactions in HCP <sup>4</sup>He. **A.L. Barnes, R.J. Hinde**

**1:50 COMP 621.** Thermoelectric properties of iodine-substituted bismuth telluride using WIEN2k. **A. Dumi, J.D. Madura, M.N. Srnec**

**2:10 COMP 622.** Temperature dependence of excited state decay rates in medium-to large-size molecules. **S. Banerjee, A. Baiardi, J. Bloino, V. Barone**

#### 2:40 Intermission.

**2:55 COMP 623.** Comparison of the set of dipeptides containing two aromatic rings. **M.A. Shebel, J.A. Thomas**

**3:25 COMP 624.** Close connection between  $\pi$  aromaticity of hydrocarbons and three-dimensional aromaticity of closo borohydrides. **J. Poater**

**3:55 COMP 625.** Reaction exploration for transition metal-catalyzed C-H activation. **A.L. Dewey, P.M. Zimmerman**

**4:15 COMP 626.** Composite approach towards accurate predictions of lanthanide and actinide thermochemistry. **C.C. Peterson, D.A. Penchoff, A.K. Wilson**

## Section F

San Diego Convention Center  
Room 25A

### Advances in Computer-Aided Biologics Design

#### Antibody Design & Optimization

M. R. Landon, S. Vajda, *Organizers*

D. Pearlman, *Organizer, Presiding*

#### 1:30 Introductory Remarks.

**1:35 COMP 627.** Knowledge-based methods for computational antibody design. **J. Adolf-Bryfogle, R. Dunbrack**

**2:05 COMP 628.** Atomistic modeling of H3 loops: Is it necessary for protein-protein docking? **D. Hall**

**2:35 COMP 629.** Cloud computing and multi-template large-scale antibody modeler validation: How to model > 2200 antibodies in 1 hour. **E. Metwally**

#### 3:05 Intermission.

**3:20 COMP 630.** *In silico* profiling of commercial antibodies. **S. Sirin, W.B. Stine**

**3:50 COMP 631.** Probing electrostatic interactions between amino acids and urea using *ab-initio* calculations. **B. Wei, B. Safina, J.L. Gunzner, T. Pillow, G. Zhao, J. Nonomiya, K. Kozak, Y. Liu, J.A. Flygare**

**4:20 COMP 632.** Relative binding affinity predictions in HIV antibody-antigen complexes using fep/REST. **A. Clark, T. Gindin, L. Wang, F. Xu, R. Friesner**

## Multiscales Chemistry

### Sustainable

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### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Powering the Future: Novel Materials for Solar Cell Technologies

Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY

### Computer-Aided Drug Design

#### New Modalities RNA

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

## THURSDAY MORNING

### Section A

San Diego Convention Center  
Room 28A

#### Time-Dependent Dynamics & Electronic Excited States

B. M. Wong, *Organizer, Presiding*

#### 8:30 Introductory Remarks.

**8:35 COMP 633.** Quantum dynamics simulations of photoinduced charge transfer processes in donor-bridge-acceptor systems. **M.B. Oviedo, B.M. Wong**

**9:10 COMP 634.** Excited-state dynamics of mPlum fluorescent protein. **S. Faraji, A. Krylov**

**9:45 COMP 635.** Modeling excited states of large molecular systems using hybrid QM/QM methods with point charge embedding. **A. Biancardi, J.S. Barnes, M. Caricato**

10:20 Intermission.

10:35 **COMP 636.** Charge-transfer dynamics of light-harvesting systems in complex environments. **B.M. Wong**, M. Oviedo

11:10 **COMP 637.** New computational tools for photochemistry, solvatochromatic shifts, and excitation energy transfer. **J. Herbert**, X. Zhang, J. Liu, A. Morrison

11:45 **COMP 638.** Excited-state absorption from real-time, time-dependent density functional theory. **N. Govind**, S. Fischer, C.J. Cramer

## Section B

San Diego Convention Center  
Room 26B

### Drug Discovery

#### SAR Modeling Examples

M. R. Landon, Y. Tseng, *Organizers*

S. M. Gathiaka, *Presiding*

8:30 **COMP 639.** Ferulic acid and vanillin analogues as potential influenza neuraminidase inhibitors: Modelling, synthesis and biological activities. **M. Hariono**, N. Abdullah, E. Kamarulzaman, N. Mohamed, S. Syed Hassan, S. Shamsudin, **H. Wahab**

8:50 **COMP 640.** Discovery of novel Myc inhibitors using structure and ligand-based drug design. **M. Liosi**, D. Stellas, A. Efstratiadis, **Z. Cournia**

9:10 **COMP 641.** Computational studies of allosteric regulation of BRAF kinases: Combining multiscale modeling and network analysis in design of conformation-specific and allosteric modulators targeting oncogenic BRAF mutants. **G. Verkhivker**, K. Blacklock, A. Tse

9:30 **COMP 642.** Rational development of a new type of HBV capsid inhibitors by a combination of microsecond-scale molecular dynamics and docking. **A. Pavlova**, M. Korablyov, J. Gumbart

9:50 **COMP 643.** Insight into the mechanisms of resistance-associated variants of HCV NS3 protease binding to MK-5172: A computational study. **Z. Guo**

10:10 **COMP 644.** Probing the S2 subsite of the anthrax toxin-lethal factor. **E.A. Amin**, E.K. Kurbanov, K.M. Maize, T. Chiu, J. Solberg, J. Fernandez, S. Francis, R.L. Johnson, J. Hawkinson, M.A. Walters, B. Finzel

10:30 Intermission.

10:45 **COMP 645.** On the use of homology models for binding free energies predictions. **D. Cappel**, **W. Sherman**

11:05 **COMP 646.** Homology modeling of class A GPCRs in the inactive conformation: A quantitative analysis of the correlation between model-/template-sequence identity and model accuracy. **S. Costanzi**, M. Skorski, A. Deplano, B. Habermehl, M. Mendoza, J. Dawson, J. Gao

11:25 **COMP 647.** Does flexibility control the specificity of protein-protein and protein-drug interfaces? **K. Liedl**

11:45 **COMP 648.** Unraveling DNA repair catalyzed by Y-family polymerases. **V. Genna**, R. Gaspari, M. Dal Peraro, **M. De Vivo**

## Section C

San Diego Convention Center  
Room 25C

### Molecular Mechanics

#### Materials

M. Feig, *Organizer*

S. P. Hirakis, *Presiding*

8:30 **COMP 649.** Phase transitions in quasi 1-D and 2-D nanoconfined water. **M. Raju**, A.C. Van Duin, M. Ihme

8:55 **COMP 650.** Multiscale MD/CFD simulations of a supersonic reactive gas flow within a nanopore. **A.V. Popov**, R. Hernandez

9:20 **COMP 651.** Dynamic free-energy surfaces for sodium diffusion in type II silicon clathrates. **C.M. Maupin**

9:45 **COMP 652.** Characterization of tetra-n-butyl ammonium chloride electrolyte at varying concentrations and temperatures using molecular dynamics. **R.L. Napoleon**, D. Szucs, P.B. Moore

10:10 **COMP 653.** Elucidating the properties of fuel mixtures using molecular dynamics. **B.H. Morrow**, M. Gustafson, J. Schall, M. Knippenberg, J.A. Harrison

10:35 Intermission.

10:50 **COMP 654.** Computational studies of guest-dependent, flexible metal organic frameworks. **J.C. Pearson**, A.K. Wilson

11:15 **COMP 655.** Modeling ethane and ethylene separation in the metal-organic framework Fe<sub>2</sub>(dobdc). **J.C. Sung**, K.N. Youmans, J.I. Siepmann

11:40 **COMP 656.** Computer-aided design of helical arylamide foldamers for selective encapsulation of monosaccharides. **Z. Liu**, E.C. Fluck, A. Lai, A. Abramyan, V. Pophristic

12:05 **COMP 657.** On the cis/trans isomerization of amide bonds for classical simulation of peptoids. **K. Cunha**, **R. Lins**

## Section D

San Diego Convention Center  
Room 26A

### Quantum Mechanics

*Cosponsored by PHYS*

S. E. Wheeler, *Organizer*

M. R. Jones, *Presiding*

8:30 **COMP 658.** Vibrational spectra of medium-to-large systems at the anharmonic level. **J. Bloino**, M. Biczysko

9:00 **COMP 659.** Withdrawn.

9:20 **COMP 660.** Cluster-weighted modeling approach to potential energy surface fitting. **J.B. Maddox**

9:50 Intermission.

10:05 **COMP 661.** Optimization of a hybrid-density functional for use on endohedral metallofullerenes. **T.J. Fuhrer**, J. Snelgrove

10:35 **COMP 662.** Suitability of dispersion-corrected and nonlocal density functionals for predicting vapor-liquid equilibria. **H. Goel**, Z. Windom, C. Butler, **N. Rai**

11:05

**COMP 663.** Density functionals' performance for the mechanism of CH<sub>3</sub>OH decomposition by Cu<sub>4</sub> clusters. **S. Moncho Escriva**, E. Brothers, B.G. Janesko

11:35 **COMP 664.** Alcohol dehydration kinetics over various zeolites in experimental and theoretical methods for catalytic fast pyrolysis. **S. Kim**, L. Kunz, R. McDonough, L. Bu, M.R. Nimlos, R.S. Paton, D. Robichaud

12:05 **COMP 665.** DFT modeling of SCR catalyst Cu-CHA. **X. Yang**, D. Crandell, H. Zhu, M. Baik, J. Hochmuth

## Big Data Science

### Accessing Chemical Space & Better Modeling

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDJ and PHYS*

### Computational Materials & Nanoscience: Theory Meets Experiment

### Forum: The Future of Spectroscopies: Quantum & Classical Fields; Theoretical Perspectives

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

### Computer-Aided Drug Design

#### New Modality Therapeutics

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDJ and PHYS*

## THURSDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 28A

### Time-Dependent Dynamics & Electronic Excited States

B. M. Wong, *Organizer*, *Presiding*

1:30 **COMP 666.** Coarse-gained model of exciton dynamics on long-chain conjugated polymer system. **E.M. Lee**, W.A. Tisdale, A.P. Willard

2:05 **COMP 667.** Computational screening of two-photon absorption in fluorescent protein chromophores made from non-canonical amino acids. **M. Salem**, A. Brown

2:40 **COMP 668.** Optical spectra of molecules, molecular complexes, and solids from optimally-tuned, time-dependent, range-separated, hybrid density functional theory. **L. Kronik**

3:15 Intermission.

3:30 **COMP 669.** Polarization-induced spontaneous charge separation in perovskite photovoltaics: A large-scale TDDFT study. **X. Zhang**, **G. Lu**

4:05 **COMP 670.** Understanding the fundamental connection between electronic correlation and decoherence. **A. Kar**, L. Chen, **I. Franco**

4:40 **COMP 671.** Simple and accurate method for time-dependent transport along nanoscale junctions. **L. Chen**, **I. Franco**

## Section B

San Diego Convention Center  
Room 26B

### Drug Discovery

#### SAR Modeling Examples

M. R. Landon, Y. Tseng, *Organizers*

S. M. Gathiaka, *Presiding*

1:30 **COMP 672.** Further development of the movable-type energy sampling method and its application in the biomolecular systems. **Z. Zheng**, D.S. Cerutti, N. Bansal, K.M. Merz

1:50 **COMP 673.** Using multisite lambda dynamics for the calculation of 512 binding free energies of HIV-RT in ~1.5  $\mu$ s. **K. Armacost**, G. Goh, C.L. Brooks

2:10 **COMP 674.** Dependence of multiparameter optimization results on descriptors variation. **E.A. Sosnina**, D.I. Osolodkin, E.V. Radchenko, V.A. Palyulin, N.S. Zefirov

2:30 **COMP 675.** CCSD(T)-F12 re-evaluation of the S66x8 noncovalent interaction and YMPJ amino acid conformer space benchmarks: Assessment of more approximate methods. **M.K. Kesharwani**, B. Brauer, A. Karton, **J.M. Martin**

2:50 **COMP 676.** Catalytic, enantioselective dibromination of allylic alcohols: A computational perspective. **R.P. Pemberton**, D.X. Hu, N.Z. Burns, D.J. Tantillo

3:10 **COMP 677.** Technology development and design of novel 1, 3, 5-tri substituted-1H-indole-2, 3-dione: HIV-1 inhibitors with displays-strategic, nanomolar cytotoxicity. **R.A. Hajare**, **R.S. Paranjape**, S.S. Kulkarni

3:30 Intermission.

3:45 **COMP 678.** Medicinal chemistry: From intuitive rules and examples to chemical patterns. **S. Bietz**, K. Schomburg, **M. Rarey**

4:05 **COMP 679.** Conformer compatibility filtering based on matching distances between features. **L. Zaslavsky**, S. Kim, E. Bolton

4:25 **COMP 680.** Computational methods for understanding structure-activity relationships in NSAIDs. **Y.S. Khan**

4:45 **COMP 681.** Synthesis, chemical characterization, DNA interaction, antioxidant, and computational study of new ferrocene-based N,N-disubstituted ureas. **F. Asghar**, A. Badshah, A. Hussain Raja, I.S. Butler

## Section C

San Diego Convention Center  
Room 25C

### Molecular Mechanics

#### Lipids, Membranes & Proteins

M. Feig, *Organizer*

S. P. Hirakis, *Presiding*

1:30 **COMP 682.** Adventures in the world of lipids: Towards the routine simulation of membranes. **R.C. Walker**, B. Madej, C. Lin, C. Dickson, A. Skjervek, K. Teigen, L. Yang, I.R. Gould

1:55 **COMP 683.** Evolving allostery of the 3-ketosteroid family of nuclear receptors. **B. Kossman**, W. Hudson, I.N. Ivanov, E. Ortlund

2:20 **COMP 684.** Channelrhodopsin: Proton transport and mutation studies. **M.R. VanGordon**, S.W. Rick, S.L. Rempe

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## ENFL

## Division of Energy and Fuels

X. Wang and D. Heldebrant, Program Chairs

## SUNDAY MORNING

## Section A

Wyndham San Diego Bayfront  
Porthole

## Solar Cells

## Organic

Y. H. Hu, R. T. Koodali, *Organizers, Presiding*

## 8:30 Introductory Remarks.

**8:35 ENFL 1.** Control of nanoscale architecture in organic photovoltaic materials: From plastic solar cells to biomimetic assemblies with extremely long-lived carriers. **S.H. Tolbert****9:15 ENFL 2.** Perspectives on earth-abundant, multinary photovoltaics and how we can make them better. **R. Haight****9:55 ENFL 3.** Effects of molecular weight and crystallization on the donor-acceptor composition ratio of spin-coated, blended, organic semiconductor films. **M. Weintraub, A. Austin, J.M. Szarko**

## 10:15 Intermission.

**10:25 ENFL 4.** Organic-based semiconductors for high-performance photovoltaic devices. **G. Li****11:05 ENFL 5.** Triplet excitons, singlet fission, and prospects for improved organic photovoltaics. **M.J. Tauber****11:45 ENFL 6.** Photophysical characterization of porphyrin donor-acceptor materials for photochemical applications. **D.M. Marin, K. Ren, M. Kaushal, D. Cohen, J. Kolesar, S.J. Hall, M. Walter****12:05 ENFL 7.** Dye-controlled, interfacial electron transfer for high-current indium tin oxide photocathodes. **M. He, Z. Huang, M. Yu, K.A. Click, D.R. Beauchamp, Y. Wu**

## 12:25 Concluding Remarks.

## Section B

Wyndham San Diego Bayfront  
Pacific C

## Fuel Cells

*Cosponsored by CATL*S. Cha, Z. Iqbal, *Organizers*T. Kim, E. Lee, *Organizers, Presiding*

## 8:30 Introductory Remarks.

**8:35 ENFL 8.** Enhancing the power and current density of hydrogen fuel cells operating at low temperatures, using oblate-metal and metal-alloy nanoparticles. **H. Li, C. Pan, S. Zhao, C. Kao, P. Liu, Y. Zhu, M. Rafailovich****9:15 ENFL 9.** Ag-composite cathode for high-performance, intermediate temperature, solid oxide fuel cells. **M. Kim, N. Chean, Y. Li, H. Choi, J. Shim****9:35 ENFL 10.** Perovskite-type oxide films synthesized via an electrochemical route and its application in SOFC interconnects. **J. Lee, B. Park, R. Song, S. Lee, T. Lim, S. Park**

## 9:55 Intermission.

**10:15 ENFL 11.** Synthesis of nitrogen-doped graphene catalyst by wet-ball milling for electrochemical systems. **S. Zhuang, B. Nunna, L. Lei, E. Lee****10:35 ENFL 12.** Fe/C/N nonprecious metal catalyst prepared from spherical polyimide. **Y. Nabae, S. Nagata, T. Hayakawa, H. Niwa, Y. Harada, M. Oshima, A. Isoda, A. Matsunaga, K. Tanaka, T. Aoki****10:55 ENFL 13.** Metal-organic framework-derived, porous carbons as highly efficient electrocatalysts for oxygen reduction reactions. **Y. Wang, P. Feng****11:15 ENFL 14.** Structural characterization and electrochemical performance of Mo<sub>3</sub>O<sub>7</sub> and Pt-black composite used to enhance methanol oxidation. **F. Yang, F. Li, Y. Wang, X. Chen, D. Xia, J.L. Liu**

## Section C

Wyndham San Diego Bayfront  
Pacific D

## Advances in Methane Technology

## Mechanism &amp; Kinetics

*Financially supported by Custom Solutions Group LLC*Z. He, J. Zhang, *Organizers, Presiding*

## 8:30 Introductory Remarks.

**8:35 ENFL 15.** Fixed-bed reactor model for the gas-phase Fischer-Tropsch synthesis. **P. Mills****9:20 ENFL 16.** Finding new methane oxidation (NEMO) sites in metal-exchanged zeolites: Insights from the tandem oxidation and carbonylation of methane to acetic acid in Cu-MOR. **Y. Roman-Leshkov****9:55 ENFL 17.** Catalytic transformations of methane, ethane, and propane to lower olefins in the presence of hydrogen chloride and oxygen. **Q. Xie, J. Kang, J. He, Q. Zhang, Y. Wang**

## 10:30 Intermission.

**10:45 ENFL 18.** Effect of Pd crystallite size and oxygen vacancies on the partial oxidation of methane on Pd/Al<sub>2</sub>O<sub>3</sub>. **J. Doodson, S. Wang, L. Grabow, W. Epling****11:20 ENFL 19.** Stability of Zn/HZSM-5 catalysts towards methane dehydroaromatization reaction. **V. Abdelsayed, M.W. Smith, D. Shekhawat****11:55 ENFL 20.** Effect of La<sub>2</sub>O<sub>3</sub> additive on catalytic performance of Ni/ZrO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> catalyst for syngas methanation. **C. Guo, H. Zhang, X. Li, W. Li**

## Section F

Wyndham San Diego Bayfront  
Pacific B

## Advances in Chemistry of Energy &amp; Fuels

## Catalysis of Fuels

X. Wang, *Organizer*D. J. Heldebrant, *Organizer, Presiding*Z. He, L. Li, *Presiding***8:30 ENFL 21.** Iron(III) catalyzed dimerization of cycloolefins: Synthesis of high-density fuel candidates. **R. Arias-Ugarte, F.S. Wekesa, S. Schunemann, M. Findlater****8:50 ENFL 22.** Methyl ester production by acid-catalyzed ester interconversion processes. **J.A. Struss, D.J. Amato, L.R. Grubb, D. Pett, K. Shah****9:10 ENFL 23.** FCC technology for enhancing propylene production and its development. **C. Xie, X. Wei, J. Long****9:30 ENFL 24.** Oxidative ring-opening of aromatics: Effect of water on reaction selectivity. **N. Montoya Sanchez, R. Feng, A. De Klerk**

## 9:50 Intermission.

**10:00 ENFL 25.** Electrochemically-assisted oxidative dehydrogenation (ODH) of lower alkanes to olefins. **U.S. Ozkan, A. Fuller, D. Dogu, K. Binkley, N. Kramer, A. Co****10:20 ENFL 26.** Catalysts for the electrochemical oxidation of renewable polyalcohols in alkaline media. **J. Haan, J. Estrada, O. Muneeb, S. Hu, L. Scudiero, S. Ha****10:40 ENFL 27.** Polymorphic CoSe<sub>2</sub> with mixed orthorhombic and cubic phases for highly efficient hydrogen evolution reaction. **X. Zhang**

## 11:00 Intermission.

**11:10 ENFL 28.** Thermodynamic equilibrium calculation and experimental investigation of olefin products in catalytic cracking. **G. Liu****11:30 ENFL 29.** Computational investigation of a catalyst for olefin purification: Copper bis(oxathiolene) complexes. **D.N. Sredojevic, E. Brothers, M.B. Hall****11:50 ENFL 30.** Influence of fuel structures on molecular weight growth kinetics in hydrocarbon conversions: A comparative study of the C<sub>3</sub> & C<sub>4</sub> alkenes pyrolysis. **K. Wang, S. Villano, A.M. Dean**

## Catalytic Materials for Methane Conversion

## Combustion &amp; MTO

*Sponsored by CATL, Cosponsored by ENFL*

## Computational Chemistry Across Catalysis

## Modeling Complex Reaction Networks in Catalysis

*Sponsored by CATL, Cosponsored by COMP, ENFL and WCC*

## Fundamental Surface Chemistry of Non-oxide Transition Metal Ceramic Catalysts: Carbides, Nitrides, Sulfides, Phosphides, Selenides

*Sponsored by CATL, Cosponsored by ENFL*

## SUNDAY AFTERNOON

## Section A

Wyndham San Diego Bayfront  
Porthole

## Solar Cells

Y. H. Hu, R. T. Koodali, *Organizers, Presiding***1:30 ENFL 31.** Non-hermitian optics and parity-time photonics. **X. Zhang****2:10 ENFL 32.** Avoiding the kinetics of the bulk heterojunction: Sequential processing and self-assembly for conjugated, polymer-based photovoltaics. **B.J. Schwartz****2:50 ENFL 33.** Last progresses in photosynthetic solar cells. **B. Su**

## 3:25 Intermission.

**3:30 ENFL 34.** Transparent composite electrode for flexible and stretchable OPVs. **Q. Pei****4:10 ENFL 35.** Iodide-passivated colloidal PbS nanocrystals for application in hybrid solar cells. **R.L. Brutchey****4:50 ENFL 36.** Optimization and simplification of polymer-fullerene solar cells through polymer and active layer design. **B.C. Thompson****2:45 COMP 685.** Molecular simulations unravel the key factors of lipid selection in fatty acid amide hydrolase and suggest a general mechanism of lipid-processing in the parent enzymes. **G. Palermo, I. Bauer, P. Campomanes, A. Cavalli, A. Armirotti, S. Girotto, M. De Vivo****3:10 COMP 686.** Molecular simulations of water within ion channels. **P.B. Moore, T.H. Nguyen, Z. Liu**

## 3:35 Intermission.

**3:50 COMP 687.** Membrane protein folding via computer simulations. **J. Domanski, P. Stansfeld, M.S. Sansom, R.B. Best****4:15 COMP 688.** Towards an energy landscape of G protein-coupled receptor (GPCR) activation using hybrid methods. **S.S. Dong, R. Abrol, W.A. Goddard****4:40 COMP 689.** Conformational changes in the angiotensin II type 1 (AT1) receptor under shear stress. **M. Malta de Sa, S.M. Modestia, C. Oliveira Rangel-Yagui, J.E. Krieger****5:05 COMP 690.** Computational discovery of activating and repressing states for the liver receptor homologue 1 ligand binding domain. **B. Kossmann, P. Musille, I.N. Ivanov, E. Orlund**

## Section D

San Diego Convention Center  
Room 26A

## Quantum Mechanics

*Cosponsored by PHYS*S. E. Wheeler, *Organizer*M. R. Jones, *Presiding***1:30 COMP 691.** Quantum properties from machine learning in chemical space. **O. von Lilienfeld****2:00 COMP 692.** Quantum chemistry on diverse computational platforms: Tradeoffs among cost, accuracy, and speed. **R. Thackston, A. Ringer McDonald, R.C. Fortenberry****2:30 COMP 693.** Ontology for quantum chemistry. **N.S. Ostlund, M. Sopek, L.A. Burns, J.W. Bloom, B. Wang**

## 3:00 Intermission.

**3:15 COMP 694.** Variational density fitting of the full electron-electron interaction. **B.I. Dunlap, M.C. Palenik****3:45 COMP 695.** Diagrammatic screening approach to configuration interaction calculations. **M. Bayne, A. Chakraborty****4:05 COMP 696.** Configuration interaction under the presence of a density functional. **C. Hoyer, D. Ma, J. Olsen, D.G. Truhlar, L. Gagliardi****4:25 COMP 697.** Diagnosis and implications of spurious poles in the quadratic response of approximate, electronic structure method. **S.M. Parker, S. Roy, F.U. Furch**

## Big Data Science

## Interpreting Pharmacology

*Sponsored by MPPG, Cosponsored by BIOL, CINP, COMP, MEDI and PHYS*

## Computational Materials &amp; Nanoscience: Theory Meets Experiment

## Forum: Exciting Aspects of Excitation Dynamics &amp; Dissociation at the Nanoscale

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

**Section B**

Wyndham San Diego Bayfront  
Pacific C

**Fuel Cells**

*Cosponsored by CATL*

S. Cha, Z. Iqbal, *Organizers*

T. Kim, E. Lee, *Organizers, Presiding*

**1:30 ENFL 37.** Clicked, comb-shaped anion exchange membranes with pendent quarternary ammonium groups. N. Li

**1:50 ENFL 38.** Using direct alcohol fuel cells to extract electricity from ongoing fermentations. J. Jahnke, M. Benyamin, J. Sumner, D. Mackie

**2:10 ENFL 39.** Effect of H<sub>2</sub> diffusion on the hydrogen-evolution reaction kinetics. J. Zheng, Y. Yan, B. Xu

**2:30 ENFL 40.** Studies on physical and electrochemical modifications of the carbon-supported Pt/Ru electrocatalyst induced by different synthetic methodology for fuel cell applications. B. Lal, A. Altaf, A. Badshah

**2:50 ENFL 41.** Thermally cross-linked, chemically robust poly(2,6-dimethyl-1,4-phenylene oxide)-b-poly(vinylbenzyltrimethylammonium) diblock copolymer anion-exchange membrane for fuel cell applications. A.M. Herring, T. Pandey, H. Sarode

**3:10** Concluding Remarks.

**Section C**

Wyndham San Diego Bayfront  
Pacific D

**Advances in Methane Technology****Novel Materials & Processes**

*Financially supported by Custom Solutions Group LLC*

Z. He, J. Zhang, *Organizers, Presiding*

**1:30 ENFL 42.** Withdrawn.

**2:05 ENFL 43.** TiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub>-supported Ni catalysts for CO methanation. C. Guo, H. Zhang, J. Zhang

**2:40 ENFL 44.** Structure influence of nickel-based catalysts on methane conversion and their coke-resistant properties. Y. Zhang, C. Liu

**3:05** Intermission.

**3:20 ENFL 45.** Low-temperature, active, oscillation-resistant PdNi(allyl)/Ni-foam catalyst with enhanced heat transfer for coalbed methane deoxygenation via catalytic combustion. Q. Zhang, G. Zhao, Y. Lu

**3:55 ENFL 46.** Nickel catalysts supported on amino-functionalized MCM-41 for syngas methanation. M. Zhu, B. Dai, B. Wen

**4:30 ENFL 47.** Production of inherently separated syngas streams via chemical looping. A. More, C. Hansen, G. Veser

**Section D**

Wyndham San Diego Bayfront  
Pacific A

**Heavy Oil Upgrading, Production & Characterization****Upgrading**

J. J. Adams, C. Mesters, *Organizers, Presiding*

**1:30 ENFL 48.** Thiophene mitigates high-temperature fouling of metal surfaces in oil refining. D. Mitlin

**1:55 ENFL 49.** Effect of asphaltene stability in crude oils on fouling rate and fouling morphology. C.M. Holt, J. Haagsma, V.T. Sauer, J.J. Adams

**2:20 ENFL 50.** Bottom cracking FCC catalyst for processing high-basic nitrogen feedstock. Y. Zhu, Y. Luo, F. Ren, M. Xu, J. Zheng

**2:45 ENFL 51.** Distribution of basic nitrogen aromatic species in FCC process. Y. Zhu, Y. Liu, F. Ren, J. Deng

**3:10 ENFL 52.** Selective asphaltene adsorption from hydroconverted bottoms. J.J. Adams, J.F. Schabron, J.F. Rovani, J. Boysen, F.G. van den Berg, C. Mesters

**3:35 ENFL 53.** Diolefin characterization in thermally cracked naphtha. N.Y. Paez Cardenas, A. De Klerk

**4:00 ENFL 54.** Characterization of crude oil and water emulsion, interfacial material. J.J. Adams, J.F. Schabron, R.W. Grimes, J.L. Loveridge, H. Qu, L. Goual

**4:25 ENFL 55.** Supercritical water treatment of fractions of crude oil: Quantification of the products and model compound studies. S. Gudiyella, L. Lai, A. Lui, A. Carr, W.H. Green

**4:50 ENFL 56.** Filtration behavior of fine solids in bitumen froth before and after hydrothermal treatment. Q. Chen

**Section D**

San Diego Convention Center  
Room 4

**Research Opportunities for Future Energy Technologies**

M. Kidder, D. G. Schmidt, *Organizers*

M. V. Buchanan, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:40 ENFL 57.** The quadrennial technology review: Creating a clean energy future. F.M. Orr

**2:10 ENFL 58.** Basic research for carbon capture and storage (CCS). D. DePaolo

**2:40 ENFL 59.** Structural materials needs for energy technologies. K. Luthra

**3:10 ENFL 60.** Modern materials and chemical science: Enabling nuclear power into the future. J.T. Busby

**3:40 ENFL 61.** Additive manufacturing. P.D. Olmsted

**4:10 ENFL 62.** Hydrogen generation and fuel cells. T.F. Jaramillo

**4:40 ENFL 63.** Energy storage for transportation and the electricity grid: Challenges and opportunities. G. Crabtree

**Section F**

Wyndham San Diego Bayfront  
Pacific B

**Advances in Chemistry of Energy & Fuels****Supercapacitors & Batteries**

X. Wang, *Organizer*

D. J. Heldebrant, *Organizer, Presiding*

Z. He, L. Li, *Presiding*

**1:30 ENFL 64.** Synthesis of sulfur-doped porous carbon for high-performance lithium-ion batteries. Y. Sun, G. Ning, J. Gao

**1:50 ENFL 65.** Preparation of water-based slurry of S-doped CNTs as conductive additive for lithium-ion battery. C. Qi

**2:10 ENFL 66.** Synthesis of dual S, N-doped graphene fibres and their application as high-performance electrodes in supercapacitors. Y. Kan, G. Ning

**2:30 ENFL 67.** Pursuit of bulk graphene prevented by side reactions. D. Zugell, J.W. Baldwin

**2:50** Intermission.

**3:00 ENFL 68.** Interactions of nanostructured TiO<sub>2</sub> with nonaqueous electrolytes for Na-ion batteries. K. Smith, R. Parrish, P.L. Barnes, E.J. Dufek, H. Xiong

**3:20 ENFL 69.** Withdrawn.

**3:40 ENFL 70.** Visible light-responsive, dual-functional photocatalytic fuel cell. Y. He

**4:00 ENFL 71.** Double-acceptor dye design for p-type, dye-sensitized solar cells. K.A. Click, D.R. Beauchamp, B. Garrett, Z. Huang, C.M. Hadad, Y. Wu

**4:20 ENFL 72.** Reactivity studies using single-events methodology. B. Celse

**Catalytic Materials for Methane Conversion****Oxidation & Oxidative Coupling of Methane**

*Sponsored by CATL, Cosponsored by ENFL*

**Computational Chemistry Across Catalysis****QMMM & Reaction Pathway Sampling**

*Sponsored by CATL, Cosponsored by COMP, ENFL and WCC*

**Fundamental Surface Chemistry of Non-oxide Transition Metal Ceramic Catalysts: Carbides, Nitrides, Sulfides, Phosphides, Selenides**

*Sponsored by CATL, Cosponsored by ENFL*

**MONDAY MORNING****Section A**

Wyndham San Diego Bayfront  
Porthole

**Solar Cells****Dye-Sensitized & Perovskite**

Y. H. Hu, R. T. Koodali, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 73.** Light-induced structural change and degradation in organometal halide perovskite solar cells. J.Z. Zhang

**9:15 ENFL 74.** Dynamic effects of bulk and contacts at lead-halide perovskite solar cells. J. Bisquert

**9:55 ENFL 75.** Mesoporous titanium dioxide materials for dye-sensitized solar cells. L. Mahoney, H. Elbohy, S. Rasalingam, C. Wu, Q. Qiao, R.T. Koodali

**10:25** Intermission.

**10:35 ENFL 76.** Novel counter electrode materials for highly efficient dye-sensitized solar cells (DSSCs). Y.H. Hu

**11:15 ENFL 77.** Tuning the energetics of components and kinetics of key steps in dye-sensitized solar cells. D. Jiang, N. Darabedian, S. Ghazarian, Y. Hao, M. Zhgamadze, N. Majjaryan, R. Shen, F. Zhou

**11:55 ENFL 78.** High-transparency graphene films as counter electrodes for bifacial dye-sensitized solar cells. W. Yang, Z. Li, X.W. Xu, Y. Li

**12:15 ENFL 79.** Molecular monolayers as electrical passivation for silicon solar cells. J. Veerbeek, N. Firet, J. Huskens

**12:35** Concluding Remarks.

**Section B**

Wyndham San Diego Bayfront  
Pacific C

**ENFL Distinguished Researcher Award: Symposium in honor of Stu Soled****Conventional Energy**

J. G. Santiesteban, *Organizer*

E. Iglesia, *Organizer, Presiding*

**8:45** Introductory Remarks.

**8:50 ENFL 80.** Investigation of sulfur tolerance in supported Pt-Pd catalysts for aromatic saturation. M.P. Lanci, S. Soled, S. Miso, C. Kiewer, P. Stevens, J. Baumgartner, Y. Joshi, J. Guzman, T. Green, J. McConnachie

**9:20 ENFL 81.** Insights into the flexibility of porous, organic frameworks and its impact in adsorption. Y. Du, B. Wooler, K. Mao, S.C. Weston, M. Nines, P. Kortunov, P. Ravikovitch, C. Paur

**9:50 ENFL 82.** Innovation in heterogeneous catalysis research. D. Levin

**10:20 ENFL 83.** Advances in distillate catalytic dewaxing. J.G. Santiesteban

**10:50** Intermission.

**11:05 ENFL 84.** Emission and trapping of adatoms during Ostwald ripening. A.K. Datye, C. Carrillo, T. Johns, H. Xiong, R. Goeke, G. Qi, S. Oh, M. Wiebenga, M. Balogh

**11:35 ENFL 85.** Selective oxidation at the Au/TiO<sub>2</sub> interface. M. Neurock

**Section C**

Wyndham San Diego Bayfront  
Pacific D

**Advances in Methane Technology****Novel Materials & Processes**

*Financially supported by Custom Solutions Group LLC*

Z. He, J. Zhang, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 86.** Co-production of power and hydrogen by combined processes of chemical looping, combustion, and methane decomposition/reforming. H. Tian, R.V. Sirinwardane

**9:10 ENFL 87.** Methane steam reforming: Using external electric fields to enhance the catalytic performance of Ni. F. Che, J.T. Gray, S. Ha, J. McEwen

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)



**9:45 ENFL 88.** Gas uptake and safety evaluation of porous materials used in shale gas storage. B. Martinez, U. Okakpu, X. Wang, Y. Chen, H. Zhou, S. Bashir, J.L. Liu

**10:20** Intermission.

**10:35 ENFL 89.** Methane to gasoline conversion using STG+ technology. E. Tenenbaum, G. Boyajian, E. Gal, Z. He, H. Fang

**11:10 ENFL 90.** Advanced coal gasification process for SNG. G. Wang, Y. Nie, Z. Ma, X. Jing

**11:45 ENFL 91.** Methane production from oil refinery, waste-activated sludge by two-phase anaerobic digestion. Q. Wang, C. Chen, S. Guo

**12:20** Concluding Remarks.

## Section D

Wyndham San Diego Bayfront  
Pacific A

### Novel Materials for Energy & Fuels

#### Solar Energy Materials

X. Wang, X. Xu, Y. Yang, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 92.** Materials and catalysts for solar energy conversion and electrical energy storage. Y.H. Hu

**9:05 ENFL 93.** Organolead halide perovskite solar cells enabled by flow-enabled self-assembly. Z. Lin, M. He, B. Li, C. Zhang

**9:35 ENFL 94.** Withdrawn.

**10:05** Intermission.

**10:20 ENFL 95.** Strategies towards improved efficiency in photocatalytic hydrogen evolution from aqueous media. K. Striegler, R. Glaeser

**10:50 ENFL 96.** Synthesis, optical properties, and exciton dynamics of organolead bromide perovskite quantum dots. J.Z. Zhang

**11:20 ENFL 97.** Controlled fabrication of copper-indium-selenide (CIS) nanotube arrays for high-efficiency solar energy conversion. W. Liyanage, M. Nath

**11:40 ENFL 98.** Strategies for designing highly efficient and stable photoanodes for solar water splitting. Y. Li

## Section E

Wyndham San Diego Bayfront  
Harborside

### CO<sub>2</sub> Conversion & Utilization

#### Conversion

*Cosponsored by CATL*

E. J. Biddinger, H. Lin, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 99.** CO<sub>2</sub> hydrogenation activity and selectivity dependency on crystal facets of cobalt oxide catalysts. C. Wen, J. Hattrick-Simpers, J. Lauterbach

**9:15 ENFL 100.** Structure sensitivity and deactivation of copper-based catalysts in carbon dioxide hydrogenation to methanol. S. Natesakhawat, J. Lakse, P.R. Ohodnicki, J.P. Baltrus, B.H. Howard, X. Deng, C. Matranga

**9:40 ENFL 101.** Importance of metal-oxide and metal-carbide interfaces in the activation of CO<sub>2</sub>: Novel catalysts for methanol synthesis. J. Rodriguez, P. Liu, S.D. Senanayake, D.J. Stacchiola, J. Evans, J. Graciani, J.F. Sanz, F. Vines, F. Illas

**10:05 ENFL 102.** Enhanced CO<sub>2</sub> hydrogenation to methanol over Ga-modified Cu/ZnO catalysts. E. Tsang, M. Li

**10:30** Intermission.

**10:45 ENFL 103.** Catalytic performance of Ni-Co/SBA-15-CD in carbon dioxide reforming of methane at high pressure. H. Wu, Q. Zhu, H. Liu, W. Yang, D. He

**11:10 ENFL 104.** Mechanistic insights into CO<sub>2</sub> hydrogenation on transition metal surfaces: A DFT-based microkinetic analysis. T. Avanesian, P. Christopher

**11:35 ENFL 105.** Catalytic CO<sub>2</sub> hydrogenation over carbon-supported Fe-Cu-K catalysts. M. Rafati, A. Shahabzi, L. Wang

**12:00 ENFL 106.** Synthesis of cyclic 2-oxazolidenes by chemical CO<sub>2</sub> fixation. T. Niemi, J.E. Perea-Buceta, I. Fernández, T. Repo

## Section F

Wyndham San Diego Bayfront  
Pacific B

### Advances in Chemistry of Energy & Fuels

#### Fuel Chemistry

X. Wang, *Organizer*

D. J. Heldebrant, *Organizer, Presiding*

Z. He, L. Li, *Presiding*

**8:30 ENFL 107.** Electrochemical and spectroscopic investigations of fuel additives based on butylated phenols. N. Zabik, S. Martic

**8:50 ENFL 108.** Microwave-assisted pyrolysis of low-rank coals. V. Abdelsayed, D. Shekhawat, M.W. Smith

**9:10 ENFL 109.** Ionic liquid extraction of polycyclic aromatic hydrocarbons from petroleum source rock. A. Akinlua

**9:30 ENFL 110.** Birch reduction of asphaltene. M. Verma, B. Brinson, L. Alemany, S. Wellington, M. Shammai, W.E. Billups

**9:50** Intermission.

**10:00 ENFL 111.** Red mud catalytic pyrolysis of auto shredder residue. F.A. Agblevor, O. Hietsoi, K. Christian, B. Sargent

**10:20 ENFL 112.** Bioinspired MOF design for lignin catalysis: Role of co-factor on enzymatic lignolysis. P. Ramakrishnan, V. Stavila, B.A. Simmons, M. Allendorf, K. Sale

**10:40 ENFL 113.** Withdrawn.

**11:00 ENFL 114.** Nitrogen-containing compounds in thermally cracked naphtha. Y. Rao, A. De Klerk

**11:20 ENFL 115.** Molecular characterization of N-methyl-2-pyrrolidone (NMP) extracts from a lignite coal. Q. Shi, H. Ni, L. Yan, C. Ma, C. Xu

**11:40 ENFL 116.** DFT studies of CO<sub>2</sub> reduction to CO and methanol on ceria (110) surface. N. Kumari, M. Haider, N. Sinha, S. Basu

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Environmental Chemistry/Water Chemistry

*Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC*

#### WCC 2016 Rising Stars Awards Symposium

*Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE*

#### Catalytic Materials for Methane Conversion

#### Methane Reforming

*Sponsored by CATL, Cosponsored by ENFL*

### Computational Chemistry Across Catalysis

#### Towards Chemical Accuracy

*Sponsored by CATL, Cosponsored by COMP, ENFL and WCC*

## MONDAY AFTERNOON

### Section A

Wyndham San Diego Bayfront  
Porthole

#### Solar Cells

Y. H. Hu, R. T. Koodali, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 ENFL 117.** Enabling advances in solar cell performance through materials integration. M. Goorsky

**2:15 ENFL 118.** Multiscale modeling and operation of PECVD of thin-film solar cells. M. Crose, P. Christofides

**2:55 ENFL 119.** Core-shell structured solar cells. J.G. Lu

**3:35** Intermission.

**3:45 ENFL 120.** Dilute-nitride GaN(As) P-based solar cells. C. Tu

**4:25 ENFL 121.** Engineering defects to enable cost-effective solar cells. E. Magaña, Y. Luo, A. Morishige, J. Hofstetter, M. Ann Jensen, S. Castellanos, J. Maser, B. Lai, V. Rose, M. Bertoni, T. Buonassisi, D. Fenning

**4:55 ENFL 122.** High-performance, microscale silicon photovoltaics enabled with nanoscale photon management and spectral modification. J. Yoon

**5:25** Concluding Remarks.

### Section B

Wyndham San Diego Bayfront  
Pacific C

### ENFL Distinguished Researcher Award: Symposium in honor of Stu Soled

#### Renewable Energy

E. Iglesia, *Organizer*

J. G. Santiesteban, *Organizer, Presiding*

**1:45 ENFL 123.** CO<sub>2</sub> conversion using catalysis and electrocatalysis. J.G. Chen

**2:15 ENFL 124.** Catalytic and chemical reaction engineering challenges in the refining and petrochemical industries: The decade ahead. T.F. Degnan

**2:45 ENFL 125.** Isomerization of acyclic and cyclic alkanes: Acid strength and metal-acid site proximity effects on turnover rates and selectivities. W. Knaeble, E. Iglesia

**3:15** Intermission.

**3:30 ENFL 126.** Carbon dioxide: What can we do with it? B.H. Davis

**4:00 ENFL 127.** Experimental study of adsorption and low-temperature reactions of pentene on ZSM-5. S. Schallmoser, G.L. Haller, M. Sanchez, J.A. Lercher

**4:30 ENFL 128.** Enhanced stability of catalytic surfaces by bimetallic core-shell structures and the concept of differential surface free energies of the core and shell components. J.R. Monnier, J.R. Regalbuto, K. O'Connell, W. Diao, A. Wong

### Section C

San Diego Convention Center  
Halls B/C

### Advances in Chemistry of Energy & Fuels

D. J. Heldebrant, X. Wang, *Organizers*

**2:00 - 4:00**

**ENFL 129.** Electrospun anatase TiO<sub>2</sub>/carbon-composite nanofiber as an anode material for sodium-ion batteries. K. Jung, M. Park, J. Lee

**ENFL 130.** Novel metal-doped, ceria-decorated, aminated graphene for high-performance supercapacitor. R. Kumar

**ENFL 131.** Compilation of gas-phase enthalpies of formation for hydrogen-oxygen (H<sub>2</sub>O<sub>x</sub>) species. D.R. Burgess

**ENFL 132.** Diaxially substituted P(V) porphyrin as a new photosensitizer for TiO<sub>2</sub>-based solar cells. M.P. Gajewski, F.F. Rodriguez

**ENFL 133.** Control of defects in organo-halide perovskite materials for solar energy conversion. J. Paige, R. Stewart, J.B. Asbury

**ENFL 134.** Preparation of S-doped nanomesh graphene based on the post-treatment methodology: A high-performance electrode for supercapacitor. X. Ma

**ENFL 135.** Improved performance of organic solar cells with Ag nanoparticles through dispersion control and layer-evolved bulk-heterojunction. D. Wang, S. Ahn, W. Jang, J. Park

**ENFL 136.** Use of nano-catalysts to improve performance of hybrid-model vehicle driven by H<sub>2</sub> fuel and solar cells. E. Hager-Hahn, P. Villarreal, K. Kuypers, J. Mendoza, M. Ruelas, Y. Bhakta, W. Beatty, J.L. Liu

**ENFL 137.** Protonic transfer steps in yttrium-doped barium zirconite. M. Gomez, D. Pan, D. Fry, F. Haibach

**ENFL 138.** Investigating synthesis of hybrid metal sulfide nanocrystals from ethyl xanthate metal salts for solution-processed solar cells. M. Leal, T. Trad, M. Uddin, J. Moore

**ENFL 139.** Withdrawn.

**ENFL 140.** Dye-sensitized photovoltaic cells with enhanced exciton-hole separation and barrier characteristics. H.J. Moore, M. Leal, G.E. Grissom, T. Trad, N. Islam, A. Touhami, J. Uddin

**ENFL 141.** Exsolution mechanism of nanoparticles on double-layered perovskite under reduction condition. K. Kim, J. Han

**ENFL 142.** Hyperpolarized <sup>129</sup>Xe nuclear magnetic resonance studies of Si nano-composite electrode materials. Y. Mao, M. Song, R. Hopson, N. Karan, P. Guduru, L. Wang

**ENFL 143.** Novel approach to double-junction tandem solar cells using organo-metallic-organic hybrid device structure. S. Sahare, H.P. Rathnayake

**ENFL 144.** Organic polymeric materials for renewable batteries. L.S. Aakerlund, M. Sjödin, M. Stromme

**ENFL 145.** Effect of reflection on the performance of dye-sensitized solar cell (DSSC) using MoS<sub>2</sub>-based counter electrode. I.R. Stephenraj

**ENFL 146.** Adsorption mechanism of thiophene, benzothiophene, and dibenzothiophene on carbon nanotubes-titania. T.A. Saleh, M.N. Siddiqui, A.A. Al-Artaj

**ENFL 147.** Desulfurization of fuel oils using membrane-assisted flow reactor. M.M. Suliman, C. Basheer, M.N. Siddiqui

- ENFL 148.** Looking at alkali, pre-extraction conditions and its effect on the composition of different hybrid poplar cultivars. **S. Polk**, H. David, R. Stoklosa
- ENFL 149.** Density functional theory calculations for resisting sulfur poisoning on Ni-based bimetallic alloys/YSZ in solid oxide fuel cell anode. **B. Hwang**, J. Ko, J. Han
- ENFL 150.** Effects of water dynamic process and water retaining zeolites on the performance of self-humidifying proton exchange membrane. V. Sim, R. Deng, W. Han, W. Hui, K. Yeung
- ENFL 151.** Novel PEMFC with promoted performance under high temperature. R. Deng, V. Sim, W. Han, W. Hui, K. Yeung, M.V. Martinez-Huerta, X. Ouyang
- ENFL 152.** Simultaneous adsorption of organosulfur compounds on a novel, Al-modified, activated carbon adsorbent: Insight into competitive effect of sulfur-compounds on adsorption capacity. S. Ganiyu, K.R. Alhooshani, I.A. Bakare, T.A. Saleh
- ENFL 153.** Effect of heterocyclic groups in copolymers on cold flowability of waxy crude oils. H. Zhao, T. Li, T. Wang, J. Xu, X. Guo
- ENFL 154.** Rheology and stability improvement of coal water slurry by poly(styrene-co-maleic anhydride aminobenzene sulfonate)s. X. Guo, K. Meng, K. Huang, L. Li
- ENFL 155.** Development of new borate delayed crosslinkers for oilfield applications. **D.M. Schubert**, M. McCray
- ENFL 156.** Synergistic effects of tetrahydrofuran and sodium dodecyl sulfate on methane hydrate formation. A. Saingsai, B. Kitiyanan, P. Rangsunvigit, S. Kulprathipunya
- ENFL 157.** Implementation of multiphase-integrated systems for organic waste treatment coupled with biogas production in family farms at the northern Caribbean region of Costa Rica. V. Chaves-Villarreal, C. Villarreal
- ENFL 158.** Preparation of ordered silica nanotubes and its application on PEMFC. **Y. Chen-Yang**
- ENFL 159.** Adsorptive desulfurization performances of nitrogen-doped active carbon from slurry oil. X. Song, G. Ning, J. Gao
- ENFL 160.** Prediction of atmospheric distillates (199-371°C+) from its raw crude oils by FTIR-ATR and multivariate analysis. **B. Murcia**, E. Mejía-Ospino
- ENFL 161.** Selective and efficient methane activation by novel organometallic catalyst. N. Zargari, J. Chen, K. Kaneshiro, A. Coward, J. Lee, K.W. Jung
- ENFL 162.** Investigation into the efficacy of the IP-143 method for the separation of asphaltenes from bulk crude oils. **M. Rizor**, G.C. Klein
- ENFL 163.** Enhanced desulfurization of model fuel oil at ambient temperature using aluminum-doped activated carbon. S. Ganiyu, K.R. Alhooshani, K. Sulaiman, M. Qamaruddin
- ENFL 164.** Composite materials for the conversion of methane to synthesis gas. **K. Dossomov**
- ENFL 165.** Withdrawn.
- ENFL 166.** Cu nanowires for electrochemical reduction of CO<sub>2</sub> and CO. **D. Raciti**, C. Wang
- ENFL 167.** Modeling and investigation of CO<sub>2</sub> diffusivity in formation water in CO<sub>2</sub>-EOR process. **S. Pourjafar**, H. Jabbari
- ENFL 168.** Amine-based adsorbents for CO<sub>2</sub> capture from simulated flue gas. **G. Xue**
- ENFL 169.** Hydrogen production from solar water splitting: Preventing electron and hole recombination using structured TiO<sub>2</sub>. F. Rusinque, N. Ha, L. Li, X. Wang
- ENFL 170.** Paper microfluidic formate fuel cell. L. Pham, K. Purohit, K. Domalaon, V. Galvan, F.A. Gomez, J. Haan
- ENFL 171.** Formate: An energy-storage and -transport bridge between carbon dioxide and formate fuel cell. **S. Saric**, M. Guntenspergen, B. Biggs, C. Nguyen, S. Mayoral, J. Haan
- ENFL 172.** Abatement of CO<sub>2</sub> emission in the Chinese petroleum refining industry. **M. Du**, H. Ge, Z. Lyu
- ENFL 173.** Metal oxides impact on mesoporous carbon structure and CO<sub>2</sub> adsorption performance. **M. Li**
- ENFL 174.** CO<sub>2</sub> hydrogenation to methanol over Cu/ZnO/ZrO<sub>2</sub> catalysts prepared by chemical reduction. **D. Xiaosu**
- ENFL 175.** PdCu/C catalysts for the electrochemical oxidation of renewable polyalcohols. **O. Muneeb**, J. Flores, K. Nguyen, S. Hu, L. Scudiero, S. Ha, J. Haan
- ENFL 176.** Pd/CNT catalysts for electrochemical oxidation of small organic molecules in alkaline media. **J. Estrada**, J. Flores, K. Nguyen, S. Hu, L. Scudiero, S. Ha, J. Haan
- ENFL 177.** Generation of hydrogen from formic acid in the presence of ruthenium-containing catalysts. **M. Czaun**, A. Goepfert, J. Kothandaraman, R.M. Haiges, S.G. Prakash, G.A. Olah
- ENFL 178.** Effect of acid treatment time of Fe-BEA zeolite on its catalytic performance for N<sub>2</sub>O conversion. **J. Jeong**, J. Park, J. Baek, K. Yi
- ENFL 179.** Redox characteristics and kinetics of Ni-based oxygen carrier for chemical looping combustion (CLC). **J. Park**, J. Jeong, J. Baek, K. Yi
- ENFL 180.** Catalytic characteristic of Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst for WGS reaction: Effect of Al precursor addition time. **J. Baek**, J. Park, J. Jeong, K. Yi
- ENFL 181.** Effect of the method of catalysts preparing for their activity in the Fischer-Tropsch synthesis. **K. Dossomov**
- ENFL 182.** First-principles calculations for catalytic activation and dissociation of carbon dioxide on pure, bimetallic surfaces. **J. Ko**, J. Han
- ENFL 183.** Iron-nickel layered double hydroxide combined with Ru(II)-diimine as visible-light photosensitizer in water oxidation electrocatalysis. **D.F. Sranko**, Z. Horvath, M. Chamam, J. Pap
- ENFL 184.** Thermophysical properties of LiFePO<sub>4</sub>: DFT+U computations combined with a thermodynamically self-consistent (TSC) method. **A. Seifitokaldani**, A.E. Gheribi, M. Dolle, P. Chartrand
- ENFL 185.** High-performance, plate-frame, microfluidic fuel cell with flow-through porous electrodes: Breaking the size limitation. **L. Li**, M.K. Leung
- ENFL 186.** Octane number prediction using density functional theory. **P. Ramakrishnan**, J. Gladden, N. Hillson, S. Singh, B.A. Simmons
- ENFL 187.** Energetics of H<sub>2</sub>O elimination from aliphatic alcohols. **D.R. Burgess**, C. Rosado-Reyes, J.A. Manion
- ENFL 188.** Degradation of organic matter under geological conditions: A route towards thermodynamic solid/fluid equilibrium using replica exchange, molecular dynamics simulations. **L. Atmani**, J. Leyssale, C. Bichara, R. Pellenq, H.J. Van Damme, F. Ulm
- ENFL 189.** Suppressing cation segregation on perovskite surfaces to design high-performance cathode materials in solid oxide fuel cells. **H. Kwon**, **J. Han**
- ENFL 190.** Improved design of a commercial, diffuse reflectance reactor for *in-situ*, ultraviolet-visible spectroscopy studies. **P.D. Srinivasan**, J.J. Bravo-Suarez
- ENFL 191.** Trends in activity of spinel-type ferrite MFe<sub>2</sub>O<sub>4</sub> (M=Mn, Fe, Co, Ni, Zn) for oxygen evolution reaction. **C. Hsu**, N. Suen, S. Lin, H. Chen
- ENFL 192.** *In-operando* identification of geometrical-site-dependent water oxidation activity of spinel Co<sub>3</sub>O<sub>4</sub>. **H. Wang**, S. Hung, H. Chen, T. Chan, H. Chen, B. Liu
- ENFL 193.** Propene pyrolysis at low to intermediate temperatures. **K. Wang**, S. Villano, A.M. Dean
- ENFL 194.** Withdrawn.

## Section D

Wyndham San Diego Bayfront  
Pacific A

## Novel Materials for Energy & Fuels Solar Energy & Energy Storage Materials

X. Wang, X. Xu, Y. Yang, *Organizers, Presiding*

1:30 Introductory Remarks.

**1:35 ENFL 195.** Efficient hydrogen generation from liquid-chemical hydrogen storage materials over functional-supported, metal nanoparticles at room temperature. **X. Gu**, **H. Su**

**2:05 ENFL 196.** Development in high-performance membranes for efficient hydrogen purification. **Z. Wang**, X. Cao, Z. Qiao, J. Wang, S. Wang

**2:35 ENFL 197.** Achieving sustainable water purification: Visible light-responsive, graphitic carbon nitride for the removal of persistent contaminants. **D. Shuai**, Q. Zheng, D. Durkin, N. Banek, M.J. Wagner

3:05 Intermission.

**3:20 ENFL 198.** Functional energy materials from 1D and 2D polymers to 3D carbon nanomaterials. **M. Wang**, Q. Dai, X. Chen, **N. Dai**

**3:50 ENFL 199.** Inorganic-biological hybrid systems for solar-to-chemical production. **K.K. Sakimoto**, P. Yang, C. Liu

**4:20 ENFL 200.** Nanoporous metals for optical-electrical energy applications. **Y. Zhao**, **Y. Ding**

**4:50 ENFL 201.** Mechanistic study of N<sub>2</sub>MWNTs synthesis and its oxygen reduction reaction activity. **Z. Wu**, E. Benchafia, Z. Iqbal, **X. Wang**

## Section E

Wyndham San Diego Bayfront  
Harborside

## CO<sub>2</sub> Conversion & Utilization

### Capture & Utilization

*Cosponsored by CATL*

E. J. Biddinger, H. Lin, *Organizers, Presiding*

1:30 Introductory Remarks.

**1:35 ENFL 202.** Energy issues in the utilization of CO<sub>2</sub> in the synthesis of chemicals: The case of direct carboxylation of alcohols to dialkyl-carbonates. **A. Dibenedetto**, **M. Aresta**, A. Dutta

**2:00 ENFL 203.** Highly efficient formate production by hydrogenation of captured CO<sub>2</sub>. **H. Lin**

**2:25 ENFL 204.** CO<sub>2</sub>-based chemicals in a renewable natural gas context. **C.S. Park**, P.S. Roy, K. Kim, A. Raju

**2:50 ENFL 205.** Methane partial oxidation and CO<sub>2</sub> reduction via a cyclic redox scheme. **J. Zhang**, **F. Li**

3:15 Intermission.

**3:30 ENFL 206.** Pathway toward reducing CO<sub>2</sub> emissions in the industrial sector. **P.C. Psarras**, J. Wilcox

**3:54 ENFL 207.** Small-molecule thickeners for CO<sub>2</sub> EOR. **R.J. Perry**, M. O'Brien, M.D. Doherty, J. Lee, R.M. Enick, A. Dhuwe, E.J. Beckman, S. Cummings

**4:18 ENFL 208.** Fabrication of faujasitic zeolite membranes with roller assembly for CO<sub>2</sub> capture. **B. Wang**, P. Dutta

**4:42 ENFL 209.** Carbon-dioxide capture using polyethylenimine impregnated titanate nanotubes. **H. Du**, M. Stewart, X. Shen, **R.R. Kommalapati**

**5:06 ENFL 210.** On the origin of preferred bicarbonate production from carbon dioxide (CO<sub>2</sub>) capture in aqueous 2-amino-2-methyl-1-propanol (AMP). **H. Stowe**, L. Vilciauskas, E. Paek, G.S. Hwang

## Section F

Wyndham San Diego Bayfront  
Pacific B

## Nanomaterials for Energy Conversion & Storage

### Energy Conversion

*Cosponsored by CATL*

Y. Lee, *Organizer*

Z. Wu, H. Zhao, *Organizers, Presiding*

**1:30 ENFL 211.** Challenges and opportunities for perovskite solar cells. **T. Xu**, Q. Jiang

**2:00 ENFL 212.** Hybrid organic-inorganic perovskite solar cells: Impact of atomic structure and dynamics on optoelectronic properties and device performance. **J.J. Choi**

**2:30 ENFL 213.** *In situ*-grown graphene 3D hybrids for the photoanode of dye-sensitized solar cells. **C. Villarreal**, T.M. Terse, P. Ramnani, G. Madrigal, A.K. Mulchandani

**2:50 ENFL 214.** Towards low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics. **M.A. Niedermeier**, B. Su, L. Song, S.V. Roth, **P. Mueller-Buschbaum**

**3:10 ENFL 215.** Nanoengineered films for sustainable energy. **Y. Yang**

3:30 Intermission.

**3:40 ENFL 216.** Photoinduced electron injection from ruthenium complex to Ni/Ni(OH)<sub>2</sub> core/shell nanoparticles. **J. Huang**, Y. Tang

**4:10 ENFL 217.** *In situ* synchrotron x-ray studies of nanomaterials for energy conversion and storage applications. **Z. Feng**

**4:40 ENFL 218.** Characterization and reactivity studies of nanocatalysts by small-angle x-ray scattering. **R.E. Winans**, S. Lee, T. Li, J. Wang, S. Seifert, B. Lee

**5:10 ENFL 219.** Increased hydrogen production from DNA-assembled TiO<sub>2</sub>-CdS photocatalytic material. **K. Ma**, O. Yehzekeli, D. Domaille, H.H. Funke, J. Cha

## WCC 2016 Rising Stars Awards Symposium

*Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE*

## Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

### Environmental Chemistry/Water Chemistry

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

### Computational Chemistry Across Catalysis

### Oxide Catalysts & Key Industrial Reactions

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

## MONDAY EVENING

### Section A

San Diego Convention Center Halls D/E

#### Sci-Mix

X. Wang, *Organizer*

#### 8:00 - 10:00

2, 7, 22, 26, 30, 38, 46, 65, 67, 94, 107, 113, 191-192, 203-204, 211, 215. See previous listings.

225, 259, 261, 264-265, 272, 301, 303, 307-308, 312-313, 321, 337-338, 341, 343, 347-348, 366, 372, 407, 422. See subsequent listings.

## TUESDAY MORNING

### Section A

Wyndham San Diego Bayfront Porthole

#### Batteries & Supercapacitors

#### Li-Ion Battery Materials Synthesis & Characterization

X. Ji, X. Li, K. Xu, *Organizers*

J. Guo, H. Xiong, *Organizers, Presiding*

#### 8:30 Introductory Remarks.

**8:35 ENFL 220.** Progress on chemistries and materials for inherently robust EV batteries. P. Liu

**9:05 ENFL 221.** 3D distribution of the conductive carbon-binder domains in Li-ion batteries. S.J. Harris, C. Li, J. Gelb, P.R. Shearing

**9:35 ENFL 222.** Hierarchical molybdenum sulfide: Carbon microspheres for high-performance lithium-ion battery anode. G. Chen, H. Luo

**9:55 ENFL 223.** Nano-rod boron anode materials for lithium ion batteries.

C. Deng, R. Parrish, H. Barkholtz, L. Luo, C. Wang, T. Xu, H. Xiong

#### 10:15 Intermission.

**10:30 ENFL 224.** Nanoscale structural and chemical evolution of electrode and their correlation with TEH capacity fading. C. Wang

**11:00 ENFL 225.** Mesoscale metal-oxide-based composite electrodes: Impact of crystallite size and aggregation on battery electrochemistry. A.C. Marschilok, E.S. Takeuchi, K.J. Takeuchi

**11:30 ENFL 226.** Hierarchical mesoporous SnO<sub>2</sub>@C@TiO<sub>2</sub> nanochains as a high-performance anode materials for lithium-ion batteries. X. Yu

**11:50 ENFL 227.** Li-ion battery based on quinone-derivatives: First-principles modeling approach. K. Kim, S.W. Lee, S.S. Jiang

**12:10 ENFL 228.** Phases hybridizing and hierarchical structuring of mesoporous TiO<sub>2</sub> nanowire bundles for high-rate and high-capacity lithium batteries. B. Su, J. Jin, Y. Li

### Section B

Wyndham San Diego Bayfront Pacific C

#### ENFL Distinguished Researcher Award: Symposium in honor of Stu Soled

#### Renewable Energy

E. Iglesia, J. G. Santesteban, *Organizers*

D. Levin, *Presiding*

**9:00 ENFL 229.** Effects of spatial distribution of supported nanoparticles in catalysis. K. De Jong

**9:30 ENFL 230.** Operando imaging of PEFC electrocatalysts by time/space-resolved XAFS. M. Tada

**10:00 ENFL 231.** Hydrodesulfurization studies on phosphide catalysts. S.T. Oyama

#### 10:30 Intermission.

**10:45 ENFL 232.** Metastability: The key to new catalyst discovery. S. Soled

**11:25 ENFL 233.** Using cascading catalysis concepts to design heterogeneous catalysts for CO<sub>2</sub> hydrogenation. L.T. Thompson

### Section C

Wyndham San Diego Bayfront Pacific D

#### Application of Computational Chemistry for Energy & Fuel Production

#### Computational Catalysis in Research

Cosponsored by CATL

L. Wang, *Organizer*

Y. Chen, H. Xin, *Organizers, Presiding*

**8:30 ENFL 234.** Atomic-dispersed Pt and Au atoms on ZnO surface for methanol steam reforming. W. Li

**9:00 ENFL 235.** Hydrogen storage system based on the reversible interconversion between H<sub>2</sub>/CO<sub>2</sub> gas and formic acid in water using molecular catalysts. J.T. Muckerman, M.Z. Ertem, E. Fujita, Y. Himeda

**9:30 ENFL 236.** Exploring the impact of density-functional approximation tuning in predictions of bonding, energetics, and magnetic properties of transition metal catalysts. H.J. Kulik, Q. Zhao, E. Ioannidis

**10:00 ENFL 237.** Thermodynamic and kinetic investigation on the selectivity of water-gas shift reaction on Ni catalyst. M. Zhou, B. Liu, T.N. Le, L.K. Huynh

#### 10:20 Intermission.

**10:30 ENFL 238.** Modern catalytic technologies for converting biomass to renewable aromatics. D.G. Vlachos

**11:00 ENFL 239.** Screening approaches in computational heterogeneous catalysis. F. Abild-Pedersen

**11:30 ENFL 240.** Stability, reactivity, and activity of nano-structured oxides supported on gold. A. Vojvodic, M. Bajdich, M. Garcia-Melchor

**12:00 ENFL 241.** Kinetic barriers of photocatalytic oxygen evolution on anatase TiO<sub>2</sub> (101). A. Selloni, Y. Li

### Section D

Wyndham San Diego Bayfront Pacific A

#### Novel Materials for Energy & Fuels

#### Heterogeneous Catalytic Materials

X. Wang, X. Xu, Y. Yang, *Organizers, Presiding*

**8:30 ENFL 242.** Small molecules directed synthesis of catalytic materials: The surface interfaces and structure regulation. B. Chen

**9:00 ENFL 243.** Design of ceria thin-film catalyst support for capillary microreactor application. A. Tanim, K.R. Alhooshani

**9:20 ENFL 244.** Atomic cobalt on nitrogen-doped graphene for hydrogen generation. H. Fei, J. Dong, D. Chen, J.M. Tour

**9:50 ENFL 245.** Developing highly active catalysts for the production of methanol from waste glycerol. P. Smith, N.F. Dummer, D.W. Knight, S.H. Taylor, G. Hutchings

#### 10:20 Intermission.

**10:30 ENFL 246.** Catalysis and the nature of mixed-metal oxides at the nanometer level: Special properties of MOx/TiO<sub>2</sub>(110) (M= Ru, Ce) surfaces. D.J. Stacchiola, S.D. Senanayake, P. Liu, J. Rodriguez

**11:00 ENFL 247.** Mechanistic insights into metal Lewis acid-mediated catalytic transfer hydrogenation reactions. B. Xu, D.G. Vlachos, M. Gilkey

**11:30 ENFL 248.** MOF-derived nitrogen-doped porous carbon as metal-free catalysts for acetylene hydrochlorination. X. Li, C. Guo, W. Li, J. Zhang

### Section E

Wyndham San Diego Bayfront Harborside

#### CO<sub>2</sub> Conversion & Utilization

#### Electroreduction

Cosponsored by CATL

E. J. Biddinger, H. Lin, *Organizers, Presiding*

#### 8:30 Introductory Remarks.

**8:35 ENFL 249.** Investigating the electroreduction pathway of carbon dioxide to fuels. J. Billy, K. Muhlenkamp, A. Co

**9:00 ENFL 250.** Exploring CO<sub>2</sub> reduction on heteroatom-doped nanoporous carbons. W. Li, M. Sereych, T. Bandoz

**9:25 ENFL 251.** Low-overpotential electrochemical reduction of CO<sub>2</sub> and CO enabled by Cu nanowires. C. Wang

**9:50 ENFL 252.** Copper nanoparticle/carbon nanospire as a synergic catalyst for CO<sub>2</sub> reduction reaction towards enhanced activity and selectivity. Y. Song, A. Rondinone, D. Hensley

**10:15 ENFL 253.** Importance of substrate metals in Cu nanoparticle-based catalysts for CO<sub>2</sub> electroreduction. A.N. Karauskakis, S. Shrestha, E.J. Biddinger

#### 10:40 Intermission.

**10:55 ENFL 254.** Design of catalysts for the selective electrochemical reduction of CO<sub>2</sub> to C<sub>2</sub> hydrocarbons and oxygenates. A.T. Bell

**11:35 ENFL 255.** Extremely efficient, carbon negative electrochemical CO<sub>2</sub> conversion with atomically precise Au<sub>25</sub> nanocatalysts. D. Kauffman, D. Alfonso, C. Matranga, P.R. Ohodnicki, J. Thakkar, R. Siva, R. Jin

**12:00 ENFL 256.** Facet dependence of CO<sub>2</sub> electroreduction on Cu catalysts. A.R. Asthagiri, W. Luo, X. Nie, M.J. Janik

### Section F

Wyndham San Diego Bayfront Pacific B

#### Nanomaterials for Energy Conversion & Storage

#### Energy Conversion: Characterization/Application

Cosponsored by CATL

H. Zhao, *Organizer*

Y. Lee, Z. Wu, *Organizers, Presiding*

**8:30 ENFL 257.** Probing structural stability and transitions in MOFs using PDF analysis. K.W. Chapman, A. Platero-Prats, L.C. Gallington

**9:00 ENFL 258.** Redox-active, porous, organic framework for efficient energy storage in Na-ion batteries. C. Deng, J. Mok, J. Lu, R. Cutler, J. Zhang, H. Xiong

**9:30 ENFL 259.** Pore tuning towards highly active nitrogen doped carbon electrocatalysts. J. Pampel, M. Antonietti, T. Fellinger

**9:50 ENFL 260.** Frameless hexahedron bimetallic nanostructure for electrochemically catalyzing oxygen reduction: Synergistic plasmonic effects to alter reaction toward 4-electron pathway. S. Lin

**10:10 ENFL 261.** Solar-driven waste-to-fuels: Rational design of a hybrid photoelectrochemical reactor. J. Radich, R. Zhao

#### 10:30 Intermission.

**10:40 ENFL 262.** GUITAR: A new carbon allotrope and application in ultracapacitors. I.F. Cheng, H. Zhu, I. Gyan, J. Foutch

**11:10 ENFL 263.** Study of nanoparticle formation in zeolites using simultaneous pair distribution function & infrared spectroscopy measurements. T.M. Nenoff, H. Zhao, K.A. Beyer, M. Newton, K. Chapman, P. Chupas

**11:40 ENFL 264.** Morphology and atomic structures of gold on ceria nanostructures: The role of surface structure and oxidation state of ceria supports. Y. Lin, Z. Wu, J. Wen, K. Ding, K.R. Poeppelmeier, L. Marks

**12:10 ENFL 265.** Controlling the active sites of sulfur-doped carbon nanotube-graphene nanolobes for highly efficient oxygen evolution and -reduction catalysis. A. El-Sawy, I.M. Mosa, D. Su, C.J. Guild, S. Khalid, R. Joesten, J.F. Rusling, S.L. Suib

## Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

### Microbial Processes & Treatment

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

### Computational Chemistry Across Catalysis

#### Electrocatalysis & Photocatalysis

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

#### Condensed Phase Catalysis

Sponsored by CATL, Cosponsored by ENFL

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:

[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## TUESDAY AFTERNOON

## Section A

Wyndham San Diego Bayfront  
Porthole

## Batteries &amp; Supercapacitors

## Electrolytes &amp; Interface

J. Guo, X. Ji, X. Li, *Organizers*

H. Xiong, K. Xu, *Organizers, Presiding*

## 1:30 Introductory Remarks.

**1:35 ENFL 266.** Effectively suppressing dissolution of manganese from spinel lithium manganate via nanoscale surface-doping approach. J. Lu, C. Zhan, X. Qiu, K. Amine

**2:05 ENFL 267.** *In silico* screening and rank-order of electrolytes for Li-ion batteries and beyond. G. Kamath, H. Xiong, S. Sankaranarayanan

**2:35 ENFL 268.** Lithium-ion solvation and intercalation at anode-electrolyte interface from first principles. M. Ong, V. Lordi, E. Draeger, J. Pask

**2:55 ENFL 269.** Synthesis and characterization of bis(tetrahydrofurfuryl) ether, a novel electrochemical solvent. P.A. Goodman, J. Stenger-Smith, A. Chafin, L. Baldwin

## 3:15 Intermission.

**3:30 ENFL 270.** Design solid electrolyte materials with enhanced stability and ionic conductivity using first-principles computation. Y. Mo

**4:00 ENFL 271.** Understanding ionic interactions and dynamics in battery electrolytes with multinuclear NMR spectroscopy. M. Gobet, J. Peng, S. Greenbaum

**4:30 ENFL 272.** Understanding chemical stability in size-selective membranes cast from polymers of intrinsic microporosity. S.E. Doris, A. Ward, P.D. Frischmann, B. Helms

**4:50 ENFL 273.** Effect of copolymer composition on performance of poly(3-hexylthiophene)-b-poly(ethylene oxide) (P3HT-b-PEO) block copolymers in lithium batteries. M.P. Bhatt

## Section B

Wyndham San Diego Bayfront  
Pacific C

## ENFL Distinguished Researcher Award: Symposium in honor of Stu Soled

## Other

E. Iglesia, J. G. Santiesteban, *Organizers*

Y. Du, *Presiding*

**1:30 ENFL 274.** Factors that affect olefin hydrogenation in supported single-site tetrairidium cluster catalysts. A.S. Katz

**2:00 ENFL 275.** On the reaction mechanism and the nature of the active site for standard, selective catalytic reduction of NO<sub>x</sub> on Cu/SSZ-13 zeolites. F. Ribeiro, N. Delgass, R. Gounder, J.T. Miller, W.F. Schneider, A. Yezzerets, A.A. Parekh, C. Paolucci, I. Khurana, J. Albarracin, J.R. Di Iorio, A. Shih

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**2:30 ENFL 276.** Rectifying the chemisorption-XRD particle size discrepancy: The roles of residual chloride and carbon decoration. R. Banerjee, J. Tengco, J.R. Regalbuto

## 3:00 Intermission.

**3:15 ENFL 277.** Reaction pathways in the reductive catalytic cleavage of aryl ethers. J. He, D. Mei, E. Barath, J.A. Lercher

**3:45 ENFL 278.** Importance of site-selectivity in zeolite catalysts: A resurgence in interest in small pore zeolites. S.I. Zones

**4:15 ENFL 279.** Heterogeneous tetrahedral Sn oxo center catalyst. H. Kung, M. Kung, E. Beletskiy

## 4:45 Concluding Remarks.

## Section C

Wyndham San Diego Bayfront  
Pacific D

## Application of Computational Chemistry for Energy &amp; Fuel Production

## Computational Catalysis in Research

*Cosponsored by CATL*

L. Wang, *Organizer*

Y. Chen, H. Xin, *Organizers, Presiding*

**1:30 ENFL 280.** Aligning electrochemical energy levels at metal/water interfaces using DFTMD. J. Le, M. Iannuzzi, A. Cuesta, J. Cheng

**2:00 ENFL 281.** On the way toward efficient perovskite photovoltaics. S. Tretiak

**2:30 ENFL 282.** Electron dynamics of large systems from real-time TDDFTB. B.M. Wong, M. Oviedo, N. Ilavre

**3:00 ENFL 283.** Modelling environment-induced electronic processes. V. Vaissier, M. Mavros, T.A. Van Voorhis

## 3:20 Intermission.

**3:30 ENFL 284.** Detailed reaction mechanisms for oxygen-reduction and CO<sub>2</sub>-reduction reactions at electrode surfaces. W.A. Goddard, T. Cheng, H. Xiao

**4:00 ENFL 285.** Ligand structure of passivated quantum dots. N. Geva, J.J. Shepherd, T.A. Van Voorhis

**4:30 ENFL 286.** Excited-state dynamics at nanoscale interfaces for solar light harvesting. O.V. Prezhdo

**5:00 ENFL 287.** Non-adiabatic energy dissipation in dissociation on catalytic surface. M. Montemore, R.A. Hoyt, E. Kaziras

## Section D

Wyndham San Diego Bayfront  
Pacific A

## Novel Materials for Energy &amp; Fuels

## Heterogeneous Catalytic Materials

X. Wang, X. Xu, Y. Yang, *Organizers, Presiding*

## 1:30 Introductory Remarks.

**1:35 ENFL 288.** Effect of contact time, reaction temperature, and reactant pressure on reaction sequences: The case of guaiacol hydrodeoxygenation on Ni phosphide catalysts. S.T. Oyama, P. Yang, A. Takagaki, R. Kikuchi

**2:05 ENFL 289.** Dry reforming over doped Ni-based pyrochlores. J.J. Spivey, N. Kumar

**2:35 ENFL 290.** Promoter effects on Pt/TiO<sub>2</sub> for highly effective hydrodeoxygenation of guaiacol. Z. He, M. Hu, X. Wang

**2:55 ENFL 291.** Mechanistic insights of ethanol steam-reforming over Ni-CeO<sub>x</sub>(111): The importance of hydroxyl groups for suppressing coke formation. Z. Liu, T. Duchon, H. Wang, E.W. Peterson, Y. Zhou, J. Rodriguez

## 3:15 Intermission.

**3:30 ENFL 292.** Metal-insulator-metal (MIM) structures for CO<sub>2</sub> activation. H. Freund

**4:00 ENFL 293.** Study of nickel-based catalysts in steam reforming of tar using simulated toluene as a model compound in hot-gas cleanup of syngas. T. Ahmed

**4:20 ENFL 294.** Design of the catalysts containing both microporous zeolite and mesoporous materials for the hydrorefining of gasoline and diesel fuel. Z. Zhao, A. Duan, H. Wu, T. Li, D. Zhang, Q. Huo

**4:50 ENFL 295.** Phosphate-promoted hydrogen evolution reaction on copper. Z. Xu, J. Zhao

## Section E

Wyndham San Diego Bayfront  
Harborside

CO<sub>2</sub> Conversion & Utilization

## Electroreduction

*Cosponsored by CATL*

E. J. Biddinger, H. Lin, *Organizers, Presiding*

## 1:30 Introductory Remarks.

**1:35 ENFL 296.** Cathode and anode catalysts for efficient electroreduction of CO<sub>2</sub>. P.J. Kenis

**2:15 ENFL 297.** Efficient electrochemical conversion of CO<sub>2</sub> to ethylene and ethanol in an alkaline electrolyzer. S. Ma, M. Sadakiyo, M. Yamauchi, P.J. Kenis

**2:40 ENFL 298.** Poly(4-vinylpyridine) as a new platform for robust CO<sub>2</sub> electroreduction. I. Chernyshova, S. Ponnurangam, C. Yun, P. Somasundaran

**3:05 ENFL 299.** Pd-catalyzed electrohydrogenation of CO<sub>2</sub> to formate with high conversion rates and low overpotential. X. Min, M. Kanan

## 3:30 Intermission.

**3:45 ENFL 300.** *In-operando* optical studies of CO<sub>2</sub> electrolysis. S.N. Qadri, J. Kirtley, D.A. Steinhurst, J. Owrutsky

**4:10 ENFL 301.** Electrochemically augmented biosynthetic platform of CO<sub>2</sub> fixation. C. Liu, B.C. Colon, P.A. Silver, D.G. Nocera

**4:35 ENFL 302.** Mechanistic study of the electro-carboxylation of alkenes. S.N. Steinmann, C. Michel, R. Schwiedernoch, M. Wu, P. Sautet

**5:00 ENFL 303.** Calculations of electrochemical reduction of CO<sub>2</sub> to methane and the competing H<sub>2</sub> formation. J. Hussain, H. Jonsson, E. Skulason

## Section F

Wyndham San Diego Bayfront  
Pacific B

## Nanomaterials for Energy Conversion &amp; Storage

## Energy Storage: Synthesis/Characterization

*Cosponsored by CATL*

Z. Wu, *Organizer*

Y. Lee, H. Zhao, *Organizers, Presiding*

**1:30 ENFL 304.** Accelerating materials discovery with hard x-ray tools. P. Chupas, N. Bechtold, K.W. Chapman

**2:00 ENFL 305.** 2D nanosheet-based photocatalysts efficient for visible light-induced H<sub>2</sub> and O<sub>2</sub> production. S. Hwang

**2:30 ENFL 306.** Metal oxide-carbon network structure for lithium-ion battery electrodes. H. Luo

**2:50 ENFL 307.** Graphene-based assemblies for efficient lithium storage. H. Yen, H. Tsai, A. Chen, G. Wu, H. Wang

**3:10 ENFL 308.** Redox mediators control electrodeposition of Li<sub>2</sub>S in lithium-sulfur batteries. L.C. Gerber, P.D. Frischmann, F. Fan, S. Doris, X. Qu, A. Scheuermann, K. Persson, Y. Chiang, B. Helms

## 3:30 Intermission.

**3:40 ENFL 309.** Engineering platinum-alloy electrocatalysts in nanoscale for PEMFC application. T. He

**4:10 ENFL 310.** Block copolymer-directed functional-ordered, mesoporous materials for energy devices: From functional materials to hierarchical materials. J. Lee

**4:40 ENFL 311.** Probing surface structural and chemical evolution at the atomic scale in bi-metallic catalysts using *in situ* STEM. M. Chi, C. Wang, G. Wang, K. More

**5:10 ENFL 312.** Silver-, gold-, and bi-metallic-nanoclusters for photoelectrochemical revolution and photovoltaics. W. Fan

## Computational Chemistry Across Catalysis

## From Metallic Nanoparticles to Isolated Metal Active Site

*Sponsored by CATL, Cosponsored by COMP, ENFL and WCC*

## Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Sponsored by CATL, Cosponsored by ENFL*

## WEDNESDAY MORNING

## Section A

Wyndham San Diego Bayfront  
Porthole

## Batteries &amp; Supercapacitors

## Beyond Li-Ion: Li-S &amp; Na-Ion Batteries

X. Li, H. Xiong, K. Xu, *Organizers*

J. Guo, X. Ji, *Organizers, Presiding*

## 8:30 Introductory Remarks.

**8:35 ENFL 313.** Sulfides for Li-ion batteries and beyond Li-ion batteries. C. Wang

**9:05 ENFL 314.** Comprehensive approach to produce industrially relevant lithium-sulfur cathodes. H. Su, J. Guo

**9:25 ENFL 315.** Ternary hybrid material structures for high-performance lithium-sulfur batteries. H. Wang

**9:45 ENFL 316.** Withdrawn.

**10:05 ENFL 317.** Molecular level understanding of reactivity of lithium polysulfides with ether solvents from first principles. R. Surendran Assary

## 10:25 Intermission.

**10:40 ENFL 318.** Development of stable, intermetallic alloy anodes for Li-ion/Na-ion batteries. D. Wang

**11:10 ENFL 319.** Lithiation-delithiation mechanism of covalently bonded sulfur. C. Fu, J. Guo

**11:30 ENFL 320.** Sodiation mechanisms in Si, Ge, and Sn for Na-ion battery anodes: A first-principles study. C. Chou, M. Lee, G.S. Hwang

**11:50 ENFL 321.** Nanoporous MoS<sub>2</sub> as an electrode material exhibiting high levels of pseudocapacitive charge storage with both Li and Na-ions. **J.B. Cook**, H. Kim, Y. Yan, J. Ko, B. Dunn, S.H. Tolbert

## Section B

Wyndham San Diego Bayfront  
Pacific C

### In Situ & Operando Characterization & Modelling of Reaction Kinetics

#### In Situ Studies, Oxidation & Gold Catalysts

Cosponsored by CATL

J. J. Bravo-Suarez, F. Tao, Y. Yang, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 322.** Efficient manufacturing, better industrial catalysts: Shifting the focus to composition/kinetics. **A.M. Gaffney**

**9:15 ENFL 323.** Unraveling the dynamics of surface- and bulk-phase transition of Pt-based, bi-metallic clusters and their kinetic consequences during oxidation catalysis. **J. Shangquan**, J. Howe, Y. Yang, W. Tu, D.D. Perovic, **Y. Chin**

**9:45 ENFL 324.** Liquid interfaces investigated by photoelectron spectroscopy. **H. Blumh**

**10:15 ENFL 325.** How stable are methanol species on oxide? A SSITKA study. **Y. Yang**, C. Mims, C.H. Peden, C.T. Campbell, J.H. Kwak

**10:35** Intermission.

**10:45 ENFL 326.** Catalyst and reactor engineering for carbon-neutral CO<sub>2</sub> conversion. **C. Matranga**, D. Kauffman, C. Wang, S. Hammache

**11:25 ENFL 327.** Understanding CO oxidation and PROX over supported Au catalysts. **J. Saavedra**, H. Doan, C.J. Pursell, L. Grabow, **B.D. Chandler**

**11:55 ENFL 328.** Catalytic role of ligands in supported Au<sub>n</sub>P<sub>m</sub> nanoclusters for gas phase reactions. **Z. Wu**

**12:25** Concluding Remarks.

## Section C

Wyndham San Diego Bayfront  
Pacific D

### Application of Computational Chemistry for Energy & Fuel Production

#### Computational Catalysis in Research

Cosponsored by CATL

L. Wang, *Organizer*

Y. Chen, H. Xin, *Organizers, Presiding*

**8:30 ENFL 329.** First-principles investigations of aqueous phase CO<sub>2</sub> reduction by borohydrides. **M. Groenenboom**, J.A. Keith

**9:00 ENFL 330.** Ethanol electrooxidation mechanism based on new insights from PM-IRRAS and DFT studies on palladium. **E. Monyoch**, **S.N. Steinmann**, C. Michel, E. Baranova, T.K. Woo, P. Sautet

**9:30 ENFL 331.** Development of new semiconductors for water splitting and photovoltaic devices based on DFT computed properties. **T. Le Bahers**, P. Sautet, S. Melissen, K. Takanabe

**10:00 ENFL 332.** Withdrawn.

**10:30 ENFL 333.** Electronic structure theory applied to modeling catalysis of the CO<sub>2</sub>-reduction reaction for artificial light harvesting. **M. Cheng**, J. Goodpaster, A.T. Bell, **M.P. Head-Gordon**

**11:00 ENFL 334.** Theoretical investigation of the oxygen reduction reaction in Li-O<sub>2</sub> batteries. **W.C. McKee**, G. Dathar, W.A. Shelton, **Y. Xu**

**11:30 ENFL 335.** Design core-shell nanocatalysts for oxygen reduction reaction from first principles. **P. Liu**, W. An

**12:00 ENFL 336.** Computational design for active catalysts of oxygen evolution reactions in Li-O<sub>2</sub> batteries. **J. Liu**, J. Zhu, X. Ren

## Section D

Wyndham San Diego Bayfront  
Pacific A

### Novel Materials for Energy & Fuels

#### Biological Materials

X. Wang, X. Xu, Y. Yang, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 337.** Rational design of carbon/inorganic composite nanostructures for energy storage and conversion. **Z. Jin**, J. Liu

**9:05 ENFL 338.** Hybrid DNA-templated gold nanocluster enhances enzymatic electroreduction of oxygen. **S. Chakraborty**, S. Babanova, R.C. Rocha, K. Artyushkova, A. Desireddy, P.B. Atanassov, J.S. Martinez

**9:25 ENFL 339.** Evolutionary design of low-molecular weight organic anolyte materials for applications in non-aqueous redox flow batteries. **C.S. Sevon**

**9:45 ENFL 340.** Hybrid polymer-metal organic framework fibers for mercaptan removal from natural gas. **G. Chen**, C.W. Jones, W. Koros

**10:05** Intermission.

**10:20 ENFL 341.** Developing a biodegradable, photoluminescent hydrogel. **X. Xu**

**10:50 ENFL 342.** Cyclopentadiene-containing  $\pi$ -conjugated macromolecules: Structure/property correlations and comparisons to their aromatic congeners. **L. Chen**, K. Wang, S. Mahmood, **A. Pietrangelo**

**11:20 ENFL 343.** Highly dispersible, thermally stable core/shell proppants for subsurface stimulation. **C. Fernandez**, M. Endres, I. Childers, K. Carroll, C. Burns, A. Bonneville, B. Garcia, J. Moore

## Section E

Wyndham San Diego Bayfront  
Harborside

### CO<sub>2</sub> Conversion & Utilization

#### Conversion

Cosponsored by CATL

E. J. Biddinger, H. Lin, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 344.** Electrocatalytic reduction of carbon dioxide to organic oxygenates: From chemical concept to scaled-up electrochemistry. **A.B. Bocarsly**, J.L. White, J. Pander, M.F. Baruch, J. Kaczur, P. Majsztrik

**9:10 ENFL 345.** Design of Lewis pair-functionalized metal organic frameworks for CO<sub>2</sub> hydrogenation. **J. Ye**, K. Johnson

**9:35 ENFL 346.** Molecular electrocatalysts for the reduction of CO<sub>2</sub> and the effects of bioinspired, secondary-sphere interactions on mechanism. **C.P. Kubiak**, C.W. Machan, S.A. Chabolla

**10:00** Intermission.

**10:15 ENFL 347.** Catalytic reduction of CO<sub>2</sub> by renewable organo-hydrides. **C. Musgrave**, C. Lim, A.M. Holder, J.T. Hynes

**10:50 ENFL 348.** Bio-electrochemical reduction of carbon dioxide to formate in enzymatic fuel cells. **L. Zhang**, S.F. Li

**11:15 ENFL 349.** Bicarbonate hydrogenation by iron: How the choice of solvent can reverse the reaction. **R. Marcos**, L. Xue, R. Sanchez-De-Armas, **M. Ahlquist**

**11:40 ENFL 350.** Carbon dioxide utilization via carbonate-promoted C-H carboxylation. **A. Banerjee**, G. Dick, M. Kanan

**12:05 ENFL 351.** Acetic acid from CH<sub>4</sub> and CO<sub>2</sub> in a continuous, fixed-bed reactor over metal-supported catalysts. **A. Rabie**, R. Kulkarni, S. Lee, H. Choi, **S. Park**

## Section F

Wyndham San Diego Bayfront  
Pacific B

### Nanomaterials for Energy Conversion & Storage

#### Energy Storage: Computational/ Application

Cosponsored by CATL

Y. Lee, Z. Wu, H. Zhao, *Organizers, Presiding*

**8:30 ENFL 352.** Chemical stabilization and mechanism of hydrogen evolution reaction, 1T MoS<sub>2</sub>. **D. Jiang**

**9:00 ENFL 353.** Machine-learning-augmented chemisorption model for CO<sub>2</sub> electroreduction catalyst screening. **X. Ma**, Z. Li, L.E. Achenie, **H. Xin**

**9:30 ENFL 354.** On the influence of polarization effects in predicting the interfacial structure and capacitance of graphene-like electrodes in ionic liquids. **E. Paek**, A.J. Pak, G.S. Hwang

**9:50 ENFL 355.** Synthesis and characterization of highly dense Cu nanowires for electrocatalytic applications. **D. Raciti**, C. Wang

**10:10 ENFL 356.** Heterojunction of zinc Blende/Wurtzite in Zn<sub>1-x</sub>Cd<sub>x</sub>S solid solution for efficient solar hydrogen generation: X-ray absorption/diffraction spectroscopy approach. **Y. Hsu**, N. Suen, S. Hong, T. Chan, S. Chen, H. Chen

**10:30** Intermission.

**10:40 ENFL 357.** Introduction of defects to nano-sized MOS<sup>2</sup> using organic solvents. **H. Zhang**, **Y. Zheng**

**11:10 ENFL 358.** Tuning catalytic selectivity on metal oxide through doping nonmetallic atoms. **F. Tao**, J. Liu, S. Zhang, D. Jiang, J. Fan

**11:40 ENFL 359.** Method for preparing cobalt nanoparticles supported on porous carbon for effective, adsorptive desulfurization. **T.A. Saleh**, K.R. Alhooshani, S.A. Al-Hammadi, A.A. Al-Shaikh

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Water Use & Reuse

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Computational Chemistry Across Catalysis

#### From Heterogeneous to Homogeneous Catalysis

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Materials Genome & Materials Informatics

Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY

#### Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

Sponsored by CATL, Cosponsored by ENFL

## WEDNESDAY AFTERNOON

### Section A

Wyndham San Diego Bayfront  
Porthole

#### Batteries & Supercapacitors

#### Beyond Li-Ion: Mg-Ion, Redox Flow, K-Ion & Li-Air

J. Guo, X. Ji, H. Xiong, *Organizers*

X. Li, K. Xu, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 ENFL 360.** Development of electrodes for vanadium redox flow battery at Pacific Northwest National Laboratory. **B. Li**, Z. Nie, X. Wei, J. Kizewski, W. Duan, E. Thomsen, J. Liu, W. Wang, D. Reed, V. Sprenkle

**2:05 ENFL 361.** Confession of Mg battery. **J. Muldoon**, C.B. Bucur, A.I. Lita

**2:35 ENFL 362.** Codependence of Mg and Al speciation in advanced Mg electrolytes: Identifying the active complexes in the MACC electrolyte. **K.A. See**, K.W. Chapman, L. Zhu, K.W. Wladerek, O. Borkiewicz, C.J. Barile, P.J. Chupas, A.A. Gewirth

**2:55 ENFL 363.** Halide-free electrolyte for rechargeable Mg batteries with wide electrochemical window. **O. Tutusaus**, R. Mohtadi, T. Arthur, F. Mizuno, E. Nelson, Y. Sevryugina

**3:15** Intermission.

**3:30 ENFL 364.** One electron at a time: Rechargeable K-O<sub>2</sub> and K-ion-O<sub>2</sub> batteries. **Y. Wu**

**4:00 ENFL 365.** X-ray absorption spectroscopy: Exploring batteries at APS beamline 9-BM. **T. Wu**

**4:30 ENFL 366.** Aqueous energy storage utilizing layered vanadium pentoxide electrodes with high-specific capacity in a KCl electrolyte. **D. Charles**, X. Shan, M. Feygenson, W. Xu, D. Su, X. Teng

**4:50 ENFL 367.** Lithium-gas energy storage using ionic liquids. **F. Mizuno**, C. Roberts, N. Singh, K. Takechi, P.T. Fanson, T. Song, S. Seo, J.F. Brennecke

**5:10 ENFL 368.** Insight into the catalytic mechanism of bimetallic platinum-copper core-shell nanoparticles for nonaqueous oxygen evolution reaction in lithium-oxygen batteries. **L. Ma**, X. Luo, T. Wu, J. Lu, K. Amine

### Section B

Wyndham San Diego Bayfront  
Pacific C

### In Situ & Operando Characterization & Modelling of Reaction Kinetics

#### Microkinetics & Renewables

Cosponsored by CATL

J. J. Bravo-Suarez, F. Tao, Y. Yang, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 ENFL 369.** Lewis-Brønsted acid sites interplay on vanadia-based catalysts for  $\text{NH}_3\text{-SCR}$ : A combined operando, isotopic, and chemometric study on an integral monolithic reactor. S.B. Rasmussen, P. Bazin, R. Portela, P. Avila, S. Mossin, A. Godiksen, M. Daturi, **M.A. Banares**

**2:15 ENFL 370.** Computational investigation of Lewis acidity in metal-doped mesoporous silicates. **M. Caricato**, A. Biancardi

**2:45 ENFL 371.** Mechanistic insights into syngas conversion through first-principles-based microkinetics simulations. **E. Hensen**

**3:15 ENFL 372.** Structural mechanism study on Ni-Co dry reforming catalysts. **H. Zhao**, M. Shakouri, H. Wang, K. Chapman, P.J. Chupas

**3:45** Intermission.

**3:55 ENFL 373.** Speciation at liquid-solid interfaces in the processing of renewable fuels. D.C. Cantu, Y. Wang, Y. Yoon, V. Glezakou, R. Rousseau, **R.S. Weber**

**4:35 ENFL 374.** Effect of alkali metal ions on H- $\beta$  zeolite structure and their catalytic activity on transesterification of green seed canola (GSC) oil. **C. Barol**, A.K. Dalai

**5:05 ENFL 375.** Kinetic modeling of isothermal degradation of lignin under conventional pyrolysis and oxidative pyrolysis conditions. **M. Xu**, L. Khachatryan, J. Kibet, S. Lomnicki, H.B. Dellinger

**5:25** Concluding Remarks.

## Section C

Wyndham San Diego Bayfront  
Pacific D

### Application of Computational Chemistry for Energy & Fuel Production

#### Computational Catalysis in Research

*Cosponsored by CATL*

L. Wang, *Organizer*

Y. Chen, H. Xin, *Organizers, Presiding*

**1:30 ENFL 376.** Screening for activity and selectivity in small metal-based oxidation catalysts. S.L. Pellizzeri, L. Monteith, A. Samstag, C.T. Campbell, **R. Getman**

**2:00 ENFL 377.** Withdrawn.

**2:30 ENFL 378.** Withdrawn.

**3:00 ENFL 379.** Using high-quality, atomic point charges for metal-organic frameworks to enable high-throughput screening of materials for contaminant removal from methane. **D. Nazarian**, P. Ganesh, J. Camp, D. Sholl

**3:20** Intermission.

**3:30 ENFL 380.** Theoretical investigation of metal-organic frameworks for electrochemical device applications. **S. Patwardhan**, G.C. Schatz

**4:00 ENFL 381.** Combined catalytic conversion of  $\text{CH}_4$  and  $\text{CO}_2$  over doped ceria surface. **Y. Zhao**, X. Zhu, H. Wang, J. Han, **Q. Ge**

**4:30 ENFL 382.** Role of oxygen vacancies in the surface evolution of H at  $\text{CeO}_2(111)$ . **X. Wu**, X. Gong

**5:00 ENFL 383.** Computational catalyst design for selective methane oxidation using first-principles methods. **B. Liu**

## Section D

Wyndham San Diego Bayfront  
Pacific A

### Novel Materials for Energy & Fuels

#### Electrocatalysis & Battery Materials

X. Wang, X. Xu, Y. Yang, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 ENFL 384.** Synthesis of  $\text{Ni}_3\text{P}_4$  films and their use as electrocatalysts for the hydrogen and oxygen evolution reaction. **M. Ledendecker**, S. Krick-Calderón, C. Papp, H. Steinrueck, M. Antonietti, M. Shalom

**2:05 ENFL 385.** Towards rechargeable hydrogen battery for renewable energy storage. **H. Lin**

**2:35 ENFL 386.** Probing structures and porosity in novel nanostructured electrode materials. **Y. Mao**, K. Dokyoung, M.J. Sailor, **L. Wang**

**3:05 ENFL 387.** Highly efficient storage of high-frequency pulse energy in  $\text{Li}_3\text{V}_2(\text{PO}_4)_3/\text{C}$  cathode Li-ion batteries. **G. Cao**, X. Nan

**3:35** Intermission.

**3:50 ENFL 388.** Relevant influence of calcium precursors on  $\text{CO}_2$  capture performance of coal fly ash stabilized, CaO-based sorbents. **F. Yan**, J. Jiang

**4:20 ENFL 389.** Material degradation problems with metallic electrodes in microbial, electrochemical technologies. **K. Chilkoor Gopala**, N. Shrestha, S. Star, V.R. Gadhamshetty

**4:40 ENFL 390.** Surface-charge-enabled photolytic hydrogen generation in nanocorjugates. **S. Varghese**, C. Walgama, M. Wilkins, S. Krishnan, **A. Kalkan**

**5:00** Concluding Remarks.

## Section E

Wyndham San Diego Bayfront  
Harborside

### $\text{CO}_2$ Conversion & Utilization

#### Photoconversion

*Cosponsored by CATL*

E. J. Biddinger, H. Lin, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 ENFL 391.** Iron<sup>II</sup> porphyrins as catalysts of the  $\text{CO}_2$ -to- $\text{CO}$  electrochemical conversion: An illustration of current issues in molecular catalysis. **J. Saveant**, I. Azcarate, C. Costentin, M. Robert, A. Tatin

**2:15 ENFL 392.** Withdrawn.

**2:40 ENFL 393.** Visible light photocatalytic  $\text{CO}_2$  conversion. **Y.H. Hu**

**3:20** Intermission.

**3:35 ENFL 394.** Solar energy utilization in the direct photocarboxylation of 2,3-dihydrofuran using  $\text{CO}_2$ . **A. Dibenedetto**, T. Baran, M. Aresta, S. Szymon Wojtyla, W. Macyk

**4:00 ENFL 395.** How do surface reconstructions affect  $\text{CO}_2$  reduction over GaP, CdTe, and  $\text{CuInS}_2$  photoelectrodes? **T. Sentle**, E.A. Carter

**4:25 ENFL 396.** 3D-ordered, macroporous  $\text{TiO}_2$ -supported Pt@CdS core-shell nanoparticles for efficient, photocatalytic  $\text{CO}_2$  conversion. **J. Jiao**, Y. Wei, Z. Zhao, J. Liu, A. Duan, G. Jiang

**4:50 ENFL 397.** Optimization of photocatalytic conversion of  $\text{CO}_2$  into fuels: Dependence on reductant ( $\text{water}/\text{H}_2$ ), pressure, and thickness of photocatalysts. **S. Kawamura**, H. Zhang, **Y. Izumi**

## Section F

Wyndham San Diego Bayfront  
Pacific B

### George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in honor of Mieczyslaw M. Boduszynski

*Cosponsored by CATL*

R. Malhotra, C. E. Rechsteiner, R. P. Rodgers, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:45 ENFL 398. Award Address** (George A. Olah Award in Hydrocarbon or Petroleum Chemistry sponsored by the (George A. Olah Award in Hydrocarbon or Petroleum Chemistry sponsored by the George A. Olah Award Endowment). Molecular composition of petroleum: The continuity model. **M.M. Boduszynski**

**2:15 ENFL 399.** Attainable product-yield distribution curve: A roadmap to crude oil composition. **C.E. Rechsteiner**, M.M. Boduszynski

**2:45 ENFL 400.** Advances in instrumentation and data reduction for characterization of petroleum crude oil by Fourier transform ion cyclotron resonance mass spectrometry. **A.G. Marshall**, Y. Corilo, C. Enke, C.L. Hendrickson, N.K. Kaiser, L.C. Krajewski, D.F. Smith, R.P. Rodgers

**3:15 ENFL 401.** Petroleomics: Applications of targeted analysis for heteroatom chemistries. **R.P. Rodgers**, A.G. Marshall, D.C. Podgorski, V. Lobodin, S. Rowland, P. Lalli, J. Putman, A. Clingenpeel, J. Lu, W.K. Robbins

**3:45** Intermission.

**3:55 ENFL 402.** Ultra high-resolution mass spectrometry of abiogenic organic chemicals in olivine crystals from deep mantle. **R. Malhotra**, F. Freund, J. Mellon, R.P. Rodgers, U. Kamakolun

**4:25 ENFL 404.** Superior properties of oil sands derived crudes in refinery operation. **P. Rahimi**

**4:55 ENFL 403.** Extension of structure-oriented lumping to vacuum residua. **S. Jaffe**

**5:25** Concluding Remarks.

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Water Use & Reuse/Water Treatment

*Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC*

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Powering the Future: Novel Materials for Solar Cell Technologies

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

### Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Sponsored by CATL, Cosponsored by ENFL*

## THURSDAY MORNING

### Section A

Wyndham San Diego Bayfront  
Porthole

### Batteries & Supercapacitors

#### Supercapacitors

J. Guo, H. Xiong, K. Xu, *Organizers*

X. Ji, X. Li, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 405.** Brick-and-mortar self-assembly synthesis of electrode architectures. **S. Dai**

**9:05 ENFL 406.** Development of pseudocapacitance in nanosized  $\text{MoO}_3$ . **H. Kim**, J.B. Cook, S.H. Tolbert, **B. Dunn**

**9:35 ENFL 407.** Graphene-dichalcogenide-based electrodes for supercapacitors. **A. Gigot**, R. Giardi, M. Fontana, M. Castellino, M. Serrapede, S. Bianco, A. Lamberti, S.L. Marasso, S. Marco, C.F. Pirri, E. Tresso, P. Rivolo

**9:55 ENFL 408.** Supercapacitor electrodes with high-volumetric capacitance and outstanding stability using ligand exchange-induced, multi-stacking of high-energy CNT hybrids and conductive CNTs. **S. Dongyeeb**, J. Cho

**10:15** Intermission.

**10:25 ENFL 409.** Understanding pseudocapacitive charge storage in transition metal oxides from fundamental interfacial processes to 3D electrode design. **J.W. Long**, M.B. Sassin, C.N. Chervin, J.M. Wallace, D.R. Rolison

**10:55 ENFL 410.** Using nanoporous materials for fast and stable electrochemical energy storage. **S.H. Tolbert**

**11:25 ENFL 411.** Understanding capacitive energy storage. **D. Jiang**

**11:55 ENFL 412.** Electrochemical capacitors: Renewable materials and fabrication strategies for potential AC line-filtering. **U. Graham**, C.R. Swartz, S.M. Lipka

### Section B

Wyndham San Diego Bayfront  
Pacific C

### In Situ & Operando Characterization & Modelling of Reaction Kinetics

#### In Situ Techniques & Electrocatalysis

*Cosponsored by CATL*

J. J. Bravo-Suarez, F. Tao, Y. Yang, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ENFL 413.** Observation of structures of catalysts through *in-situ* microscopy. **F. Tao**, L.T. Nguyen, **S. Zhang**

**9:15 ENFL 414.** Response of the atomic structure of copper surfaces to reactant molecules at ambient pressures. **B. Eren**

**9:45 ENFL 415.** Combined, in situ XAFS and XRD study of terbium-doped fibrous alumina. **K. Bando**, T. Kodaira, E. Kobayashi, T. Okajima, N. Nagai, F. Mizukami

**10:15 ENFL 416.** *In situ* modeling of reaction pathways and kinetics at a sliding, solid-solid interface. **H. Adams**, A. Martini, **W.T. Tysoe**

**10:35** Intermission.

**10:45 ENFL 417.** *In situ* XAFS and XPS for various electrochemical processes at solid/liquid interfaces. **T. Masuda**, K. Uosaki

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**11:25 ENFL 418.** Cocatalyst for overall water splitting: Its function by electrochemical investigation. A.T. Garcia-Esparza, D. Sokaras, T. Weng, D. Nordlund, K. Takanabe

**12:05 ENFL 419.** *In-operando*, optical investigations of carbon gasification by steam in solid oxide fuel cells. J. Kirtley, S.N. Qadri, D.A. Steinhurst, J. Owrutsky

**12:25** Concluding Remarks.

## Section C

Wyndham San Diego Bayfront  
Pacific D

### Application of Computational Chemistry for Energy & Fuel Production

#### Computational Catalysis in Research

*Cosponsored by CATL*

L. Wang, *Organizer*

Y. Chen, H. Xin, *Organizers, Presiding*

**8:30 ENFL 420.** Fundamental insights into catalytic conversion of lignin-derived model ether compound over supported transition metal catalysts. D. Mei, J. He, J.A. Lercher

**9:00 ENFL 421.** Density functional theory study of aldol condensation reactions between acetone and biomass-derived aldehydes in delta clusters of HZSM-5. A.N. Migués, S. Vaitheeswaran, A.N. Muskat, W. Sherman, S.M. Auerbach

**9:30 ENFL 422.** Coking wastewater treatment via supercritical water: ReaxFF-reactive molecular dynamics simulation. Y. Han, D. Jiang, J. Zhang, W. Li, M. Zhang

**10:00 ENFL 423.** First-principles reaction engineering at the solid-liquid interface. B. Wang, R. Bababrik, Z. Zhao, A. Avolian, A. Rozenblit, D.E. Resasco

**10:30 ENFL 424.** Insights into energy-efficient gas separation. D. Jiang

**11:00 ENFL 425.** Computational modeling insights into the competing chemical and solvation interactions that control the process of non-aqueous extraction of bitumen from oil sands. S.R. Stoyanov, Y. Xu, A. Kovalenko, T. Dabros

**11:30 ENFL 426.** Scalable algorithms in automatic mechanism generation for complex fuel systems. N. Vandewiele, K. Han, W.H. Green

**12:00 ENFL 427.** Water on graphene: Friction and diffusion from molecular simulations. A. Michaelides

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Modeling

*Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC*

#### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: The Future of Spectroscopies: Quantum & Classical Fields; Theoretical Perspectives

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

#### Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Sponsored by CATL, Cosponsored by ENFL*

## THURSDAY AFTERNOON

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Regulatory Aspects

*Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC*

#### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Exciting Aspects of Excitation Dynamics & Dissociation at the Nanoscale

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

#### Fischer-Tropsch Catalysis: From Fundamentals to Industrial Practice

*Sponsored by CATL, Cosponsored by ENFL*

## ENVR

### Division of Environmental Chemistry

S. Al-Abed, *Program Chair*

#### OTHER SYMPOSIA OF INTEREST:

**Functional Lignocelluloses & Nanotechnology** (see CELL, Sun, Mon, Tue, Wed)

**Basic Research in Colloids, Surfactants & Nanomaterials** (see COLL, Sun, Mon, Tue, Wed, Thu)

**Geochemical Reactivity of Nanoparticles, Aggregates, Coatings & Organo-Nanoparticle Flocculates** (see GEOC, Sun, Wed)

**Nanomaterials for Energy Conversion & Storage** (see ENFL, Mon, Tue, Wed)

**Chemistry of Materials: Nanomaterials** (see INOR, Sun, Wed, Thu)

**Applied Nanotechnology for Food & Agriculture** (see AGFD, Tue)

#### SOCIAL EVENTS:

**Reception, 6:30 PM:** Tue

#### BUSINESS MEETINGS:

**Program Planning Meeting, 2:00 PM:** Sun

**Long Range Planning Meeting, 3:00 PM:** Sun

**Executive Committee Meeting, 7:00 PM:** Sun

## SUNDAY MORNING

### Section A

Omni San Diego Hotel  
Grand Ballroom C

#### Characterization & Toxicity of Airborne Particulate Matters (PMs) in East Asia

S. L. Simonich, *Organizer*

X. Li, S. Tao, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 ENVR 1.** Silicon stable isotopes as a tracer for atmospheric fine particulate matters. G. Jiang, Q. Liu, D. Lu

**8:35 ENVR 2.** Effects of particulate matter from different sources: An *in vitro* study. W. Jin, S. Su, B. Wang, S. Tao

**9:05 ENVR 3.** Essential approaches to investigation on chemical origins of proinflammatory components of diesel exhaust and wood smoke particulate matter. A. Kubatova, K. Ondrusova, R. Cochran, J. Rousova, A. Totlandsdal, J. Øvrevik, P. Schwarze, M. Lag

**9:30 ENVR 4.** Dissolved black carbon released from biochar: Structural characterization and potential environmental impacts. X. Qu, H. Fu, B. Wang, D. Zhu

**9:55** Intermission.

**10:15 ENVR 5.** Multi-pollutants emitted from major agricultural residues burning and the impact on air quality in China. C. Li, J. Chen, Z. Ma, D. Donaldson

**10:40 ENVR 6.** Identification of potentially aerosolized nanoparticles in road dust from Shanghai. M.E. Vance, A.J. Tiwari, F. Tou, Y. Yang

**11:05 ENVR 7.** Mercury stable isotope compositions in airborne particulate matters in remote areas of China. X. Fu, H. Zhang, X. Yang, L. Ming, X. Li, X. Feng

**11:30 ENVR 8.** Evaluation of China's mercury emission controls in the coal-fired power industry: Projection for the health and welfare effects in East Asia. W. Zhang, G. Zhen, L. Chen, X. Ye, H. Wang, X. Wang

### Section B

Omni San Diego Hotel  
Grand Ballroom E

#### New Challenges on Metals & Metalloids: Chemistry, Treatment & the Impacts on Water Quality

#### Hexavalent Chromium Removal

D. Giammar, *Organizer*

H. Liu, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:10 ENVR 9.** Reductive immobilization of hexavalent chromium by polysulfide-reduced lepidocrocite. B. Deng, M. Shi, J.S. Zheng

**8:30 ENVR 10.** Effect of humic acid on Cr(VI) removal from water by electrocoagulation. C. Pan, L. Troyer, P. Liao, J.G. Catalano, D. Giammar

**8:50 ENVR 11.** Reduction of Cr(VI) mediated by zero-valent magnesium (ZVMg) in water at pH 7. G. Lee

**9:10 ENVR 12.** Development and application of highly reductive TiO<sub>2</sub> photocatalyst for hexavalent chromium removal. G. Chen, H. Liu

**9:30 ENVR 13.** Withdrawn.

**9:50** Intermission.

**10:05 ENVR 14.** Adsorption of chromium and copper on electrospun hematite mesoporous silica core shell nanomaterials. S.N. Egodawatte, D.M. Cwiertny, S.C. Larsen

**10:25 ENVR 15.** Adsorptive removal of multiple metal ions from contaminated water with EDTA functionalized superparamagnetic nanoparticles: Equilibrium, kinetics and thermodynamics. Y. Huang, A.A. Keller

**10:45 ENVR 16.** Bioprocesses for simultaneously removing hexavalent chromium and 1,4-dioxane. S. Zhang, S. Guo, P. Gedalanga, S. Mahendra

**11:05 ENVR 17.** Chromium toxicity to nitrifying bacteria: Implications for wastewater treatment. V. Kapoor, J. Santo Domingo

**11:25 ENVR 18.** Direct isotope dilution measurement of trace level Cr(VI) using ion chromatography tandem mass spectrometry. V.I. Furdui, S. Maedler, T. Switzer, F. Sun, C. Tat, R. Tooley, M. Pamuku, H.M. Kingston

### Section C

Omni San Diego Hotel  
Gaslamp 1

#### Detection of Engineered Nanomaterials in Environmentally Relevant Media

B. C. Nelson, *Organizer*

C. M. Sims, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 ENVR 19.** Trophic transfer of engineered nanoparticles in terrestrial food chains. J.C. White, A. Servin, R. De la Torre Roche, S. Majumdar, L. Pagano

**8:40 ENVR 20.** Size and chemistry of modified engineered nanomaterials in environmental and biological media: How different are the nanoparticles we are exposed to from their initial form? A.P. Ault, J. Axson, D. Stark, A. Bondy, J. Keeney, C. Sun, S. Capracotta, A. Maynard, I. Bergin, M. Philbert

**9:05 ENVR 21.** Facile separation, sizing, and quantitative analysis of engineered nanoparticles in an organism model using single particle ICP-MS. M. Johnson

**9:30** Intermission.

**9:45 ENVR 22.** Withdrawn.

**10:20 ENVR 23.** Measurements of silver ions and silver nanoparticles in biologically and environmentally relevant conditions. R.I. Maccuspie, E. Petersen, J. Zook, J. Gorham

**10:45 ENVR 24.** Low concentrations of silver nanoparticles stimulated biofilm development on various materials used for water distribution systems. Y. Yang, C. Yu, P.J. Alvarez

**11:10 ENVR 25.** Identifying the effects of size and shape on the physicochemical properties of cerium oxide nanoparticles. C.M. Sims, J. Gorham, T. Cho, I. Levin, V.A. Hackley, B.C. Nelson

### Section D

Omni San Diego Hotel  
Gaslamp 2

#### Sources, Fate & Transport of Perfluorinated Alkyl Substances in the Environment: Theory, Practice & Innovation

S. T. Kurwadkar, *Organizer*

D. Kempisty, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 ENVR 26.** Determination of manufacturing origin of PFOA in global precipitation samples using isomer-specific analysis. J. Johansson

**8:30 ENVR 27.** Scratching the surface of PFASs: An attempt at closing the mass balance using four techniques in select consumer products. A. Robel, J. Rewerts, J.A. Field, S.L. Simonich, G.F. Peaslee, C. Butt, T.F. Webster

**8:55 ENVR 28.** Sorption and desorption of perfluorinated compounds to sediments of an urban water body. M. Reinhard, H. Chen, Y. Shi, K. Gin

**9:20 ENVR 29.** Adsorption of traditional and emerging perfluoroalkyl substances by powdered activated carbon. M. Sun, L. Dudley, M. Strynar, A. Lindstrom, D. Knappe

**9:45** Intermission.

**10:10 ENVR 30.** First discovery of chlorinated perfluoroalkyl ether sulfonic acids (Cl PFAESs) in humans and estimation of elimination kinetics. Y. Shi, R. Vestergren, Z. Zhou, L. Xu, C. Li, Y. Liang, Y. Cai

**10:35 ENVR 31.** Rapid screening for volatile PFASs in textiles by in-vial extraction gas chromatography mass spectrometry. **J.N. Rewerts**, S.L. Simonich, J.A. Field

**11:00 ENVR 32.** Aerobic biodegradation of N-ethyl perfluorooctane sulfonamidoethanol (EtFOSE)-based surfactants in two contrasting soils. **L.S. Lee**, L. Zhang, J. Liu

**11:25 ENVR 33.** Perfluorinated alkyl acid degradation mechanisms probed by chemical computations. **D.J. Van Hooymissen**, Z. R. Smialek, C.P. Higgins, S. Vyas

## Section E

Omni San Diego Hotel  
Gaslamp 3

### Advances & Applications in Water Sensing Technologies for Drinking Water, Reuse, Agri-Tech & Research

*Cosponsored by AGFD*

M. E. Romero-Gonzalez, P. L. Schorr, M. Tamburri, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 ENVR 34.** Concentrating microorganisms in water samples by super-absorbent polymer beads. **X. Xie**, J. Bahnemann, S. Wang, Y. Yang, M.R. Hoffmann

**8:30 ENVR 35.** Real time monitoring for cyanobacteria during an algal bloom in August 2015 as recorded at USGS 01389005. **P.L. Schorr**, J.R. Yagovic

**8:55 ENVR 36.** Withdrawn.

**9:30 ENVR 37.** Evaluation of the QA/QC performance of recently developed low cost sensors for drinking water, surface water and wastewater compared to traditional laboratory techniques (DENVR). **M. Bowkett**

**9:55** Intermission.

**10:15 ENVR 38.** On-line monitoring of organic compounds as well as chlorophyll-a in drinking water production process using spectro-fluorometry. **C. Moldaenke**, A. Dahlhaus, M. Wagner, D. Lohse

**10:40 ENVR 39.** Measuring continuous concentration of mass pollutants in the aquatic environment. **M.E. Romero-Gonzalez**, P. Skipworth, N. Morley, T. Turton, E. Holdsworth, G. Chimonides, F. Hassani, F. Clayessens

**11:05 ENVR 40.** Low-cost free-chlorine sensor. **S. Pan**, M. Deen, R. Ghosh

**11:30** Panel Discussion.

## Section F

Omni San Diego Hotel  
Gaslamp 4

### Flue Gas Cleaning & Climate Control

#### General Papers & CO<sub>2</sub> Capture

A. Riisager, *Organizer*

R. Fehrmann, *Organizer, Presiding*

**8:00 ENVR 41.** Gas cleaning by ionic liquid absorbers. **R. Fehrmann**, A. Riisager, S. Mossin, P. Thomassen

**8:20 ENVR 42.** Use of chemical scrubbing agents and advanced oxidation processes in multi-component flue gas purification and treatment. **Y.G. Adewuyi**

**8:40 ENVR 43.** Analysis of pollutant emissions from elevated point sources in the 8-counties of the Houston-Galveston-Brazoria area during 2012 summer episode. **M. Shahriar**, **R.R. Kommalapati**, Z. Huque, **H. Du**

**9:00 ENVR 44.** Removal of CO<sub>2</sub>, water and VOCs by supported ionic liquids (SILP) for minimizing energy losses due to ventilation. **L. Schill**

**9:20 ENVR 45.** Advanced hybrid process, CAER-adCCS, for CO<sub>2</sub> removal from coal-derived flue gas. **C. Lippert**, L. Widger, M. Sarma, R.A. Frimpong, K. Liu

**9:40 ENVR 46.** Influence of dissolved metals on n-nitrosamine formation under amine-based CO<sub>2</sub> capture conditions. **Z. Wang**, W. Mitch

**10:00** Intermission.

**10:20 ENVR 47.** Development of passive polymer membranes for high flux carbon dioxide separation. **T. Hong**, S. Chatterjee, S. Lai, S.M. Mahurin, D. Jiang, B.K. Long, J.W. Mays, A.P. Sokolov, **T. Saito**

**10:40 ENVR 48.** PIM-1/poly(ethylene imine) composites as solution-processable molecular baskets for CO<sub>2</sub> capture from dilute streams. **S.H. Pang**, M. Jue, J. Leisen, C.W. Jones, R.P. Lively

**11:00 ENVR 49.** Polyvinylamine based solid adsorbents for CO<sub>2</sub> capture. **C. Sullivan**, E. Chou, D.A. Schiraldi, **H. Ghassemi**

**11:20 ENVR 50.** CO<sub>2</sub> removal from natural gas using N-modified silicate fiberglass materials. **B. Bal'zhinmaev**, E. Kovalyov

**11:40 ENVR 51.** Metal organic framework-mediated synthesis of oxide-derived Cu/carbons for the electrochemical reduction of CO<sub>2</sub>. **K. Zhao**, Y. Liu, X. Quan

### Analytical & Computational Isotope Geochemistry

*Sponsored by GEOC, Cosponsored by ENVR and MPPG#*

## SUNDAY AFTERNOON

### Section A

Omni San Diego Hotel  
Grand Ballroom C

#### Characterization & Toxicity of Airborne Particulate Matters (PMs) in East Asia

S. L. Simonich, *Organizer*

X. Li, S. Tao, *Organizers, Presiding*

**1:30 ENVR 52.** Toxicity of airborne particulate matter in urban China: Quantitative contribution of metals to mixture effects. **L. Jin**, L. Ming, J. Xie, X. Li

**2:00 ENVR 53.** Withdrawn.

**2:25 ENVR 54.** In situ visualization and quantitative investigation of the bioavailability of PAHs adsorbed onto micro-zone of particulate matter. **R. Li**, Y. Zhu, Y. Zhang

**2:50 ENVR 55.** Withdrawn.

**3:15** Intermission.

**3:30 ENVR 56.** Estimation of mass scattering efficiency in Hong Kong. **S. Lee**

**3:55 ENVR 57.** Toxic effects of indoor atmospheric fine particulate matter collected from allergic and non-allergic families in Wuhan on mouse peritoneal macrophages. **H. Guo**

**4:20 ENVR 58.** Old and emerging flame retardants in atmospheric fine particles in Chinese cities: Compositions, sources and spatio-temporal variation. **D. Liu**, K. Shen, J. Li, G. Zhang

**4:45 ENVR 59.** Design and formulation of antimicrobial system for particulate air filter. **J. Lee**, Y. Lai, W. Hui, K. Yeung

**5:10** Discussion.

**5:25** Concluding Remarks.

### Section B

Omni San Diego Hotel  
Grand Ballroom E

#### New Challenges on Metals & Metalloids: Chemistry, Treatment & the Impacts on Water Quality

#### Metals, Metalloids & Nanoparticles

H. Liu, *Organizer*

D. Giammar, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:40 ENVR 60.** Sequestration of antimony by zerovalent iron: Using weak magnetic field effects to enhance performance and characterize reaction mechanisms. **P.G. Tratnyek**, C. Xu, B. Zhang, L. Zhu

**2:00 ENVR 61.** Reduction of Sb(V) by coupled biotic and abiotic processes in sulfidogenic microcosms. **C.R. Johnson**, D.A. Antonopoulos, M. Boyanov, T. Flynn, J.C. Koval, K.M. Kemner, **E.J. O'Loughlin**

**2:20 ENVR 62.** Iron electrocoagulation for treatment of selenium in wastewater from flue gas desulfurization. **Y. Bae**, D. Giammar

**2:40 ENVR 63.** Enhanced arsenite removal during Fe(III)-based Oxidative Coagulation Treatment. **W. Yan**, Y. Li

**3:00 ENVR 64.** Mechanistic understanding of impact of hematite nanoparticle (na-Fe<sub>2</sub>O<sub>3</sub>) size and shape on sustainable aqueous inorganic remediation. **A.W. Lounsbury**, N. Billmyer, J. Yamani, D. Peak, J.B. Zimmerman

**3:20** Intermission.

**3:35 ENVR 65.** Aluminum hydroxide, fluoride, and NOM: Insights using infrared spectroscopy. **M. Bartolo**, L.E. Katz, S.C. Myneni, D. Lawler, I. Gee, J. Herrboldt

**3:55 ENVR 66.** Copper speciation in wastewater-impacted surface waters. **A. Mosbrucker**, J.A. Nason

**4:15 ENVR 67.** Oxidative transformation of bisphenol A in the presence of synthetic δ-MnO<sub>2</sub>. **S.J. Balgooyen**, B. Chhouk, C.K. Remucal, M.A. Ginder-Vogel

**4:35 ENVR 68.** Environmental performance of polyetherimide composites for mitigating the metallic corrosion of steel structures. **V.R. Gadhamshetty**, V. Upadhyayula

**4:55 ENVR 69.** Concentration-dependent aggregation of citrate coated Ag NPs induced by cystine. **K. Afshinnia**, I. Gibson, R.C. Merrifield, M. Baalousha

**5:15** Concluding Remarks.

### Section C

Omni San Diego Hotel  
Gaslamp 1

#### Detection of Engineered Nanomaterials in Environmentally Relevant Media

C. M. Sims, *Organizer*

B. C. Nelson, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 ENVR 70.** Liquid nebulization / differential mobility analysis approach for size, quantification, and chemical evaluation of engineered nanoparticles in environmental water matrices. **B. Mader**, M. Elfelson, S.T. Wolf, C. Loza, C. Chan

**2:10 ENVR 71.** *In vivo* bioprocessing of engineered nanoparticles after environmental uptake: Implications for health outcomes. **U.M. Graham**, A.K. Dozier, G. Oberdoerster, A. Elder, M.E. Birch

**2:35 ENVR 72.** Uptake and accumulation of TiO<sub>2</sub> nanoparticle in rice (*Oryza sativa* L.) plants with enhanced vegetative growth under long-term exposure. **Y. Deng**, E. Petersen, B.C. Nelson, B. Xing

**3:00 ENVR 73.** Quantification of carbonaceous nanomaterials in complex matrices. **T. Nosaka**, P.K. Westerhoff, P. Herckes

**3:25** Intermission.

**3:40 ENVR 74.** Detection and quantification of nanomaterial number concentration in environmentally relevant media by atomic force and electron microscopy. **M. Baalousha**

**4:15 ENVR 75.** Three-dimensional evaluation and visualization of AuNP transport in silicon-based micromodel with SERS and μ-CT. **M. Chan**, W. Leng, S.L. Walker, D. Borschneck, J. Rose, P.J. Vikesland

**4:40 ENVR 76.** Effects of zero-valent iron nanoparticles on plants: Uptake, translocation, physiological change and its implication. **H. Yoon**, J. Kim, Y. Kang, Y. Chang

**5:05 ENVR 77.** Development of gold-labeled titanium dioxide nanoparticles for tracking behavior in complex environmental matrices. **A. Deline**, J.A. Nason

## Section D

Omni San Diego Hotel  
Gaslamp 2

#### Sources, Fate & Transport of Perfluorinated Alkyl Substances in the Environment: Theory, Practice & Innovation

D. Kempisty, *Organizer*

S. T. Kurwadkar, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 ENVR 78.** Source characterisation of perfluoroalkyl substances (PFASs) in an Arctic remote lake system: Contaminant pattern evaluation in sediment and surface waters of lake Linnevatnet (Svalbard, European Arctic). **R. Kallenborn**, J.S. Skaar, S.M. Lunde, S. Axelsson, J. Rakovic, L. Ahrens

**2:00 ENVR 79.** Withdrawn.

**2:25 ENVR 80.** Development of a linear free-energy relationship for the reductive defluorination of perfluorooctanoic acid by zero-valent metals. **J. Blotvogel**, T. Borch

**2:50 ENVR 81.** Removing perfluoroalkyl acids from potable reuse systems using carbon adsorbents: Bench-scale and pilot testing. **M. Inyang**, E. Dickenson, M. Velarde

**3:15** Intermission.

**3:40 ENVR 82.** Environmental fate of per- and polyfluoroalkyl substances (PFASs) in wildlife at the former Wurtsmith Air Force base (WAFB). **R. Delaney**, D. Bogdan, D. Corsi, G.S. Fraley, G.F. Peaslee

**4:05 ENVR 83.** Conceptual site model for measurement of per- and polyfluoroalkyl substances (PFASs). **G.F. Peaslee**, **D. Bogdan**, R. Delaney, D. Corsi, D.M. Lunderberg, E.E. Ritter

**4:30 ENVR 84.** Degradation of perfluorooctane sulfonate by enzyme catalyzed oxidative humification reactions. **Q. Huang**, Q. Luo

**4:55 ENVR 85.** Effects of environmental factors on β-cyclodextrin-perfluorinated surfactant host-guest interactions. **M.J. Weiss**, K.E. O'Shea



## Section E

Omni San Diego Hotel  
Gaslamp 3

### Advances & Applications in Water Sensing Technologies for Drinking Water, Reuse, Agri-Tech & Research

Cosponsored by AGFD

M. E. Romero-Gonzalez, P. L. Schorr, M. Tamburri, *Organizers, Presiding*

#### 1:30 Introductory Remarks.

**1:35 ENVR 86.** Specialized field operational support involving chemical warfare agents (CWA) to the Hawaii undersea military munition assessment (HUMMA) projects. J.L. Schwarz

#### 2:00 ENVR 87. Withdrawn.

**2:25 ENVR 88.** Colorimetric nanoprobes for mycotoxin deoxynivalenol detection. W. Leng, H. Gruszewski, D. Schmale, P.J. Vikesland

**2:50 ENVR 89.** Extending SERS application to lower pH: A stable platform for environmental pollutants detection. H. Wei, P.J. Vikesland

#### 3:15 Intermission.

**3:35 ENVR 90.** Facilitating innovations in environmental monitoring technologies. M. Tamburri, B. Stauffer, T. Johengen

**4:10 ENVR 91.** Development of cost effective sensors for the in-situ monitoring of eutrophication in marine waters. M. McCaul, E. McNamara, D. Diamond

**4:35 ENVR 92.** Engineering analysis and management of water reuse through water quality sensing technology. P.L. Schorr, A. Salvesson

#### 5:00 Discussion and Concluding Remarks.

## Section F

Omni San Diego Hotel  
Gaslamp 4

### Flue Gas Cleaning & Climate Control

#### Removal of CO<sub>2</sub> & Other Pollutants: Characterization, Mechanisms & Models

R. Fehrmann, *Organizer*

A. Riisager, *Organizer, Presiding*

**1:30 ENVR 93.** Imidazole-2-thiones as liquid sorbents of Hg(0): Thermal behavior, redox chemistry, and loading on solid supports. S.P. Kelley, G.P. Rachiero, J. Wang, R.D. Rogers

**1:50 ENVR 94.** Advances in gas phase separation of NO<sub>x</sub> with supported ionic liquid phase using hollow silica spheres. P. Thomassen, S. Mossin, R. Fehrmann, S. Dai

**2:10 ENVR 95.** Effect of dopants on NH<sub>4</sub>NO<sub>3</sub> formation over vanadia-based SCR catalysts under fast-SCR conditions at 150° C. L. Schill

**2:30 ENVR 96.** In-situ EPR investigations of copper substituted zeolites for NH<sub>3</sub>-SCR. A. Godiksen, S.B. Rasmussen, L.F. Lundegaard, P.N. Vennestrom, S. Mossin

**2:50 ENVR 97.** Quantification of vanadium(IV) on SCR catalysts by operando electron paramagnetic resonance (EPR) spectroscopy. S. Mossin, A. Godiksen, M.H. Velk, S.B. Rasmussen

#### 3:10 ENVR 98. Withdrawn.

#### 3:30 Intermission.

**3:50 ENVR 99.** Reaction mechanisms of aqueous piperazine with carbon dioxide from first principles modeling. H. Stowe, E. Paek, G.S. Hwang

**4:10 ENVR 100.** GCMC simulations of nitrogen-doped hierarchical mesoporous carbon adsorbents for post-combustion CO<sub>2</sub> capture. P.C. Psarras, J. Wilcox

**4:30 ENVR 101.** Mechanistic investigations on CO<sub>2</sub> capture with new amino acid-based ionic liquids. A. Riisager, S. Shunmugavel, A.J. Kunov-Kruse, R. Fehrmann

**4:50 ENVR 102.** Disulfide-linked triazine based porous polymer networks for CO<sub>2</sub> capture. E. Goren, H. Cavusoglu, M. Yavuz

**5:10 ENVR 103.** Effect of rare earth doping on structural defects and redox properties of CeO<sub>2</sub>/ZrO<sub>2</sub> based catalyst materials probed by *in situ* Raman spectroscopy. C. Andriopoulou, A. Sgoura, K. Petalidou, A.M. Efsthathiou, S. Boghosian

## Environmental Interfaces

## Surface Structures

Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡

#### Analytical & Computational Isotope Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and MPPG‡

## MONDAY MORNING

## Section A

Omni San Diego Hotel  
Grand Ballroom C

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

## Environmental Chemistry/ Water Chemistry

Cosponsored by CEI, ENFL and GEOC

D. L. Drogos, R. Kleinberg, W. Orem, W. Stringfellow, *Organizers, Presiding*

#### 8:00 Introductory Remarks.

**8:10 ENVR 104.** Frac fluid chemistry overview. D.K. Durham

**8:30 ENVR 105.** Quantitative analysis chemicals used for hydraulic fracturing in California (USA). W.T. Stringfellow, M. Camarillo, J.K. Domen, C. Varadharajan, P.D. Jordan

**8:50 ENVR 106.** Organic substances from unconventional oil and gas production and potential for environmental impacts. W. Orem, M. Varonka, A. Bates, M. Engle, J.T. Kulongoski, T.J. Gallegos, I.M. Cozzarelli

**9:10 ENVR 107.** Acidizing oil wells: The chemicals and their impact. K. Abdullah, I.H. Suffet, T. Malloy

**9:30 ENVR 108.** Organic and inorganic characterization of injected hydraulic fracturing fluids and corresponding flowback. P. Piotrowski, E. Barth-Naftilan, J. Saiers, F.L. Dorman

#### 9:50 Intermission.

**10:10 ENVR 109.** Investigating the impacts of well age and fracturing fluid type on the quality and treatability of the produced water. P. Omur-Ozbek, S. Kim, K. Carlson

**10:30 ENVR 110.** Characterization and treatment of hydraulic fracturing wastewater over time from northeast Colorado. J. Rosenblum, K. Linden, M. Thurman, I. Ferrer, A. Nelson, I. Morrissey

**10:50 ENVR 111.** Identification of polyethylene and polypropylene glycols and their carboxylates in flowback and produced water from hydraulic fracturing using LC/QTOF-MS. E.M. Thurman, I. Ferrer, J. Rosenblum, K. Linden, J.N. Ryan

**11:10 ENVR 112.** Exploring the origin of radium in shale gas produced water. W. Fan, K.F. Hayes, B. Ellis

#### 11:30 Panel Discussion.

## Section B

Omni San Diego Hotel  
Gaslamp 2

#### Innovative Materials & Technologies for Water Purification

## Photochemical Process &amp; Desalination

Cosponsored by CEI

Financially supported by AEESP

E. L. Cates, B. P. Chaplin, J. Choe, D. Shuai, W. Zhang, *Organizers, Presiding*

#### 8:00 Introductory Remarks.

**8:05 ENVR 113.** Polychromatic light for nitrosamine control in recycled wastewater. D. McCurry, W. Mitch

**8:25 ENVR 114.** Development of radiocatalytic approaches towards water treatment. S. Sahu, T. Johnson, E.L. Cates

**8:45 ENVR 115.** Achieving sustainable water treatment: Graphitic carbon nitride for persistent waterborne contaminant removal with visible light irradiation. Q. Zheng

**9:05 ENVR 116.** Visible light degradation of orange ii using hybrid TiO<sub>2</sub> photocatalysts. B.D. Stewart, G. Li

#### 9:25 Intermission.

**9:40 ENVR 117.** Development and application of nanotube- and nanofiber-enabled water treatment technologies. D.M. Cwierny

**10:10 ENVR 118.** Mechanistic study of the physical, chemical, and mechanical properties of natural organic matter on photocatalytic membranes to understand fouling mitigation. R. Zhu, A. Diaz, S. Solares, D. Shuai

**10:30 ENVR 119.** Novel capacitive desalination process using battery materials. J. Lee, C. Kim, J. Yoon

**10:50 ENVR 120.** Membrane distillation with electrically conductive membranes for scale prevention during filtration of divalent salt solutions. Z. Hendren, D. Jassby, D. Bollinger, W. Duan, A. Dudchenko, Y. Choi

**11:10 ENVR 121.** Withdrawn.

#### 11:30 Concluding Remarks.

## Section C

Omni San Diego Hotel  
Grand Ballroom D

#### Treatment of Contaminants of Emerging Concern & Their Transformation Products

Cosponsored by CEI

L. M. Blaney, *Organizer*

A. J. Hernandez-Maldonado, *Organizer, Presiding*

#### 8:00 Introductory Remarks.

**8:05 ENVR 122.** Transformation of fluoroquinolone, tetracycline, and sulfonamide antibiotics at 253.7 nm: Generation of antimicrobially active transformation products. K. Mangalgiiri, H. Adejumo, D. Ocasio, K. He, L.M. Blaney

**8:30 ENVR 123.** Withdrawn.

**8:55 ENVR 124.** Degradation and debromination of bromophenols using zinc(II)-porphyrin complex as a photosensitizer under conditions of visible light irradiation. Q. Zhu, M. Igarashi, M. Sasaki, R. Kodama, M. Fukushima

**9:20 ENVR 125.** Recyclable iron-based catalysts for environmental remediation. D. Hermosilla, B. Ren, M. Nadagouda, C. Han, A. Gascó, P. Campo Moreno, D.D. Dionysiou

#### 9:45 Intermission.

**10:05 ENVR 126.** Removal of  $\beta$ -lactam antibiotics from waters using advanced oxidation processes. T.H. Do, D. Bandari, S.P. Mezyk

**10:30 ENVR 127.** High-level quantum calculations of sulfate radical generation for remediation of contaminated groundwater. B.M. Wong, H. Liu, R. Betrabat

**10:55 ENVR 128.** Reactions of bromine radical species under advanced oxidation process condition. A. Lechner, S.P. Mezyk

## Section D

Omni San Diego Hotel  
Grand Ballroom E

#### Per- & Polyfluoroalkyl Substances Associated with Aqueous Film Forming Foams (AFFF): Chemistry, Remediation & Regulatory Issues

Financially supported by ICCE/EuChMS

W. Giger, C. P. Higgins, L. Libelo, *Organizers*  
A. C. Alder, J. A. Field, *Organizers, Presiding*

#### 8:00 Introductory Remarks.

**8:10 ENVR 129.** Historical review of fluorinated foam firefighting agents and performance requirements/environmental safeguards review. J. Farley, J. Scheffey

**8:30 ENVR 130.** 1976-2016: Forty years of saving lives, C6 fluorotelomer surfactants and their use in firefighting foams. E.K. Kleiner

**8:50 ENVR 131.** Evaluating differences in foam degradation between perfluoroalkyl and fluorine-free foams for the development of environmentally friendly firefighting alternatives. K. Hinnant, R. Ananth, M. Conroy, B. Williams

**9:10 ENVR 132.** Field deployable PFASs sensors for contaminated site screening. L. Chen, C. Lai, J. Thompson, P. Buhlmann

#### 9:30 Intermission.

**10:00 Non-paper event:** The Division of Chemistry and the Environment of the European Association for Chemical and Molecular Sciences (EuCheMS). W. Giger.

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**10:10 ENVR 133.** Application of fluorine detection by combustion ion chromatography to aqueous film forming foam concentrates and aqueous environmental samples. **F. Lange**, B. Körner, A. Hauck, J. Müller

**10:30 ENVR 134.** Validation of a novel assay for total fluorine to measure per- and polyfluorinated alkyl substances in groundwater. **D.M. Lunderberg**, E.E. Ritter, K. Barzen-Hanson, J.A. Field, R. Delaney, D. Bogdan, D. Corsi, W. DiGuiseppi, G.F. Peaslee

**10:50 ENVR 135.** Assessment of PFAS in soil and groundwater: New analytical technologies for comprehensive analysis of PFAS including precursors. **I. Ross**

**11:10** Panel Discussion.

## Section E

Omni San Diego Hotel  
Gaslamp 3

### Carbonate & Sulfate Minerals: Nucleation, Growth & Control of Scale Formation

*Cosponsored by GEOC*

H. Teng, *Organizer*

Y. Hu, *Organizer, Presiding*

**8:00 ENVR 136.** Isotopes and impurities as microprobes of the mineral surface dynamics of calcite growth. **D. DePaolo**, L.N. Lammers, J. Watkins, J. De Yoreo, I. Bourg, F.J. Ryerson, A. Hoffman

**8:45 ENVR 137.** Magnesium effect on calcite growth morphology and implications for the dolomite problem. **H. Teng**, M. Hong

**9:05 ENVR 138.** Controlling heterogeneous (Ba, Ra)SO<sub>4</sub> precipitation on oil-field equipment. **W. Yang**, C. Dai, A.G. Stack, Y. Hu

**9:25 ENVR 139.** Strontium-doping into calcite through pressure-induced crystallization from amorphous calcium carbonate. **H. Kagi**, D. Enomoto, S. Matsunuma, K. Maruyama, K. Komatsu, T. Yoshino

**9:45** Intermission.

**10:00 ENVR 140.** New approach to modeling nucleation, crystal growth, and the Ostwald step rule. **C. Steefel**, A.G. Stack, L. Yang

**10:30 ENVR 141.** Molecular dynamics based investigations of liquid-liquid phase separation in the CaCO<sub>3</sub>- and MgSO<sub>4</sub>-H<sub>2</sub>O systems. **A.F. Wallace**, Y. Ma

**11:00 ENVR 142.** Computer simulation of the speciation and growth of calcium carbonate. **M. De La Pierre**, P. Raiteri, R. Demichelis, J.D. Gale

**11:30 ENVR 143.** Investigating calcium carbonate growth at close to equilibrium conditions. **B. Cao**, A.G. Stack, C. Steefel, Y. Hu

## Section F

Omni San Diego Hotel  
Gaslamp 4

### Water Treatment Technologies to Support Food-Energy-Water Nexus Water Conservation Needs

*Cosponsored by CEI*

N. Rao, *Organizer*

S. Bushart, W. J. Cooper, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 ENVR 196.** NSF and innovations at the nexus of food, energy, and water systems. **J. Lighty**, W.J. Cooper, B.K. Hamilton, B.L. Schottel

**8:30 ENVR 197.** Composite biologically active membrane system for simultaneous wastewater treatment and energy production. **A.L. Prieto**, L. Sigtermans, A. Aksan, **W. Arnold**, P. Novak, S. Romero-Vargas Castrillon

**8:55 ENVR 198.** Efficient energy recovery from dilute organic matter in a microbial battery equipped with a low cost and easily regenerated Prussian Blue cathode. **X. Xie**, M. Ye, C.S. Criddle, Y. Cui

**9:15 ENVR 199.** Response of anode-respiring bacteria to high ammonia concentration in a microbial electrolysis cell (MEC). **M. Mahmoud**, P. Parameswaran, C. Torres, B. Rittmann

**9:35 ENVR 200.** Cost-effective microbial-electrochemical/membrane approach for enabling wastewater reuse in power plants. **N. Shrestha**, K. Chilkoor Gopala, L. Xia, J. Shi, S. Bushart, J.E. Kilduff, V.R. Gadhamshetty

**9:55 ENVR 201.** Synergizing waste management for power and wastewater facilities via low-energy electrolytic carbonation. **Z. Ren**, L. Lu, Z. Huang

**10:15** Intermission.

**10:35 ENVR 202.** Life cycle evaluation of the co-management of domestic wastewater and food waste using anaerobic membrane bioreactors. **A. Becker**, K. Yu, A. Smith

**10:55 ENVR 203.** Water reuse for agriculture. **Q. Tran**, D. Jassby, K. Schwabe

**11:15 ENVR 204.** Recovering phosphorus from poultry litter: A step towards improving food security and protecting ecologically sensitive water bodies. **U. Shashvatt**, N. Rogers, H. Aris, L.M. Blaney

**11:35 ENVR 205.** Phosphorus recovery from reverse osmosis concentrate. **T. Jain**, H. Liu

### Francis P. Garvan-John M. Olin Medal: Symposium in honor of Annie Kersting

#### Environmental Chemistry of Actinides

*Sponsored by NUCL, Cosponsored by ENVR*

#### Environmental Interfaces

#### Redox Reactions

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG†*

## MONDAY AFTERNOON

### Section A

Omni San Diego Hotel  
Grand Ballroom C

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Environmental Chemistry/ Water Chemistry

*Cosponsored by CEI, ENFL and GEOC*

D. L. Drogos, R. Kleinberg, W. Orem, W. Stringfellow, *Organizers, Presiding*

**1:30 ENVR 144.** Recycling flowback and produced water in hydraulic fracturing: Influence of organic matter on frac fluid stability. **N. Esmailirad**, C. Terry, H. Kennedy, K. Carlson, A. Prior

**1:50 ENVR 145.** Comparison of organic matter in fresh and recycled water after simulation of fracturing conditions. **S. Kim**, K. Carlson, P. Omur-Ozbek

**2:10 ENVR 146.** Geochemical characterization of brine spills associated with hydraulic fracturing in North Dakota. **N. Lauer**, J. Harkness, A. Vengosh

**2:30** Intermission.

**2:50 ENVR 147.** Non-ideal behavior characterization for hydraulic fracturing flowback fluids. **N. Zhang**, K. Nedunuri, R. Kandiah, X. Wei

**3:10 ENVR 148.** Discrimination of produced formation waters from local groundwater using stable strontium isotopes: Examples from southern California and the Midwestern U.S. **R.W. Hurst**

**3:30 ENVR 149.** Groundwater quality and age in the Fayetteville and Haynesville shale gas production areas, Arkansas, Louisiana, and Texas. **P. McMahon**, J.R. Barlow, P.B. Ging, R.W. Tolleitt, T.M. Kresse, A.G. Hunt

**3:50 ENVR 150.** High methane concentrations in Los Angeles groundwater. **J.T. Kulongoski**, M. Land, P. McMahon, M.T. Wright, T. Johnson, M.K. Landon

**4:10** Panel Discussion.

### Section B

Omni San Diego Hotel  
Gaslamp 2

#### Innovative Materials & Technologies for Water Purification

#### Oxidation, Reduction & Disinfection

*Cosponsored by CEI*

*Financially supported by AEESP*

E. L. Cates, B. P. Chaplin, J. Choe, D. Shuai, W. Zhang, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 ENVR 151.** Algal toxin removal from drinking water using Ozone-BAC, BAC and GAC. **Y. Liu**, J.J. Lenhart

**1:55 ENVR 152.** Comparison of chemical oxidation pathways on nanofibrous activated carbon materials. **Y. Han**, R. Li, C. Bruckner, T.M. Vadas

**2:15 ENVR 153.** Biocatalytic perchlorate reduction in spent ion exchange brine. **J.M. Hutchison**, J.L. Zilles

**2:35 ENVR 154.** Evolution of heterogeneous catalysts for oxyanion reduction: Improved sustainability of biomimetic materials with rational design. **J. Liu**, X. Su, M. Han, X. Chen, Y. Wang, J. Shapley, T.J. Strathmann, C.J. Werth

**2:55 ENVR 155.** Synthesis and characterization of bimetallic nanoparticle catalysts on sustainable, biopolymer substrates for reduction of nitrate and nitrite in aqueous solution. **D. Durkin**, T. Ye, L. Haverhals, P.C. Trulove, H. Fairbrother, D. Shuai

**3:15** Intermission.

**3:30 ENVR 156.** Enhancement of reduction kinetics of waterborne contaminants on electrospun nanofibrous Pd-polyacrylonitrile (Pd-PAN) catalysts. **T. Ye**, D. Shuai

**3:50 ENVR 157.** Catalytic hydrogenation of aqueous nitrate with low-cost ruthenium catalysts. **X. Huo**, J. Liu, S. Vyas, T.J. Strathmann

**4:10 ENVR 158.** Evolution of heterogeneous catalysts for oxyanion reduction: New opportunities in the Periodic Table. **J. Liu**, Y. Wang, X. Chen, C.J. Werth, T.J. Strathmann

**4:30 ENVR 159.** Disinfection utilizing organic acids. **M. Butkus**, M.P. Labaree, J. Starke

**4:50 ENVR 160.** Antibacterial activity of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> (MXene): Towards new antifouling membranes. **K.A. Mahmoud**, K. Rasool, M. Helal, A. Ali, C. Ren, Y. Gogotsi

**5:10** Concluding Remarks.

## Section C

Omni San Diego Hotel  
Grand Ballroom D

### Treatment of Contaminants of Emerging Concern & Their Transformation Products

*Cosponsored by CEI*

A. J. Hernandez-Maldonado, *Organizer*

L. M. Blaney, *Organizer, Presiding*

**1:30 ENVR 161.** How to gain a more comprehensive picture of transformation products formed during ozonation of wastewater? **J. Schollee**, M. Bourgin, R. Teichler, C. McArdell, J. Hollender

**1:55 ENVR 162.** Chloramine kinetic reactions with chemical contaminants in treated wastewaters. **J.M. Gleason**, S.P. Mezzyk

**2:20 ENVR 163.** Withdrawn.

**2:45 ENVR 164.** Stability of the tetrahalobisphenol A incorporated into humic acid via oxidative coupling. **R. Kodama**, T. Miyamoto, M. Igarashi, Q. Zhu, **M. Fukushima**

**3:10** Intermission.

**3:25 ENVR 165.** Discovery of benzotriazole and novel plant metabolites in Arabidopsis and food crops. **G. LeFevre**, A. Lipsky, E. Sattely, C.P. Higgins, K. Hyland, R.G. Luthy

**3:50 ENVR 166.** Biotransformation of benzalkonium chlorides by immobilized cells of *Pseudomonas* sp. biomg1 in a packed bed reactor. **U. Tezel**, F.K. Sakarya

**4:15 ENVR 167.** Stable isotope enabled pathway elucidation of 2,4-dinitroanisole metabolized by *Rhizobium* litchii. **H.W. Schroer**, K.L. Rangenfeld, C.L. Just

**4:40 ENVR 168.** Development of antibiotic resistance in *Pseudomonas putida* chronically exposed to environmentally relevant concentrations of ciprofloxacin. **T.S. Radniecki**, K. Sertich Arruda

**5:05 ENVR 169.** Efficient biodegradation of bisphenol A by enzymes packaged in vault nanoparticles. **M. Wang**, D. Abad, V. Kickhoefer, L.H. Rome, S. Mahendra

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## Section D

Omni San Diego Hotel  
Grand Ballroom E

**Per- & Polyfluoroalkyl Substances Associated with Aqueous Film Forming Foams (AFFF): Chemistry, Remediation & Regulatory Issues**

Financially supported by ICCE/EuChMs

A. C. Alder, C. P. Higgins, L. Libelo, *Organizers*  
J. A. Field, W. Giger, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 ENVR 170. Exploring chemical markers for environmental release of perfluorooctane sulfonate in aqueous fire-fighting foams using comprehensive analysis with high resolution mass spectrometry. Y. Zushi, A. Yamamoto, S. Kitai, S. Masunaga, H. Kawasaki, R. Arakawa

2:00 ENVR 171. Application of a high-resolution product ion library to screen for AFFF-derived PFASs and other components. S. Roberts, M. Noestheden, K. Hyland, K.A. Barzen-Hanson, J.A. Field, C.P. Higgins, C. Borton

2:20 ENVR 172. Closing the mass balance on per- and polyfluorinated alkyl substances in groundwater at aqueous film-forming foam (AFFF) impacted sites. K.A. Barzen-Hanson, S. Roberts, G.F. Peaslee, C.P. Higgins, J.A. Field

2:40 ENVR 173. Characterisation of local sources for perfluorinated alkylated substances (PFAS) in Arctic local communities: A comparative study from Svalbard, Norway. R. Kallenborn, L. Ahrens, S. Axelsson, J. Rakovic, J.S. Saar, S.M. Lunde

3:00 Intermission.

3:30 ENVR 174. Investigating historical impacts of AFFF and co-contaminants. I. Kalinovich, A. Thalheimer

3:50 ENVR 175. Historical and current groundwater concentrations of per- and polyfluoroalkyl substances (PFASs) at the former Wurtsmith Air Force base (WAFB). D. Bogdan, R. Delaney, D. Corsi, G.F. Peaslee

4:10 ENVR 176. Case study: Assessing and managing Australia's longest PFOS groundwater plume. D.S. Woodward

4:30 ENVR 177. Sources and fate of AFFF in wastewater treatment plants. E. Houtz, M. Wang, E. Parry, J. Park

4:50 Non-Paper Event: The International Conference on Chemistry and the Environment (ICCE 2017) in Oslo, Norway. R. Kallenborn.

5:00 Panel Discussion.

## Section E

Omni San Diego Hotel  
Gaslamp 3

**Carbonate & Sulfate Minerals: Nucleation, Growth & Control of Scale Formation**

Cosponsored by GEOC

Y. Hu, *Organizer*

H. Teng, *Organizer, Presiding*

1:30 ENVR 178. In situ view of calcium carbonate nucleation. J. De Yoreo, M. Nielsen, P. Smeets, N.A. Sommerdijk

2:00 ENVR 179. Role of surface-bound carboxyl-group density of organic matter in low-temperature dolomite formation. J. Roberts, M. Edwards, D. Fowle, L.A. Gonzalez, R.H. Goldstein, D.S. Moore

2:30 ENVR 180. Heterogeneous nucleation and growth of barium sulfate nanoparticles at organic-water interfaces. C. Dai, A.G. Stack, A. Koishi, A. Fernandez-Martinez, Y. Hu

2:50 ENVR 181. Heterogeneous calcium carbonate nucleation in saline solution: Thermodynamic and kinetic contributions. Q. Li, Y. Jun

3:10 Intermission.

3:25 ENVR 182. Metabolism induced calcium carbonate mineralization in a microfluidic pore network. C.J. Werth, R. Singh, H. Yoon, B. Fouke, R. Sanford, L.E. Katz

3:55 ENVR 183. Chemical and physical agents of microbe-carbonate interactions. H. Teng

4:15 ENVR 184. Carbon dioxide sequestration through microbially-induced calcium carbonate precipitation using ureolytic aquatic microorganisms. D.F. Rodrigues, T.O. Okyay

4:35 ENVR 185. Optimizing microbially induced calcite precipitation under radial flow conditions. N. Zambare, R. Gerlach, E. Lauchnor

## Section F

Omni San Diego Hotel  
Gaslamp 4

**Chemistry of Materials Management: Mitigation & Reuse for Sustainable Environment**

Cosponsored by CEI

S. R. Al-Abed, *Organizer*

J. Baltrusaitis, K. Kawamoto, *Organizers, Presiding*

1:30 ENVR 186. Integrated processes for waste management, energy recovery, and the production of materials for environmental applications. J.L. Goldfarb, J. Xue, S. Emenyonu

2:00 ENVR 187. Development of a multi-zonal thermodynamic equilibrium calculation model to predict the fate and speciation of inorganic elements in municipal solid waste incineration facilities. K. Yui, H. Kuramochi, H. Sakanakura, M. Osako

2:20 ENVR 188. Development of decontamination process for radioactive cesium from radiation contaminated soil and incineration bottom ash. H. Fujiwara, H. Kuramochi, K. Nomura, S. Ide, M. Ogura, N. Takeda, M. Osako

2:40 Intermission.

2:55 ENVR 189. Assessment of bioaccessibility of As, Cd and Pb in impacted soils with mining wastes. M.E. Gutierrez Ruiz, T. Garcia-Rodriguez, A. Ceniceros-Gomez

3:15 ENVR 190. Recovery of rare earth elements from coal fly ash: Identification of candidate feedstock materials. R.K. Taggart, H. Hsu-Kim, J.C. Hower, G.S. Dwyer

3:35 ENVR 191. Mitigation of alkaline leachate generated from basic oxygen furnace slags by chemical precipitation. S. Kim, S. Jeong, K. Nam

3:55 Intermission.

4:10 ENVR 192. Simultaneous treatment of landfill leachate and domestic wastewater: Evaluation of pretreatment methods. G. Bushee, K. Miller, L. Sempriani, T.S. Radniecki

4:30 ENVR 193. Rational design of humics-based remedial agents for Installation of injectable permeable reactive barriers embedded with nano zero-valent iron. I. Perminova, A. Volikov, E. Fedorova, S. Ponomarenko, D. Pankratov, K. Hatfield

4:50 ENVR 194. Withdrawn.

5:10 ENVR 195. PCB waste disposal and management in Japan. K. Kawamoto

## Environmental Interfaces

**Nucleation, Growth & Dissolution Processes**

Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG†

**Francis P. Garvan-John M. Olin Medal: Symposium in honor of Annie Kersting Environmental Chemistry of Actinides**

Sponsored by NUCL, Cosponsored by ENVR

**Adsorption of Metals by Geomedia**

**Theory & Modeling after Twenty Years**

Sponsored by GEOC, Cosponsored by ENVR, MPPG† and NUCL

**Elucidation of Mechanisms & Kinetics on Surfaces**

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

**Undergraduate Research Posters**

**Environmental Chemistry**

Sponsored by CHED, Cosponsored by ENVR and SOCED

**Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza**

Sponsored by INOR, Cosponsored by ENVR, ORGN and POLY

## MONDAY EVENING

## Section A

San Diego Convention Center  
Halls D/E

## Sci-Mix

S. R. Al-Abed, *Organizer*

8:00 - 10:00

410, 423, 426, 436, 440-441, 445-447, 449, 451, 453, 457, 459-460, 463-466, 472-473, 476-477, 479, 481, 489, 491, 495-500, 503, 507, 510-518, 520-523, 526-527, 530, 538-539, 541-544, 550, 552. See subsequent listings.

## TUESDAY MORNING

## Section A

Omni San Diego Hotel  
Grand Ballroom C

**Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing**

**Microbial Processes & Treatment**

Cosponsored by CEI, ENFL and GEOC

D. L. Drogos, R. Kleinberg, W. Orem, W. Stringfellow, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR 206. Predominance and metabolic potential of halanerobium in Marcellus Shale hydraulic fracturing produced water. D. Lipus, K. Bibby, A. Vikram

8:30 ENVR 207. Informing hydraulic fracturing produced water microbial control via analysis of gene expression. K. Bibby, D. Lipus, A. Vikram

8:50 ENVR 208. Environmental microbial community tolerance and adaptation to biocides use in hydraulic fracturing operations. M. Campa, S. Techtmann, M.L. Patterson, A. Garcia de Matos Amaral, R. Lamendella, C.J. Grant, T.C. Hazen

9:10 ENVR 209. Endocrine disruptors in hydraulic fracturing flowback: Downhole transformation of nonylphenol ethoxylates. G. Kahrilas, J. Blotvogel, T. Borch

9:30 ENVR 210. Reactive transport modeling of biocide reagents in unconventional hydrocarbon reservoirs. J. Vilcaez

9:50 Intermission.

10:10 ENVR 211. Treatment of hydraulic fracturing wastewater by algal biomass. L. Scannell, S.R. Wegst, E.J. Mullin, D.S. Aga, B.Z. Haznedaroglu

10:30 ENVR 212. Biofilm treatment approach for produced water from hydraulic fracturing using engineered microbial mats. B. Akyon, E. Stachler, K. Bibby

10:50 ENVR 213. Inhibition of biodegradation of hydraulic fracturing fluid organic compounds in groundwater by the biocide glutaraldehyde. J.D. Rogers, S. Tummings, A.R. Bielefeldt, J.N. Ryan

11:10 ENVR 214. Multistage microbial-electrochemical approach for simultaneous desalination and wastewater treatment of super-saline backflow water. N. Shrestha, K. Chilkoor Gopala, V.R. Gadhamshetty

11:30 Panel Discussion.

## Section B

Omni San Diego Hotel  
Gaslamp 3

**Innovative Materials & Technologies for Water Purification**

**Adsorption**

Cosponsored by CEI  
Financially supported by AEESP

E. L. Cates, B. P. Chaplin, J. Choe, D. Shuai, W. Zhang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 215. Highly effective adsorption of organic aromatic molecules by electronically sorted single-walled carbon nanotubes. R.E. Rogers, J.R. Rocha, A.B. Dichiaro, R.C. Capasse

8:25 ENVR 216. Anomalous carbon rods that adsorb water vapor at low humidity and release liquid droplets at higher humidity. D.J. Heldebrant, S.K. Nune, D. Lao, J. Liu, M. Olszta, R. Kukkadapu, L. Gordon, M. Nandasiñi, D. Gotthold, T. Schaeff

8:45 ENVR 217. Facile and cost-effective technique for separation of oil from water using polymer-coated iron oxide nanoparticles. S. Mirshahghassemi, J.R. Lead

9:05 ENVR 218. Three-dimensional graphene oxide hydrogels for water treatment applications. T.A. Duster, K. Swarup, L.F. Greenlee

9:25 ENVR 219. Ligand-associated activated carbon system for the treatment of hazardous waste from research laboratories. T.M. Ditttrich, S.K. Mohanty, R. Bogle

9:45 Intermission.

10:00 ENVR 220. Engineered crumpled graphene oxide nanocomposite membrane assemblies for advanced water treatment processes. Y. Jiang, P. Biswas, J. Fortner

**10:30 ENVR 221.** Modified mesoporous silica nanoadsorbent for water purification application. **Y. Zou, Y. Wang**

**10:50 ENVR 222.** Novel technique for enhancement of phosphorus removal in aqueous system using CeO<sub>2</sub>-covered PAN nanofiber. **Y. Chun, S. Kim, U. Choi, J. Lee, S. Lee, Y. Jung**

**11:10 ENVR 223.** Application of porous materials modified with Fe<sub>3</sub>O<sub>4</sub> nanoparticles for arsenic removal in drinking water. **A. Puente-Urbina, V. Montero-Campos**

**11:30 ENVR 224.** Selenium removal from power plant waste water using solid phase extraction materials. **M. Li, C.K. Chan**

**11:50 Concluding Remarks.**

### Section C

Omni San Diego Hotel  
Grand Ballroom D

#### Treatment of Contaminants of Emerging Concern & Their Transformation Products

*Cosponsored by CEI*

**L. M. Blaney, A. J. Hernandez-Maldonado, Organizers, Presiding**

**8:00 ENVR 225.** Design of transition metal based composite adsorbents for the selective removal of contaminants of emerging concern from water. **A.J. Hernandez-Maldonado, K. Ortiz, W.A. Cabrera-Lafaurie, K.M. Gonzalez-Ramos**

**8:25 ENVR 226.** Impact of biologically active carbon on the removal of emerging DBPs and their precursors. **R. Marfil-Vega, L.A. Weinrich, M. Surmeier, M. Kreminskaya, Z. Bukhari**

**8:50 ENVR 227.** Unintended consequences of GAC on emerging DBPs. **C.T. Lee, S.W. Krasner, P.K. Westerhoff, N. Fischer, D. Hanigan, T. Karanfil, W. Beita-Sandi, L. Taylor-Edmonds**

**9:15 ENVR 228.** Novel approach for investigating mechanisms of nanoparticle filtration. **C. Chen, S.L. Walker**

**9:40 Intermission.**

**10:00 ENVR 229.** Water treatment options and challenges for perfluoroalkyl substances and fluorinated alternatives. **D. Knappe, L. Dudley, E. Arevalo, M. Sun, M. Strynar, A. Lindstrom**

**10:25 ENVR 230.** Sustainable removal of poly- and perfluorinated alkyl substances (PFASs) from groundwater using synthetic media. **S. Woodard, M.G. Nickelsen, N. Hagelin, B. Newman**

**10:50 ENVR 231.** Activated carbon surface chemistry: Significance of oxygen functional groups for mercury adsorption. **R. Rodriguez, D.W. Mazzyk**

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### Section D

Omni San Diego Hotel  
Grand Ballroom E

#### Per- & Polyfluoroalkyl Substances Associated with Aqueous Film Forming Foams (AFFF): Chemistry, Remediation & Regulatory Issues

*Financially supported by ICCE/EuChMs*

**A. C. Alder, J. A. Field, W. Giger, Organizers**

**C. P. Higgins, L. Libelo, Organizers, Presiding**

**8:00 Introductory Remarks.**

**8:10 ENVR 232.** Biotransformation of fluorotelomer thioether amido sulfonate (Lodyne) in AFFF. **K. Harding, E. Houtz, S. Yi, J.A. Field, D.L. Sedlak, L. Alvarez-Cohen**

**8:30 ENVR 233.** Sorption of anionic, zwitterionic, and cationic polyfluorinated alkyl substances in AFFF to soil and sediment. **K. Barzen-Hanson, M. Kleber, J.A. Field**

**8:50 ENVR 234.** Remediation of PFC contaminated soil at Norwegian airports. **Å. Hoisæter, B. Straith, S. Hale, G. Slinde, G. Breedveld, P. Cappelen, K. Moe, M. Jartun**

**9:10 ENVR 235.** Investigation of in-situ chemical oxidation techniques for AFFF treatment in soil-water microcosms. **J.J. Bishop, J. Hatton, D. Berggren, J.A. Field, K. Barzen-Hanson, T. Bruton, W. DiGiuseppe**

**9:30 Intermission.**

**10:00 ENVR 236.** Destruction of PFOS in groundwater: A new in situ remediation technology for per / polyfluorinated alkyl substances. **I. Ross, J. Burdick, T. Pancras, M. Ahmad**

**10:20 ENVR 237.** Per- and polyfluoroalkyl substances: EU-regulation and dialogue with fire fighters in Germany. **L. Verke, C. Staude, A. Biegel-Engler, E. Fetter, C. Schulte**

**10:40 ENVR 238.** Addressing releases of perfluoroalkyl substances: EPA programs and authorities. **L. Gaines, M. Cooke, M. Scozzafava**

**11:00 ENVR 239.** U.S. EPA regulatory update on per and polyfluoroalkyl substances (PFASs). **T. Krasnic**

**11:20 Panel Discussion.**

**11:55 Concluding Remarks.**

### Section E

Omni San Diego Hotel  
Gaslamp 1

#### Carbonate & Sulfate Minerals: Nucleation, Growth & Control of Scale Formation

*Cosponsored by GEOC*

**Y. Hu, H. Teng, Organizers, Presiding**

**8:00 ENVR 240.** Scale control in oil and gas industries and new insight into carbonates and sulfates mineral nucleation, precipitation and inhibition. **A. Kan, Z. Dai, F. Zhang, F. Yan, N. Bhandari, G. Ruan, Z. Zhang, Y. Liu, M.B. Tomson**

**8:30 ENVR 241.** Influence of polyamide membrane surface chemistry on gypsum scaling. **D. Shaffer, M. Tousley, M. Elimelech**

**8:50 ENVR 242.** Removing whitening particles (CaCO<sub>3</sub>, calcite) from water by different organic and inorganic flocculants. **X. He, E. Wert**

**9:10 ENVR 243.** Carbonate mineral formation in fractured basalt at geologic carbon sequestration related conditions. **W. Xiong, R. Wells, P. Skemer, D. Giammar**

**9:30 ENVR 244.** CO<sub>2</sub> fixation process through mineral carbonation of ultramafic rocks and industrial wastes with acceleration by acids. **A. Yamasaki, M. Noguchi, A. Iizuka**

**9:50 Intermission.**

**10:05 ENVR 245.** Characterization of structure and transformation kinetics of amorphous phases using total scattering methods. **R.J. Reeder, M. Schmidt**

**10:35 ENVR 246.** Consideration on the controlling factor of the metastable formation of CaCO<sub>3</sub> polymorphs. **J. Kawano**

**11:05 ENVR 247.** Microscopic dynamics in amorphous carbonates: The significance of ACC polymorphism. **A. Fernandez-Martinez, A. Koishi, M. Jimenez Ruiz, B. R. Ruda, F. Zontone, R. Poloni**

### Section F

Omni San Diego Hotel  
Gaslamp 4

#### Chemistry & Application of Advanced Oxidation Processes for Water Purification, Treatment & Reuse

**D. D. Dionysiou, K. E. O'Shea, X. Quan, Organizers**

**G. Li Puma, D. Minakata, Organizers, Presiding**

**8:00 Introductory Remarks.**

**8:05 ENVR 248.** Determination of aqueous-phase radical reaction rate constants for predicting the fate of transformation byproducts in advanced oxidation processes using experimental and theoretical methods. **D. Minakata, D. Kamath, D. Perram**

**8:40 ENVR 249.** Development of a quantitative structure-activity relationship model to predict the degradation of halogenated disinfection byproducts by UV-hydrogen peroxide (UV/H<sub>2</sub>O<sub>2</sub>) advanced oxidation treatment. **Y. Chuang, K.M. Parker, W. Mitch**

**9:05 ENVR 250.** Effect of Fermi level of electron mediator on construction and performance of Z-scheme photocatalyst. **H. Li, X. Quan, H. Yu, S. Chen, Y. Zhang**

**9:30 ENVR 251.** Investigation of radical chlorine species reactivity under advanced oxidation process conditions. **J. Castillo, S.P. Mezyk**

**9:55 Intermission.**

**10:10 ENVR 252.** Non-photochemical activation of peroxide and hydrogen peroxide for reactive oxidants production. **W. Choi, A. Bokare, D. Kim**

**10:45 ENVR 253.** Detailed product and kinetic studies of the ultrasonically induced degradation of the popular antihistamine, diphenhydramine. **D. Cui, C. Zhao, L.E. Arroyo-Mora, K.E. O'Shea**

**11:10 ENVR 254.** Oxidation of chloramphenicol in water using hydrodynamic cavitation. **G.A. Loraine, G. Chahine**

**11:35 ENVR 255.** Synthesis and applications of Ag/AgCl @ chiral TiO<sub>2</sub> nanofibers. **D. Wang, Y. Li, G. Li Puma**

### Environmental Interfaces

#### Surface Adsorption

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡*

#### Adsorption of Metals by Geomedia

#### Thermodynamics & Kinetics Experimental Study

*Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL*

### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

#### Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza

*Sponsored by INOR, Cosponsored by ENVR, ORGN and POLY*

## TUESDAY AFTERNOON

### Section A

Omni San Diego Hotel  
Grand Ballroom C

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Geochemistry

*Cosponsored by CEI and GEOC*

**D. L. Drogos, R. Kleinberg, W. Orem, W. Stringfellow, Organizers, Presiding**

**1:30 ENVR 256.** Trends in oil and gas production technology. **R. Kleinberg**

**2:10 ENVR 257.** Fluid-rock interactions between hydraulic fracturing fluid and shale oil & gas reservoirs: Experimental insights. **J. Kaszuba, J. Bratcher, R. Herz-Thyhsen, V. Maroon**

**2:30 ENVR 258.** Investigating radioactivity and trace element leaching from shale in unconventional oil and gas exploration. **N. Mehta, B. Kocar, C. Harvey**

**2:50 ENVR 259.** Pyrite-dazomet interactions: Reactivity of a hydraulic fracturing fluid additive. **N. Consolazio, G. Lowry, J. Hakala, A. Karamalidis**

**3:10 Intermission.**

**3:30 ENVR 260.** Shale matrix controls on the chemistry of residual treatment waters (RTW) associated with hydraulic fracturing of organic-rich gas-bearing shales. **L. Bryndzia**

**3:50 ENVR 261.** Increasing the production efficiency and reducing the water usage of hydraulic fracturing. **H. Viswanathan, J. Carey, S. Karra, M. Porter, Q. Kang, E. Rougier**

**4:10 ENVR 262.** Marcellus shale energy and environment laboratory (MSEEL). **T.R. Carr**

**4:30 ENVR 263.** Computer simulation of the buoyant ascent and liquid-gas-water repartitioning of petroleum hydrocarbons in the deep water column during the Deepwater Horizon disaster. **J.S. Arey, J. Gros, S.A. Socolofsky, A.L. Dissanayake, I. Jun, R.K. Nelson, C.M. Reddy**

**4:50 Panel Discussion.**

### Section B

Omni San Diego Hotel  
Gaslamp 3

#### Innovative Materials & Technologies for Water Purification

#### Electrochemical & Biological Process

*Cosponsored by CEI Financially supported by AEESP*

**E. L. Cates, B. P. Chaplin, J. Choe, D. Shuai, W. Zhang, Organizers, Presiding**

**1:30 Introductory Remarks.**

**1:35 ENVR 264.** Multi-layer anode for saline wastewater treatment: Manipulating oxidant generation pathway by TiO<sub>2</sub> thin film deposition. **Y. Yang, M.R. Hoffmann**

**1:55 ENVR 265.** Electrolytic dedegradation of halogenated contaminants in water using activated carbon-based electrode. Y. Li, W. Mitch

**2:15 ENVR 266.** Electrically conductive composite carbon nanotubes UF membranes for hexavalent chromium removal. A. Ronen, W. Duan, S.L. Walker, D. Jassby

**2:35 ENVR 267.** Flow-through electrochemical reduction and adsorption of nitrate on activated carbon. K.R. Muller, D. Jassby

**2:55 ENVR 268.** Electrochemically reduced TiO<sub>2</sub> nanotube array as an oxidant-generating anode for water treatment. C. Kim, S. Kim, J. Lee, J. Kim, J. Yoon

**3:15 ENVR 269.** Redox-mediated electrochemical separations as a novel technology for water remediation and removal of trace contaminants. X. Su, T.F. Jamison, T. Hatton

**3:35** Intermission.

**3:45 ENVR 270.** Composite CNTs-polyaniline electrically conducting and anodically stable membranes. W. Duan, A. Ronen, S.L. Walker, D. Jassby

**4:05 ENVR 271.** Solar powered system for the removal of arsenic using chemical free electrolytic oxidant production and disinfection. L. Romero, P. Otter, U. Feistel, T. Grischek

**4:25 ENVR 272.** Comparison of vegetable oil nanoemulsion formulations with other commercial enhancers on the biodegradation of 1,1-DCE and VC in groundwater. T. Chen, S. Chang

**4:45 ENVR 273.** Evaluation of a facultative anaerobes isolated from the Sanford Underground Research Laboratory for lignin degradation in microbial electrochemical systems. A. Shende, N. Shrestha, R. Jaswal, V.R. Gadhamshetty

**5:05 ENVR 274.** Pilot study on bioremediation of chlorinated solvent-contaminated aquifer using vegetable oil nanoemulsion. S. Chang, J. Sung, T. Chen

**5:25** Concluding Remarks.

## Section C

Omni San Diego Hotel  
Grand Ballroom D

### Treatment of Contaminants of Emerging Concern & Their Transformation Products

*Cosponsored by CEI*

L. M. Blaney, A. J. Hernandez-Maldonado, *Organizers*

A. M. Noce, *Presiding*

**1:30 ENVR 275.** Understanding the scale and origins of 1,4-dioxane in public water supplies. T.K. Mohr

**1:55 ENVR 276.** Occurrence of 1,4-dioxane in North Carolina surface water and evaluation of possible treatment options. D. Knappe, C. Lopez-Velandia, M. Sun

**2:20 ENVR 277.** Managing high iron levels while removing 1,4-dioxane from groundwater. S. Woodard, D. Samorano, R. Luhrs, A. Bishop

**2:45 ENVR 278.** Bioaugmented sorbents for removing 1,4-dioxane and CVOCs from water. M. Myers, S. Zhang, Y. Liu, P. Gedalanga, S. Mahendra

**3:10** Intermission.

**3:30 ENVR 279.** Laboratory and field studies on aerobic cometabolic biodegradation of 1,4-dioxane and co-contaminants. M. Chu, P. Bennett, M. Dolan, M. Hyman, A. Peacock

**3:55 ENVR 280.** Withdrawn.

**4:20 ENVR 281.** Water treatment panel discussion: A look at emerging contaminants. A.M. Noce, S. Woodard, D. Knappe, S. Mahendra, M. Chu

**4:55** Concluding Remarks.

## Section D

Omni San Diego Hotel  
Gaslamp 1

### Opportunities & Progress in Computational Prediction of Contaminant Toxicity, Fate & Transport Properties

*Cosponsored by CCOMP*

W. A. Alexander, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 ENVR 282.** Prediction of contaminant toxicity, fate, and transport properties to support disaster response: Looking beyond the 2014 Elk River, West Virginia chemical spill. W.A. Alexander, N.J. Deyonker

**2:00 ENVR 283.** Online QSAR prediction platform to support the environmental sciences. T. Cathey, C. Fowler, C. Grulke, R. Judson, K. Mansouri, A. Richard, A.J. Williams, D. Zang

**2:25 ENVR 284.** Prediction of physical properties and environmental fate properties with EPISuite™. P.H. Howard, W.M. Meylan, A. Hueber, J.L. Tunkel

**2:50 ENVR 285.** In silico compound profiling and risk assessment: Current capabilities and perspectives. K. Kassam, D. Adams, S.K. Bhal, K. Lanevskij

**3:15** Intermission.

**3:35 ENVR 287.** Computational approaches to reducing animal use in toxicology. E. Maull, X. Chang, D. Zang, J. Strickland, N. Kleinstreuer, W. Casey

**4:00 ENVR 286.** Methylmercury exposure and risk from rice consumption for vulnerable populations in a traditional fish eating area in china. Y. Tong, X. Wang, W. Zhang

**4:25 ENVR 288.** Unique challenges of toxicity prediction for environmentally relevant chemicals: Prediction of human plasma protein binding through quantitative structure-activity relationship (QSAR) models. B.L. Ingle, B.C. Veber, J.W. Nichols, R. Tornero-Velez

**4:50 ENVR 289.** Prediction of environmental fate properties for novel munitions compounds. P.G. Tratnyek, A.J. Salter-Blanc, M.A. Lyon, E.J. Bylaska

**5:15** Discussion.

## Section E

Omni San Diego Hotel  
Grand Ballroom E

### Science & Perception of Climate Change

*Cosponsored by CEI*

S. O. Obare, E. Schoffers, *Organizers, Presiding*

**1:30 ENVR 290.** How culture shapes the climate change debate. A. Hoffmann

**2:00 ENVR 291.** The ACS climate science toolkit: What's next? J.A. Bell

**2:30 ENVR 292.** Evaluating 10 ways to communicate climate change issues. R.G. Landolt

**2:50 ENVR 293.** Climate change, extreme events, are regional impacts. N. Moore

**3:10** Intermission.

**3:25 ENVR 294.** Metal-organic framework as single site catalyst and catalyst support. A. Peters, Z. Li, H. Beyzavi, C.J. Cramer, L. Gagliardi, J.T. Hupp, O.K. Farha

**3:45 ENVR 295.** Getting people excited about the science of climate change. K.L. Klingenberg, S. Underwood, R. Reddick, T. Greenwood, A. Hoffman, T. Scherban

**4:05 ENVR 296.** Lost in translation: A scientist's perspective on how the media portrays climate change. E. Schoffers

**4:25 ENVR 297.** Global warming in unequivocal: ACS and its members can help point the way for meaningful action. B.Z. Shakhshiri

**4:55** Panel Discussion.

## Section F

Omni San Diego Hotel  
Gaslamp 4

### Chemistry & Application of Advanced Oxidation Processes for Water Purification, Treatment & Reuse

G. Li Puma, D. Minakata, X. Quan, *Organizers*

D. D. Dionysiou, K. E. O'Shea, *Organizers, Presiding*

**1:30 ENVR 298.** Radiolysis studies on the degradation of cyclohexane methanol (MCHM). K.E. O'Shea, C. Zhao, J.R. Peller, P.V. Kamat

**2:10 ENVR 299.** Degradation kinetics and mechanism of oxytetracycline by UV-254 nm/H<sub>2</sub>O<sub>2</sub>. Y. Liu, X. He, Y. Fu, D.D. Dionysiou

**2:35 ENVR 300.** Chlorine-based radical removal of antibiotics from wastewaters. C. Rice, S.P. Mezyk

**3:00 ENVR 301.** Advanced oxidation processes on a graphite-nanoparticle modified surface: An EPR and COD investigation. M.A. Morsy, A.N. Kawde

**3:25** Intermission.

**3:40 ENVR 302.** Mineralization of phenol using a surfactant modified ZnAl LDH as photocatalyst. A. Mantilla, G. Romero-Ortiz, M. Suárez-Quezada, V. Suarez, E. Navarro, F. Tzompantzi, L. Lartundo-Rojas

**4:05 ENVR 303.** Selective remediation of pharmaceuticals in wastewater using sulfate radicals: Evidence for adsorption to dissolved organic matter. T. Reutershan, S.P. Mezyk

**4:30 ENVR 304.** Reactions of iron sulfide and surface Fe(II) compounds with persulfate, hydrogen peroxide and chlorine. R. Yin, J. Sun, C. Shang

**4:55 ENVR 305.** Withdrawn.

## Environmental Interfaces

### Complex Surface Reactions

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡*

### Adsorption of Metals by Geomedia

### Thermodynamics & Kinetics Experimental Study

*Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL*

### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

## WEDNESDAY MORNING

### Section A

Omni San Diego Hotel  
Grand Ballroom C

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Water Use & Reuse

*Cosponsored by CEI, ENFL and GEOC*

D. L. Drogos, R. Kleinberg, W. Orem, W. Stringfellow, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:10 ENVR 306.** Impacts of hydraulic fracturing on water availability and management: A case study on future water resources and stakeholder needs in the South Platte River basin. E. Walker, A.M. Anderson, T.S. Hogue

**8:30 ENVR 307.** Quantifying the impact of water use for hydraulic fracturing at local and regional scales in Colorado. T. Hogue, E. Walker, A. Anderson

**8:50 ENVR 308.** Deriving value from produced waters. W. Bellamy, J. Brant, S. Quillinan, J.F. McLaughlin

**9:10 ENVR 309.** Hydraulic fracturing: Water use, reuse, and disposal. R. Kleinberg

**9:30 ENVR 310.** Unconventional oil and gas and induced earthquakes. J. Rubinstein

**9:50** Intermission.

**10:10 ENVR 311.** Water management for hydraulic fracturing. D. Reible, V. Uddameri, S. Honarpavar

**10:30 ENVR 312.** From fracking to oil and gas development: Chemical constituents and potential implications for the beneficial reuse of produced water. S.B. Shonkoff, J.K. Domen, M. Camarillo, W. Stringfellow

**10:50 ENVR 313.** Groundwater resources and hydraulic fracturing in the Eagle Ford Shale. S. Farhat, A. Daus

**11:10 ENVR 314.** Putting produced water to beneficial use: A water management strategy whose time has come. E.L. Hagstrom

**11:30** Panel Discussion.

### Section B

Omni San Diego Hotel  
Gaslamp 2

### Aquatic Photochemistry

*Cosponsored by GEOC*

K. P. McNeill, *Organizer*

V. S. Lin, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 ENVR 315.** Stable isotope fractionation associated with the photochemical transformation of chloroanilines. M. Ratti, S. Canonica, K.P. McNeill, T.B. Hofstetter

**8:25 ENVR 316.** Molecular absorption spectra: Simulation and analysis for quantitative descriptions of pollutant phototransformation and fate in the environment. K. Terayapiwat, P. Cohen, A. Poblete, H. Rudel, S.N. Eustis

**8:45 ENVR 317.** Taking apart the aqueous photoelectron spectra and one-electron redox potentials of dissolved compounds with molecular simulations. J.S. Arey, P.R. Tentscher, J.J. Guerard, R. Seidel, B. Winter

**9:05 ENVR 318.** Comparison of photooxidation rates and patterns in glass- and water-based oil slick experiments with daily weathering observed in the Gulf of Mexico. **C.M. Sharpless**, O.C. Stewart, M. Walters, S.F. Robert, C. Aeppli, C. Reddy

**9:25 ENVR 319.** Photoinactivation of aquatic extracellular enzymes in the aquatic environment. **E. Janssen**

**9:45 ENVR 320.** Withdrawn.

**10:05** Intermission.

**10:20 ENVR 321.** Withdrawn.

**10:40 ENVR 322.** Aqueous reactions of triplet excited states with allylic compounds. **R. Kaur**, C. Anastasio

**11:00 ENVR 323.** Exploration of organic aerosol growth through photosensitized oxidation of VOCs. **M. Galloway**, M.G. Ippolito, R.A. Barron

**11:20 ENVR 324.** Effects of the local environment on photolysis kinetics of aromatic pollutants in natural waters. **J. Grossman**, A.P. Stern, M.L. Kirich, T.F. Kahan

### Section C

Omni San Diego Hotel  
Grand Ballroom E

#### ES&T @ 50: Award Winning Researchers Past, Present & Future

*Financially supported by Environmental Science & Technology; Environmental Science & Technology Letters*

B. E. Logan, *Organizer*

D. L. Sedlak, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 ENVR 325.** Status of biology in ES&T: Reflections on the last 50 years. **J.M. Suflika**

**8:50 ENVR 326.** Antibiotic resistance and water sustainability: Protecting public health in a changing world. **A. Pruden**, M. Edwards, A. Salveson, E. Garner

**9:15 ENVR 327.** Compilation and application high resolution global emission inventories of air pollutants. **S. Tao**, H. Shen, H. Chen, Q. Zhong

**9:40 ENVR 328.** Redox active metal-quinone interactions in oxic aquatic systems: Implications to metal speciation, quinone transformation and reactive oxygen species generation. **T.D. Waite**, S. Garg, C. Jiang

**10:05** Intermission.

**10:25 ENVR 329. Award Address (ACS Award for Creative Advances in Environmental Science and Technology sponsored by the ACS Division of Environmental Chemistry and the ACS Publications journal Environmental Science & Technology and Environmental Science & Technology Letters)** Microbial electrochemical technologies at the nexus of food, energy, water and climate change. **B.E. Logan**

**11:10 ENVR 330.** Water chemistry changes induced by managed aquifer recharge impact arsenopyrite dissolution and secondary mineral precipitation. **C.W. Neil**, Y.J. Yang, D. Schupp, Y. Jun

**11:35 ENVR 331.** Multiphase chemistry promotes isoprene-derived secondary organic aerosol formation in the southeastern United States. **J. Surratt**, Y. Lin, A. Gold, M. Riva, S. Budisulistiorini, T. Riedel, W. Rattanavaraha, M. Arashiro, Z. Zhang, T. Cui, Y. Chen, E. Edgerton, K. Baumann, S. Shaw, E. Knipping, K.G. Sexton, I. Jaspers, W. Vizcete, R. Fry, H. Pye, J. Thornton, C. Gaston, A. Zelenyuk-Imre, M. Glasius, D. Bell, A. Hansen, V.F. McNeill

### Section E

Omni San Diego Hotel  
Gaslamp 1

#### Green Chemistry & the Environment

*Cosponsored by CEI*

A. M. Balu, R. Luque, S. O. Obare, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 ENVR 332.** Chemistry in water: New methods for organic synthesis and applications. **C. Len**

**8:45 ENVR 333.** Analysis of products from the liquid phase reaction of furfural under reducing conditions. **L.A. Welch**, S. Ogozaly

**9:05 ENVR 334.** Greener preparation of carbohydrate-conjugated cinnamates. **M. Hunsen**

**9:25 ENVR 335.** Facile design of bimetallic nanoparticles for biomass conversion. **H.A. Al-Zubaidi**, S.O. Obare

**9:45 ENVR 336.** Catalyst activity and stability for the conversion of biologically derived muconic acid to adipic acid. **D. Vardon**, A. Settle, N. Cleveland, M. Menart, G. Beckham

**10:05** Intermission.

**10:20 ENVR 337.** Hydrodeoxygenation and hydroisomerization of algae oils to hydrocarbon fuels. **J. Kruger**, E. Christensen, T. Dong, R.L. McCormick, P. Plenkos

**10:40 ENVR 338.** Green chemistry metrics evaluation for biodiesel production. **E. Martinez-Guerra**, V. Gude

**11:00 ENVR 339.** Closing the loop: Synthesis of hematite nanoparticles (α-Fe<sub>2</sub>O<sub>3</sub>) from mine tailing sources for remediation of mine tailing contamination. **A.W. Lounsbury**, E. Rose-Willen, M. Falinski, J.B. Zimmerman

**11:20 ENVR 340.** Withdrawn.

**11:40 ENVR 341.** Incorporating green chemistry principles and risk assessment methods to support sustainability planning. **A.R. Wise**, M. Macdonell

### Section F

Omni San Diego Hotel  
Gaslamp 3

#### Chemistry & Application of Advanced Oxidation Processes for Water Purification, Treatment & Reuse

D. D. Dionysiou, G. Li Puma, D. Minakata, K. E. OShea, *Organizers*

X. Quan, *Organizer, Presiding*

J. Casas Lopez, *Presiding*

**8:00 ENVR 342.** Effect of temperature and photon absorption on the kinetics of micropollutant removal by solar photo-Fenton in raceway pond reactors. **J. Sánchez Pérez**, J. García Sánchez, J. Casas López, J. Fernández Sevilla, G. Rivas Ibañez, P. Soriano

**8:35 ENVR 343.** Solar photo-Fenton treatment of textile wastewater: An effective technology towards water reuse. **M. Vieira Martins Staring**, P. Rodrigues, F. Ribeiro de Souza, C. Costa de Amorim, M.M. Leão

**9:00 ENVR 344.** Iron-based metal organic frameworks as heterogeneous Fenton catalyst for organic pollutants treatment. **C. Gao**, X. Quan

**9:25 ENVR 345.** Withdrawn.

**9:50** Intermission.

**10:05 ENVR 346.** Alternative approaches for mild photo-Fenton process under sunlight. **A. Arques**, A. Amat, R. Vicente, R. Vercher, M. Mora, L. Santos-Juanes, S. Garcia-Ballesteros

**10:40 ENVR 347.** Micropollutant removal by photo-Fenton process using UVA-LED as radiation source. **J. Casas Lopez**, I. de la Obra Jiménez, B. Esteban García, J. Garcia Sánchez, J. Sánchez Pérez

**11:05 ENVR 348.** Intensified ozonation of water contaminants in a novel multi-orifice oscillatory baffled column reactor (MOBR). **M. Lucas**, N.M. Reis, G. Li Puma

**11:30 ENVR 349.** Statistical optimization of the solar photocatalytic degradation of a commercial dye contained in a real industrial wastewater with a pilot-scale CPC reactor. **J.A. Colina-Marquez**, D. Castilla Caballero, F. Machuca-Martinez

#### Greener Pathways to Organics & Nanomaterials: Sustainable Applications of Magnetic Nanocatalysts

*Sponsored by I&EC, Cosponsored by ENVR‡*

#### Environmental Interfaces

#### Complex Surface Reactions

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG‡*

#### Adsorption of Metals by Geomedia

#### Radionuclides: Uranium & Transuranium - Extension of ACS Garvan-Olin Medal Session

*Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL*

#### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

## WEDNESDAY AFTERNOON

### Section A

Omni San Diego Hotel  
Grand Ballroom C

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing Water Use & Reuse/Water Treatment

*Cosponsored by CEI, ENFL and GEOC*

D. L. Drogos, R. Kleinberg, W. Orem, W. Stringfellow, *Organizers, Presiding*

**1:30 ENVR 350.** Energy water nexus and water implications of energy extraction and mining. **M. Hightower**

**2:10 ENVR 351.** Use of physical/chemical data as a tool for screening potential treatment approaches for hydraulic fracturing waste streams. **M. Camarillo**, W. Stringfellow, J.K. Domen, W.L. Sandelin

**2:30 ENVR 352.** Use of polyelectrolyte complexes in Sr and Ba removal from produced waters. **E.F. Peltier**, S.J. Randtke, K. Shafer-Peltier, S. Xie

**2:50 ENVR 353.** Direct contact membrane distillation for treatment of produced water from shale gas production. **O.R. Lokare**, R.D. Vedic

**3:10** Intermission.

**3:30 ENVR 354.** Demonstration of treatment of produced water from shale oil and gas production to discharge quality standards for agricultural uses. **N. Esmailirad**, K. Carlson

**3:50 ENVR 355.** Produced water disposal in evaporation ponds: Using chemistry modeling to size them correctly. **K. Martins**

**4:10 ENVR 356.** Withdrawn.

**4:30 ENVR 357.** Corrosion-induced environmental challenges due to the backflow water from Bakken play. **G. Chilkoor**, N. Shrestha, V. Gadhamshetty

**4:50** Panel Discussion.

### Section B

Omni San Diego Hotel  
Gaslamp 2

#### Aquatic Photochemistry

*Cosponsored by GEOC*

V. S. Lin, *Organizer*

K. P. McNeill, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 ENVR 358.** Molecular probe measurements of the photochemical formation of one-electron reductants by CDOM: Relation to superoxide and hydrogen peroxide photoproduction. **Y. Zhang**, N.V. Blough

**1:55 ENVR 359.** Fluorescent molecular probes for detection of one-electron oxidants generated photochemically by dissolved organic matter. **V.S. Lin**, M. Grandbois, K.P. McNeill

**2:15 ENVR 360.** Photochemical formation of reactive oxidants by size-fractionated dissolved organic matter. **C.K. Remucal**, A. Maizel

**2:35 ENVR 361.** Photochemical production and scavenging of reactive intermediates by dissolved organic matter in natural water samples: Influence of base modification. **S.P. Mezyk**, K.D. Couch, G. McKay, F.L. Rosario

**2:55 ENVR 362.** Applications of time-resolved singlet oxygen detection: Instrumental improvements enabling low signal measurements in natural waters. **P.R. Erickson**, E. Appliani, R. Ossola, A. Linkhorst, K.P. McNeill

**3:15** Intermission.

**3:30 ENVR 363.** Reactivity differences of humic acids and their influence on nitrogen dioxide reduction in the terrestrial environment. **N. Scharko**, J.D. Raff

**3:50 ENVR 364.** Photochemical production and reactivity of reactive halogen species (RHS) in estuarine and coastal waters. **K.M. Parker**, W. Mitch

**4:10 ENVR 365.** Effect of experimental parameters on the apparent photochemical properties of dissolved organic matter. **A. Maizel**, C.K. Remucal

**4:30 ENVR 366.** Seasonal and long-term hydrologic trends in prairie potholes affect the formation rates and steady-state concentrations of photochemically-produced reactive species. **A.J. McCabe**, W. Arnold

**4:50 ENVR 367.** Photooxidation of iodide in frozen solution. **W. Choi, K. Kim, A. Yabushita**

## Section C

Omni San Diego Hotel  
Grand Ballroom E

### Advances in In Situ Pollutant Destruction by Nanoscale Zero Valent Iron & Other Engineered Nanoparticles

#### NZVI Particles: Structure, Morphology, Reactivity

A. Agrawal, S. R. Kanel, B. A. Manning, *Organizers, Presiding*

#### 1:30 Introductory Remarks.

**1:40 ENVR 368.** Approaches to characterizing the fate and effects of nano zerovalent iron. **P.G. Tratnyek, R.L. Johnson, D. Fan, Z. Shi**

**2:10 ENVR 369.** Zero-valent iron nanoparticles for soil, water and wastewater treatment: Present scenario. **S.R. Kanel, B.A. Manning**

**2:30 ENVR 370.** Use of the hydrophobic effect in the design of carbon based carriers for nanoscale zerovalent iron. **V.T. John, R. Zheng**

**2:50 ENVR 371.** More effective treatment of chlorinated solvents by Cu-amended nanoscale zero-valent iron stabilized with carboxymethylcellulose. **A. Franze, A. Agrawal**

#### 3:10 Intermission.

**3:30 ENVR 372.** Field trials with nanometals, degradation performance and enhancement through microbial activity. **D. O'Carroll, C. Kocur, L. Lomheim, H. Boparai, A. Chowdhury, K. Weber, L. Austrins, E.A. Edwards, B. Steep**

**4:00 ENVR 373.** Role of morphology and composition in reactivity of FeNi nanoparticles. **L.F. Greenlee, K. Estoque, M. Voecks, H. Weinstein, N. Rentz, N. Bedford**

**4:20 ENVR 374.** Reactivity of nano zero-valent iron (nZVI) and Ni-modified nano zero-valent iron (Ni-nZVI) stabilized with carboxymethylcellulose towards chlorinated hydrocarbons. **A. Agrawal, E. Kimmel**

**4:40 ENVR 375.** Transport of surface modified-NZVI particles in the subsurface porous media and its possible implications. **T. Raychoudhury, S. Ghoshal**

**5:00 ENVR 376.** Polymer stabilized nZVI nanoparticles for enhanced TCE degradation. **M.A. Kumar, S. Hamid, W. Lee**

#### 5:20 Concluding Remarks.

## Section D

Omni San Diego Hotel  
Gaslamp 4

### Membrane Technology for Water-Energy Sustainability

*Cosponsored by CEI*

D. Jassby, B. Mi, *Organizers, Presiding*

**1:30 ENVR 377.** Membrane technology for water purification, desalination and in energy production: Current status and challenges. **Y. Cohen**

**2:00 ENVR 378.** Potential of graphene membranes for enhanced removal neutral organic compounds. **S. Zheng, B. Mi**

**2:20 ENVR 379.** Nanostructure-enabled membranes for improved reverse osmosis processes. **J. Ray, S. Tadepalli, S.Z. Nergiz, K. Liu, L. You, Y.J. Tang, S. Singamaneni, Y. Jun**

**2:40 ENVR 380.** Water desalination and selective ion-separation using single-layer graphyne and hydrogenated graphyne membranes at realistic reverse-osmosis pressures. **M. Raju, A.C. Van Duin, M. Ihme**

**3:00 ENVR 381.** Covalent organic frameworks as novel membrane materials. **L. Valentino, J.S. Moore, B.J. Marinas**

#### 3:20 Intermission.

**3:40 ENVR 382.** Composite MD membranes with tunable surface hydrophilicity and conductivity for fouling mitigation, and process optimization. **A.V. Dudchenko, D. Jassby**

**4:00 ENVR 383.** Electrically conductive membrane for energy and resource recovery in membrane electrochemical bioreactors. **D.D. Hou, L. Lu, Z. Ren**

**4:20 ENVR 384.** Electrospun nanofiber supported thin film composite membranes prepared by molecular layer-by-layer assembly. **R. Sahadevan, T.J. Menkhaus**

**4:40 ENVR 385.** Fabrication of ultra-thin polyelectrolyte membrane for separation of botulinum toxin and vaccinia virus. **Y. Kim, S. Jeon, H. Jang, N. Lee, S. Nahm**

**5:00 ENVR 386.** Novel ceramic membrane coated by CuMn<sub>2</sub>O<sub>4</sub> particles catalytic ozonation for BP-3 degradation in aqueous: Fabrication, characterization and performance. **Y. Guo, B. Xu, F. Qi**

## Section E

Omni San Diego Hotel  
Gaslamp 1

### Green Chemistry & the Environment

*Cosponsored by CEI*

A. M. Balu, R. Luque, S. O. Obare, *Organizers, Presiding*

**1:30 ENVR 387.** Detection and quantification of various opioid compounds in urban wastewater by utilization of liquid chromatography-tandem mass spectrometry. **S.B. Reynolds**

**1:50 ENVR 388.** Multipurpose application of sacha inchi (Plukenetia volubilis L.) plant: Panacea from the Andean region. **B. Kumar, L.H. Cumbal, K. Smita**

**2:10 ENVR 389.** Degradation of naphthylazo anionic dye by Fenton and Fenton-like processes: A case study with fast sulphonic black-f. **B. Jain, A.K. Singh, V.K. Sharma**

**2:30 ENVR 390.** Deactivation of sulfide oxidizing bacteria to prevent sewer corrosion, collapse and explosion. **C. Rhee, S. Kim**

**2:50 ENVR 391.** Chemically engineered okra seed extracts: Microwave-induced synthesis of 3,5-diarylpyrazole derivatives by hydrazine hydrate treatment of the flavonoids present in okra seed extract and their potential implications in neurodegenerative diseases. **B. Dayal, J. Tuteja, B. Patel, L. Phyu, A. Mehta, S. Patel**

#### 3:10 Intermission.

**3:30 ENVR 392.** Green technology for REEs recovery. **Z. Hu, P. Kim, T. Li, P. Antonick, R. Riman, A. Eslamimanesh, A.M. Anderko, R. Shivaramaiah, A. Navrotsky, D. DePaoli, J. Zhang**

**3:50 ENVR 393.** Green, sustainable H<sub>2</sub> supply for upgrading bio-oil to biofuel: Conversion of furanic and phenolic byproducts to H<sub>2</sub> using bioelectrochemical technology. **X. Zeng, A. Borole, S.G. Pavlostathis**

**4:10 ENVR 394.** Hydrolysis of lignocellulose derived cellulose in molten salt hydrate (MSH) media. **B. Saha, S. Sadula, W. Deng, J. Kennedy, V. Nikolakis**

**4:30 ENVR 395.** Solution combustion synthesized binary oxide nanoparticles for solar fuel generation and environmental remediation. **G. Samu, A. Thomas, A. Kormanyos, K. Rajeshwar, C. Janaky**

**4:50 Discussion and Concluding Remarks.**

## Section F

Omni San Diego Hotel  
Gaslamp 3

### Chemistry & Application of Advanced Oxidation Processes for Water Purification, Treatment & Reuse

D. D. Dionysiou, G. Li Puma, K. E. O'Shea, X. Quan, *Organizers*

D. Minakata, *Organizer, Presiding*

Y. G. Adewuyi, *Presiding*

**1:30 ENVR 396.** Degradation of amoxicillin in aqueous solution by ozonation: pH effect and toxicity assessment. **F.S. Souza, V.V. da Silva, C.K. Rosin, L. Hainzenreder, L.A. F  ris, A. Arenzon**

**1:55 ENVR 397.** Naphthalene degradation in water/ethanol mixtures by catalytic ozonation based nickel oxide films. **C.M. Aguilar, J.L. Rodr  guez, I. Chairez, J.A. Galaviz, J.R. Vargas, T. Poznyak**

**2:20 ENVR 398.** Enhanced pretreatment of heavy oil refinery wastewater by charcoal-supported manganese oxides coupled with pressurized ozone. **L. Liu, W. Ma, C. Chen, X. Yan, Q.X. Li, S. Guo, Q. Wang**

**2:45 ENVR 399.** Catalyzed ozonation of organic chemicals in petroleum refinery wastewater by Mn-Fe-Mg-Ce supported Al<sub>2</sub>O<sub>3</sub>. **W. Ma, P. Wang, J. Ye, Y. Li, S. Guo, C. Chen**

#### 3:10 Intermission.

**3:25 ENVR 400.** Oxidation efficacy of ozone and chlorine on naturally occurring Microcystis protected by a colonial sheath. **X. He, E. Wertz**

**3:50 ENVR 401.** Enhanced performance of tailored TiO<sub>2</sub>-based nanotube composites towards persistent organic pollutants. **X. Li**

**4:15 ENVR 402.** Fe<sub>3</sub>O<sub>4</sub>-RGO and BiOBr nanoparticles for the removal of MB from aqueous solutions and the enhancement in its photocatalytic activity when used as a composite. **L. Miranda, J. S, S. Rani**

**4:40 ENVR 403.** Cost estimation and economic evaluations of advanced oxidation processes for emerging water pollutants. **Y.G. Adewuyi**

## Environmental Interfaces

### Complex Surface Reactions

*Sponsored by GEOC, Cosponsored by COLL, ENVR and MPPG  *

### Greener Pathways to Organics & Nanomaterials: Sustainable Applications of Magnetic Nanocatalysts

*Sponsored by I&EC, Cosponsored by ENVR  *

### Adsorption of Metals by Geomedia

### X-ray Spectroscopy

*Sponsored by GEOC, Cosponsored by ENVR, MPPG   and NUCL*

### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

## WEDNESDAY EVENING

### Section A

San Diego Convention Center  
Hall D

### Aquatic Photochemistry

*Cosponsored by GEOC*

V. S. Lin, K. P. McNeill, *Organizers*

**6:00 - 8:00 ENVR 404.** Role of dissolved organic matter in photodecomposition of methylmercury in seawater. **J. Kim, S. Han**

**ENVR 405.** Withdrawn.

### Section A

San Diego Convention Center  
Hall D

### Characterization & Toxicity of Airborne Particulate Matters (PMs) in East Asia

X. Li, S. L. Simonich, S. Tao, *Organizers*

#### 6:00 - 8:00

**ENVR 406.** Withdrawn.

### Section A

San Diego Convention Center  
Hall D

### Chemistry & Application of Advanced Oxidation Processes for Water Purification, Treatment & Reuse

D. D. Dionysiou, G. Li Puma, D. Minakata, K. E. O'Shea, X. Quan, *Organizers*

#### 6:00 - 8:00

**ENVR 407.** Quantitative removal of alkyl nitrate contaminants from wastewaters using AOP's. **B. Daws, S.P. Mezyk, M.P. Schramm**

**ENVR 408.** Ozonation of 4-phenolsulfonic acid and phenol in presence of NiO as catalyst. **E. Flores, J. Rodr  guez, T. Poznyak, I. Chairez, M. Valenzuela**

**ENVR 409.** Textile dye RB5 wastewater treatment by simple ozonation in presence of additives: A water reuse process. **A. Perez, I. Chairez, T. Pozniak**

### Section A

San Diego Convention Center  
Hall D

### General Posters

S. R. Al-Abed, *Organizer*

#### 6:00 - 8:00

**ENVR 410.** Wet weather contributions to the formation of disinfection by-products in wastewater treatment plant effluent. **F.B. Dunn, J. Wilson**

**ENVR 411.** Soil contamination interpretation by the use of monitoring data analysis. **A.E. Folorunso**

**ENVR 412.** De-ammonification and anaerobic treatment processes for alternative water reuse and energy production, case study: Using municipal wastewaters. **PL. Noophan**

**ENVR 413.** Identification and quantification of organic contaminants in impaired surface waters using high resolution mass spectrometry. **T. Anumol, L. Kennedy**

**ENVR 414.** Removal efficiency of heavy metals by two type neutralization reactor in acid mine drainage from abandoned metal mine. **J. Kim, S. Kang, J. Kim, G. Jeong, M. Lee, Y. Kim**

**ENVR 415.** Metals disrupt the enantioselective biotransformation of cis-bifenthrin in zebrafish. **J. Liu, Y. Yang**

- ENVR 416.** Degradation of trimethoprim by heterogeneous Fenton reaction using iron sulfide catalysts. **Y. Bi, H. Zhang, K. Wigginton, K.F. Hayes**
- ENVR 417.** Risk assessment of endocrine disrupting effects in agricultural soils across China. **J. Liu, R. Liu**
- ENVR 418.** Lead, mercury, sleep, and inflammatory markers in adolescents: An OMICS approach. **K.G. Bendinskas, C. Burant, J. MacKenzie, B. Gump**
- ENVR 419.** High temperature CO<sub>2</sub> sorption using amine modified silica nanotubes and nanospheres. **C. Gunathilake, A. Manchanda, P. Ghimire, M. Kruk, M. Jaroniec**
- ENVR 420.** Responses of marine microalgae *Phaeodactylum tricornutum* to the exposure of manufactured TiO<sub>2</sub> nanoparticles. **Y. Wang, X. Zhu**
- ENVR 421.** Synthesis and characterization of degradable nanocomposites based on poly(ethylene terephthalate)-poly(lactic acid) and functionalized SiO<sub>2</sub>. **S. Lu, Y. Ke, Q. Zhou, G. Zhang**
- ENVR 422.** Characterization of particulate-bound polycyclic aromatic hydrocarbons in the atmosphere in Singapore using gas chromatography mass spectrometry. **D. Urbancok, R.D. Webster**
- ENVR 423.** Photocatalytic degradation of UV-filters mediated by as-synthesized TiO<sub>2</sub>NWs. **L. Soto-Vazquez**
- ENVR 424.** Development of multilayer ClO<sub>2</sub> antimicrobial coating. **J. Lee, Y. Lai, W. Hui, K. Yeung**
- ENVR 425.** Apportioning photochemical formation of hydroxyl radical from wastewater. **J.R. Laszakovits, G. McKay, C.M. Sharpless, F.L. Rosario**
- ENVR 426.** Withdrawn.
- ENVR 427.** Degradation mechanism of algal derived odorants during chlorination and UV/chlorination processes. **T. Kim, B. Moon, T. Kim, M. Kim, K. Zoh**
- ENVR 428.** Fenton reaction as a step of chlorine-free electrochemical disinfection of water contaminated with *E. coli*: Role of hydroxyl radicals and singlet oxygen formation. **N. Barashkov, T. Sakhno, I. Irgibaeva**
- ENVR 429.** Ultraviolet disinfection of drinking water: Role of the camera's geometry and degree of mixing water during irradiation in laminar flow. **A. Semenov, T. Sakhno, N. Barashkov**
- ENVR 430.** Photochemical changes in water accommodated fractions of MC252 and surrogate oil created during solar exposure as determined by FT-ICRMS. **P.P. Vaughan, R. Kamerman, W. Jeffrey, T. Wilson, M. Hagy, A.M. McKenna, H. Chen, R.P. Rodgers**
- ENVR 431.** New approaches to the computer application of sensor networks with new device to agricultural environment. **E.J. Parish, M. Hsiao, H. Honda, T. Wei**
- ENVR 432.** Novel development to the life cycle approaches of greener products design. **E.J. Parish, S. Hyatt, G. Ren, H. Honda, T. Wei, M. Hsiao**
- ENVR 433.** Novel development of bio-based products and anaerobic digestion by compost environment standard. **E.J. Parish, H. Shyu, G. Ren, H. Honda, T. Wei**
- ENVR 434.** Novel application of environmental effects on macroeconomic energy consumption for green business marketing. **E.J. Parish, S. Lee, G. Ren, H. Honda, T. Wei**
- ENVR 435.** Novel approaches to estimation methodologies to reduce carbon emission on climate change. **E.J. Parish, G. Ren, H. Honda, T. Wei, W. Wang**
- ENVR 436.** Effect of heavy metals on nitrification activity as measured by RNA- and DNA-based function-specific assays. **V. Kapoor, J. Santo Domingo**
- ENVR 437.** Vibrational spectroscopic analysis of wetland greenhouse gas emissions resulting from nitrogen influx. **E.M. Bowers, J. Britting, D.J. Leclapain**
- ENVR 438.** Geochemistry and heavy metal distribution of plants in tailing dump of abandoned Jangun mine, Korea. **J. Kim, J. Kim, S. Kang, C. Lee, Y. Kim**
- ENVR 439.** Analysis of trace metals in bottled water samples from across the United States. **P.A. Creed, N. Hanks, J. Xue, J.T. Creed**
- ENVR 440.** Catalytic conversion of isoeugenol into high added value chemicals using supported iron oxide nanoparticles on porous materials. **A. Franco, S. De, A. Balu, A. Yezpez, A. Romero, R. Luque**
- ENVR 441.** Continuous flow design of magnetically separable nanocatalysts. **M. Marquez, A. Yezpez, A. Balu, A. Romero, R. Luque**
- ENVR 442.** Withdrawn.
- ENVR 443.** Degradation of neonicotinoid insecticides in urban stormwater runoff by UV/chlorine advanced oxidation process. **T. Bradley, W. Mitch, T. Zeng**
- ENVR 444.** Development and calibration of a passive sampler for atmospheric mercury: Influence of meteorological factors and field applications. **W. Zhang, H. Lin, H. Guo, Y. Li, T. Ren, X. Wang**
- ENVR 445.** Chromatographic separation and detection of arsenic species in sulfidic waters. **J. Zhang, A. Harper**
- ENVR 446.** Delineation of water masses in the Caribbean Sea, Gulf of Mexico, and Mediterranean Sea using stable oxygen isotope ratios. **N. Ledra**
- ENVR 447.** Ocean microplastics: Initial evaluation in a Pacific harbour region. **A. Kahl**
- ENVR 448.** Cytotoxicity of drinking water disinfection by-products produced by ferrate, monochloramine or chlorine. **C. Jaggi, C. Gray, V. Sharma, L. Chen, L. Cizmas**
- ENVR 449.** Study on the behavior of fine particles in multi-physical fields under wet condition. **L. Qi, Y. Zhang**
- ENVR 450.** Preparation, characterization and toxic dye (Basic Red 9) adsorption properties of expanded vermiculite. **T. Gurkan Polat, O. Duman, S. Tunç**
- ENVR 451.** Predicting partitioning of charged organic species using quantum chemistry (QC) and Abraham poly-parameter linear free energy relationships (pp-LFERs). **C.W. Davis, D.M. Ditoro**
- ENVR 452.** Toxicity of heavy metals and trace elements for an island population of newborns in China. **M. Tang**
- ENVR 453.** Hydrothermal carbonization of coffee wastewater as a way to obtain fine sized particles with antimicrobial properties. **P. Zuniga, J. Quesada**
- ENVR 454.** Adsorption performance of hydroxyapatite powder in the removal of dyes in wastewater. **A.A. Okoya**
- ENVR 455.** Determination of BTEX in wastewater produced by gas filling stations in the city of Bucaramanga. **J.A. Torres, J.R. Pinzon**
- ENVR 456.** Development of advanced RO membranes based on the detailed analysis of their nanostructures. **H. Shimura, K. Nakatsui, T. Sasaki, M. Kimura**
- ENVR 457.** Effect of propylamine as an amine precursor on polybenzoxazine based-carbon xerogel for CO<sub>2</sub> adsorption. **R. Dahanasamoh, T. Chaisuwan, U. Suriyapraphadilok**
- ENVR 458.** Distribution of the endocrine disruptor 4-nonylphenol as a function of fraction organic carbon in dust across the Sierra Nevada Mountains. **R.A. Lyons, J. Mendoza, A. Koons**
- ENVR 459.** Functionalized magnetic nanoparticle systems for the environmental remediation. **R. Bhandari, A. Gutierrez, B. Wahlang, P. Gupta, B. Hennig, T. Dziubla, J.Z. Hillt**
- ENVR 460.** Optimization of solid phase extraction of petroleum residues implementing green chemistry principles. **R. Kamerman, P.P. Vaughan**
- ENVR 461.** Measuring reduced organosulfur compounds in air using PTR-ToF-MS and a canister/GC-FID method. **V. Perraud, S. Meinardi, D.R. Blake, B.J. Finlayson Pitts**
- ENVR 462.** Demethylation of methamphetamine by ultra violet tertiary treatment at wastewater treatment plants. **L.M. Newberry, T.H. Boles**
- ENVR 463.** Diffusion of styrene oligomer generated from debris polystyrene surrounding Japan and the north Pacific ocean. **K. Koizumi, H. Sato, H. Katsura, B. Kwon, S. Chung, D.M. Karl, K. Takatama, Y. Koderu, K. Saïdo**
- ENVR 464.** Water-enhanced removal of ciprofloxacin from water by porous graphene hydrogel. **J. Ma, F. Yu, M. Yang, J. Zheng**
- ENVR 465.** Screening for glucocorticoid receptor activities in pesticides by *in vitro* assays. **J. Liu, J. Zhang**
- ENVR 466.** Non-invasive real-time biofouling monitoring in a gravity-driven biofilm MBR system for wastewater treatment. **L. Fortunato, T. Leiknes**
- ENVR 467.** Accelerated bromate reduction in ice phase. **D. Min, W. Choi**
- ENVR 468.** Kinetics of microalgae growth and phosphorus uptake under simulated cold region conditions. **J. Schmidt, G. Gagnon, R. Jamieson**
- ENVR 469.** Glutaraldehyde resistance drives changes in hydraulic fracturing produced water microbial populations. **D. Lipus, K. Bibby, A. Vikram**
- ENVR 470.** Radium-226 removal from hydraulic fracturing produced water using *Dunaliella salina*. **B. Akyon, T. Zhang, R.D. Vidic, K. Bibby**
- ENVR 471.** Enantioselective interactions of typical triazole fungicides with human CYP3A4 enzyme. **H. Wang, X. Lv, L. Pan, J. Wang, K. Ding**
- ENVR 472.** Toxicity of neonicotinoid insecticide paichongding to earthworm *Eisenia fetida*. **J. Zhang, J. Liu**
- ENVR 473.** Functionalized magnetic multi-walled carbon nanotubes composites for TEX removal. **F. Yu, J. Ma, J. Zheng**
- ENVR 474.** Atmospheric fates of neonicotinoid insecticides. **K. Aregahegn, B.J. Finlayson Pitts**
- ENVR 475.** Comparing the effect of replacement of the petroleum-based with bio-based polyol in polyurethane resins properties. **S.M. Albukhari, X. Ding, D.L. Richter, P. Heiden**
- ENVR 476.** Ratiometric Cu(II) sensor: Design synthesis and characterization of a bifunctional Cu(II) ligand. **M. Abdalrahman, F. Abebe, S. Burdette, R. Seitz, W.S. Kassel, R.P. Palanip**
- ENVR 477.** Electrochemical activation of titania nanotube electrode and its electrochemical response to Cu<sup>2+</sup>. **X. Zhang, D. Brodus, V. Hollimon**
- ENVR 478.** Ecological and chemical evaluation of South Dakota achillea. **M.R. Hurst, J. Ramsey**
- ENVR 479.** Selective adsorption of cesium from high salt concentration of waste water. **H. Lee, H. Kim, D. Moon, W. Lim**
- ENVR 480.** Kinetic studies on the reduction of hexavalent chromium by commercial coffee. **C. Kim**
- ENVR 481.** CO<sub>2</sub> capture via porous carbons. **Y. Tarkunde, Y. Li, J.M. Tour**
- ENVR 482.** Synthesis of phosphate modified magnetic mesoporous carbon for removal of uranium. **H. Syed Muhammad, W. Um, Y. Chang**
- ENVR 483.** Dietary exposure assessment to hexabromocyclododecane (HBCDD) in Korea. **M. Barghi, M. Son, Y. Chang**
- ENVR 484.** Photosensitized diastereoisomer-specific degradation of hexabromocyclododecane (HBCDD) in the presence of humic acid. **M. Son, Y. Kang, Y. Chang**
- ENVR 485.** Organic ligands pretreatment enhancing chromium removal by nanoscale zero-valent iron. **Y. Kang, H. Yoon, T. Thanh Le, Y. Chang**
- ENVR 486.** Nano-ecotoxicity of the environmental catalyst to the aquatic and terrestrial environment. **M. Pangging, H. Yoon, T. Thanh Le, Y. Chang**
- ENVR 487.** Removal of complex contaminants in wastewater using laccase encapsulated in magnetic copper alginate beads. **T. Thanh Le, C. Lee, C. Huong Vu, Y. Kang, Y. Chang**
- ENVR 488.** Synthesis and characterization of thiol-ene based nanoporous covalent organic polymers for CO<sub>2</sub> capture. **B. Buyukbekar, H. Cavusoglu, E. Goren, M. Yavuz**
- ENVR 489.** CYP450 enzyme-specific enantioselective metabolism of metalaxyl in HepG2 cells. **F. Yang, W. Xie**
- ENVR 490.** Photochemistry of effluent organic matter and photochemical degradation of micropollutants. **L. Bodhipaksha, A. MacKay, C.M. Sharpless**
- ENVR 491.** Mechanistic studies on the shape-based phytotoxicity of silver nanomaterials. **D.E. Gorka, N.K. Geitner, M.R. Wiesner, J. Liu**
- ENVR 492.** Tissue distribution and bioaccumulation potential of 6:2 chlorinated polyfluoroether sulfonic acid in Crucian Carp (*Carassius carassius*) under natural conditions. **Y. Shi, R. Vestergren, Z. Zhou, X. Song, L. Xu, Y. Liang, Y. Cai**
- ENVR 493.** Photoelectrochemical activity of electrochromic titania nanotube arrays for water purification. **M. Koo, K. Cho, J. Yoon, W. Choi**
- ENVR 494.** Photodegradation of phenolic compounds on titania/graphene oxide composite catalysts in liquid phase. **C. Fu, Y. Chen, C. Hsieh, R. Juang**
- ENVR 495.** Development of a risk assessment tool for petroleum vapor intrusion. **Y. Yao, I. Verginelli, E. Suuberg, J. Liu**
- ENVR 496.** Fabrication and application of magnetic nanoparticles using red mud. **Z. Katircioglu, S. Dursun, M. Yavuz**



- ENVR 497.** Assessment of microbial degradation potential of alpha-cypermethrin in soil by compound-specific stable isotope analysis. **Z. Xu, F. Yang**
- ENVR 498.** Enantioselective effect of chiral herbicide imazethapyr on the phytotoxicity of silver nanoparticles. **X. Sheng, L. Zhang, Z. Chen, J. Ma, Y. Wen**
- ENVR 499.** Ion-probe flow adsorption microcalorimetry: A new approach to the study of surface heterogeneity, acid dissociation and cation exchange behavior at the PyC-water interface. **B. Leonce, O. Harvey**
- ENVR 500.** Degradation kinetics of hexachlorobenzene (HCB) by zero-valent magnesium/graphite (ZVMg/C) and modeling of pathways using Density Functional Theory (DFT). **A. Garbou, S. Zou, M. Liu, C. Clausen, C. Yestrebtsky**
- ENVR 501.** Separation of magnetized silicotitanate from aqueous phase using a magnetic separating system. **Y. Kim, J. Kim, H. Kwon, J. Geum**
- ENVR 502.** Comparative toxicity and bioaccumulation of fenvalerate and esfenvalerate to earthworm *Eisenia fetida*. **X. Ye, J. Liu**
- ENVR 503.** Effect of pH on the wavelength dependence of hydrogen peroxide quantum yields from dissolved organic matter. **J.R. Laszakovits, C.M. Sharpless**
- ENVR 504.** Multiple-metal oxides anchored granular activated carbon based composite for fluoride removal. **S. Kalicindi, S.B. Pankaj, T. Raychoudhury**
- ENVR 505.** Reductive immobilization of selenium in sulfur-containing solution. **A. Safan, B. Jung, A. Abdel-Wahab**
- ENVR 506.** Reactive oxidants from Fe(II)-containing clay minerals for water purification. **K. Zakaria, A. Neumann**
- ENVR 507.** Withdrawn.
- ENVR 508.** Efficient CO<sub>2</sub> adsorption by disulfide-linked covalent organic polymers. **E. Goren, H. Cavusoglu, M. Yavuz**
- ENVR 509.** Development of a novel non-equilibrium passive sampling method using polyethylene with multiple thicknesses. **K. Kim, J. Jung, Y. Choi, R.G. Luthy**
- ENVR 510.** Pulsed corona discharge induced oxidation of aqueous organics: Optimization of hydrodynamic conditions and application in removal of micropollutants. **P. Ajo**
- ENVR 511.** Correlation between the odor concentration and the VOC composition of tobacco smoke. **M. Noguchi, A. Yamasaki**
- ENVR 512.** Triazine-based porous polymer networks via reaction of epoxy with amine for CO<sub>2</sub> capture. **S. Dursun, M. Yavuz**
- ENVR 513.** Array-based detection of carcinogens and carcinogen metabolites in breast milk. **L. Gareau, N. Cook, L. Prignano, M. Levine**
- ENVR 514.** Entrapment of peroxidase in porous silica particles for enzymatic degradation of drinking water contaminants. **J. Nutt, P. Edmiston**
- ENVR 515.** Biomimetic adsorbents for the removal of microcystins from water. **K.A. Carter, E. Gleason, P. Edmiston**
- ENVR 516.** Bimetallic catalysts for the aqueous phase reduction of succinic acid to 1,4-butanediol. **A. Settle, K. Steirer, K. Moyer, N. Cleveland, G. Beckham, D. Vardon**
- ENVR 517.** Methods for analyzing strontium-90 in high carbonaceous samples of soil from the Marshall Islands. **S. Herman, W.B. Connick, S. Glover, H. Spitz**
- ENVR 518.** Assessing stormwater runoff contamination effects on water quality in a nature preserve. **A.E. McGowin, J.C. McKinley**
- ENVR 519.** Assessing cytotoxicity of water soluble cadmium telluride (CdTe) quantum dots. **D. Asunskis, A.N. Coover, A.M. Benz**
- ENVR 520.** Screening for drugs of abuse in the waste water in a small college town in Southern Arkansas. **G. Geme, L. Wood**
- ENVR 521.** Water footprint of hydraulic fracturing. **A. Kondash**
- ENVR 522.** Photooxidation of squalene on titanium dioxide particles. **M.L. Kaak, M.E. Byrd, J.A. Ganske**
- ENVR 523.** Effect of water in the degradation of polychlorinated biphenyls using ZVMg and ZVMg/carbon with acidified ethanol or ethanol/ethyl lactate solvent systems. **F.M. Zullo, C. Clausen, C. Yestrebtsky**
- ENVR 524.** Cerium oxide nanomaterials for water filtration. **X. Hu, L. MacManus-Spencer, M.E. Hagerman**
- ENVR 525.** Treatment of phenolic compounds from pyrolysis wastewater by adsorption to Kenaf: Comparison of different Kenaf pre-treatments as quantified by solid-phase microextraction (SPME). **A. Bienvenu, W.E. Holmes, E. Revellame, R. Hernandez, P. Buchireddy, M. Zappi**
- ENVR 526.** Flow-injection spectrophotometric method for copper determination in natural waters. **K. Gossow-Smith, M.P. Hurst**
- ENVR 527.** Development and study of process effectivity of the novel conducting polymer based photocatalysts for reactive azo dye degradation in model waste water. **I. Peternel, Z. Katančič, Z. Hrnjak Murgic, V. Gilja**
- ENVR 528.** Speciation of arsenic (As) in tailings of Hidalgo de Parral, Chihuahua, Mexico. **I. Gavilan, A. Menchaca, G. Fernández**
- ENVR 529.** Photolysis and toxicity of ultraviolet filter chemical. **H. Stein, M.G. Paulick, L. MacManus-Spencer**
- ENVR 530.** Withdrawn.
- ENVR 531.** Removal of Nonylphenol by the electrochemical oxidation combined with carbon nanotube adsorption: Regeneration. **Y. Dai, P. Chiang, Y. Chin**
- ENVR 532.** Advanced oxidative process applied in the decolourization of real textile wastewater in original pH using bubble annular reactor. **J.C. Cardoso, G. Bessegato, M. Zanoni**
- ENVR 533.** Photolysis and product-to-parent reversion of dienogest. **M. O'Connor, E. Kolodziej, D.M. Cwitrny**
- ENVR 534.** Occurrence and composition of perfluorinated chemicals in wastewater for direct potable reuse. **B. Wang, E. Villegas, K. Dasu, A. Agrawal, M. Mills**
- ENVR 535.** Microcystin removal using powered activated carbon. **A. Bajracharya, J.J. Lenhart**
- ENVR 536.** Analytical procedure of silver nanoparticles in consumer products. **B. Lee, M. Song**
- ENVR 537.** UV/Persulfate degradation of 1,4-dioxane and kinetics modeling on radical contribution. **S.D. Patton, L. Li, K.P. Ishida, H. Liu**
- ENVR 538.** Fixation mechanism of cesium in clay minerals. **S. Park, J. Lee, K. Baek**
- ENVR 539.** Extraction characteristics of Pb using ferric-mineralogical approach. **J. Yoo, Y. Shin, G. Yoon, K. Baek**
- ENVR 540.** Role of clay minerals on Cr(VI) reduction. **S. Kwak, J. Yoo, K. Baek**
- ENVR 541.** Electrochemical activation of persulfate to remove azo-dye. **P. Jeon, S. Park, K. Baek**
- ENVR 542.** Adsorption characteristics of As(III) and As(V) onto modified alum sludge by calcination process. **E. Jeon, S. Ryu, K. Baek**
- ENVR 543.** Removal of calcium and strontium cations at concentrations found in hydraulic fracturing flowback water using pyridine based small molecules and soil bacteria. **S.G. Tajc**
- ENVR 544.** Synthesis of novel functionalized carbon nanoparticles and their potential use for water purification. **A. Gerard, F. Webster**
- ENVR 545.** Study of water adsorption/desorption isotherms on several fly ash sources. **T. Stortini, J. Greenspan, J.G. Navea**
- ENVR 546.** Effect of simulated solar radiation on the leach of iron from fly ash from various source regions. **D. Kim, J.G. Navea, H.D. Swomley**
- ENVR 547.** Quantum chemical calculations and vibrational spectroscopy of nitrate chemisorbed to SiO<sub>2</sub>. **K.C. Shi, J.G. Navea**
- ENVR 548.** Fly ash size and particle defects: A morphological study on proton-promoted iron leach from fly ash. **J.R. Borgatta, D. Kim, A. Paskavitz, J.G. Navea**
- ENVR 549.** Enhanced by computer applications. **V. Folorunso, A.E. Folorunso**
- ENVR 550.** Degradation of 2-nitrophenol using iron nanoparticles anchored to poly(acrylic acid) based electrospun fibers. **W.M. Lopez, N. Granda, W. Otaño**
- ENVR 551.** Mathematical modeling and simulation of the effect of molecular adsorption of organic compounds/TiO<sub>2</sub>-particles on six-flux-model. **M.A. Mueses, G. Li Puma, F. Machuca-Martinez**
- ENVR 553.** Evidence of lampricide photodegradation during field applications to tributaries of the Great Lakes. **C.K. Remucal, M. McConville, A.S. Ward**
- ENVR 552.** Removal of phenolic compounds from superficial water and wastewater using an inexpensive source of peroxidases. **E.P. Beiguel, S. Nasello, E.A. Hughes, J. Montserrat, A. Zalts**

## Section A

San Diego Convention Center  
Hall D

## Green Chemistry & the Environment

*Cosponsored by CEI*

A. M. Balu, R. Luque, S. O. Obare, *Organizers*

6:00 - 8:00

**ENVR 554.** Continuous flow preparation of iron oxide nanoparticles supported on mesoporous silicates. **A. Mata, A. Yezpe, A. Balu, A. Romero, R. Luque**

**ENVR 555.** Design of bionanocatalysts by mechanochemical processes and their application in alkylation reactions. **D. Rodriguez-Padron, A. Balu, M. Climent, A. Romero, R. Luque**

**ENVR 556.** Laccase catalyzed incorporation of thiol drugs into humic substances. **P. Du, H. Zhao, H. Cao**

**ENVR 557.** Withdrawn.

**ENVR 558.** Effect of rise velocity of influent of anaerobic biofilm reactor on treatment efficiency of petrochemical wastewater. **J. Li, Z. Zhang, D. Wang, L. Fang, Y. Yu, Y. Xiang, Y. Gong**

**ENVR 559.** Implication of particle size of titania on degradation of rhodamine B over TiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> mixed oxide materials. **S. Shrestha, S. Rasalingam, C. Wu, G. Mishra, R.T. Koodali**

**ENVR 560.** Process optimization studies of oil degrading *Dietzia cercidiphylli* strain X10 immobilization onto modified zeolite using response surface methodology. **X. Dai, G. Yan, L. Wang, S. Guo**

## Section A

San Diego Convention Center  
Hall D

## Science & Perception of Climate Change

*Cosponsored by CEI*

S. O. Obare, E. Schoffers, *Organizers*

6:00 - 8:00

**ENVR 561.** Understanding the mechanism of extractive electrospray ionization mass spectrometry for analyzing model secondary organic aerosols. **T.L. Longin, C. Kidd, L.M. Wingen, K. Lyster, S. Kumbhani, B.J. Finlayson Pitts**

**ENVR 562.** STEP as a chemical solution to mitigate climate change. **J. Ren, F. Li, P. Peng, J. Lau, J. Stuart, M. Lefler, J. Vicini, O. El-Ghazawi, S.L. Licht**

## Section A

San Diego Convention Center  
Hall D

## Sources, Fate & Transport of Perfluorinated Alkyl Substances in the Environment: Theory, Practice & Innovation

D. Kempisty, S. T. Kurwadkar, *Organizers*

6:00 - 8:00

**ENVR 563.** Human serum albumin binding of perfluoroalkyl acids. **A.W. Glaser, L. MacManus-Spencer**

## Section A

San Diego Convention Center  
Hall D

## Treatment of Contaminants of Emerging Concern & Their Transformation Products

*Cosponsored by CEI*

L. M. Blaney, A. J. Hernandez-Maldonado, *Organizers*

6:00 - 8:00

**ENVR 564.** Fabrication of visible-light active β-Bi<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> nanotubes array electrodes for enhanced photoelectrocatalytic glycerol oxidation. **D. Rivera, L.J. Hoyos, A.F. Gualdrón, J.L. Roper, M.E. Niño**

**ENVR 565.** Antimicrobial activity of fluoroquinolone, sulfonamide, and tetracycline antibiotics: Implications for environmental relevance. **H. Adejumo, K. He, L.M. Blaney**

**ENVR 566.** Multi-residue analysis of contaminants of emerging concern (CECs) in water and tissue samples from a freshwater environment by modified QuEChERS extraction followed by SPE-LC-MS/MS. **K. He, A. Timm, C. Welty, L.M. Blaney**

## Adsorption of Metals by Geomedia

*Sponsored by GEOC, Cosponsored by ENVR and NUCL*

## Environmental Interfaces

*Sponsored by GEOC, Cosponsored by COLL and ENVR*

## THURSDAY MORNING

## Section A

Omni San Diego Hotel  
Grand Ballroom C

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing Modeling

*Cosponsored by CEI, ENFL and GEOC*

D. L. Drogos, R. Kleinberg, W. Orem, W. Stringfellow, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 **ENVR 567.** Lessons learned about using data to understand water issues related to shale gas development in Pennsylvania: From science to sociology. **R.D. Vidic**, S. Brantley, J. Abad, D. Yoxheimer, C. Wilderman, J. Pollak, K. Brasier

8:30 **ENVR 568.** Hydraulic fracturing chemicals reporting and disclosure analysis of fracfocus data and lessons learned. **K. Konschnik**

8:50 **ENVR 569.** Climate impacts of tight oil production: Comparing the Bakken and Eagle Ford formations using detailed drilling and fugitive emissions estimates. **A. Brandt**, S. Yeh, K. Vafi, A. Ghandi, M. Wang, J. Englander

9:10 **ENVR 570.** Characteristics and environmental fate of flowback/produced water from hydraulically fractured wells in California. **C. Varadharajan**, H. Cooley, M. Heberger, W. Stringfellow, J.K. Domen, W.L. Sandelin, M. Camarillo, P.D. Jordan, M. Reagan, K. Donnelly, J. Birkholzer, J.C. Long

9:30 **ENVR 571.** Assessing occurrence and potential impacts of environmental contaminants associated with UOG waste handling and disposal practices. **I.M. Cozzarelli**, D.M. Akob, M. Engle, M.J. Focazio, K.B. Haase, D.B. Kent, A.C. Mumford, W. Orem, K. Skalak

9:50 Intermission.

10:10 **ENVR 572.** Unconventional approaches to unconventional resources: Regional-scale waste management strategies for sustainable shale gas development. **A.H. Menefee**, B. Ellis

10:30 **ENVR 573.** Evaluating the risks of surface spills at unconventional oil and gas production sites: A contaminant transport modeling study in the South Platte alluvial aquifer. **C. Kanno**, M. McLaughlin, J. Blotvogel, T. Borch, J.E. McCray

10:50 **ENVR 574.** Withdrawn.

11:10 **ENVR 575.** Water board's implementation of Senate Bill 4 requirements. **J. Zinky**

11:30 Panel Discussion.

## Section B

Omni San Diego Hotel  
Grand Ballroom E

### Aquatic Photochemistry

*Cosponsored by GEOC*

K. P. McNeill, *Organizer*

V. S. Lin, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 **ENVR 576.** Photolysis of munitions constituents in natural waters: Impact of salinity, temperature, pH, and fulvic acid concentration. **D.J. Luning Prak**, J.E. Breuer, E. Rios, D.W. OSullivan

8:25 **ENVR 577.** Decomposition of algal toxin microcystin-LR by the combination of UV irradiation and chlorination processes. **X. Duan**, X. He, D.D. Dionysiou

8:45 **ENVR 578.** Photodegradability of personal care products ingredients in the aquatic environment. **J. Lin**

9:05 **ENVR 579.** Formation of bioactive transformation products via steroid photolysis. **D.M. Cwiertny**, E. Kolodziej

9:25 **ENVR 580.** Assessing the indirect photodegradation potential of emerging contaminants in tropical urban surface water using the artificial sweetener acesulfame as a probe. **R. Ling**, M. Reinhard

9:45 **ENVR 581.** Insights into the environmental photochemistry of bacitracin, an antimicrobial non-ribosomal peptide. **R. Lundeen**, C. Chu, M. Sander, K.P. McNeill

10:05 Intermission.

10:20 **ENVR 582.** Aquatic phototransformation of fenamate-based NSAIDs. **C.A. Davis**, E. Janssen, P.R. Erickson, K.P. McNeill

10:40 **ENVR 583.** Photochemical degradation of aminoglycoside antibiotics in simulated natural waters. **W. Song**

11:00 **ENVR 584.** Withdrawn.

11:20 **ENVR 585.** Role of dissolved organic matter on imazosulfuron photolysis. **C. Rering**, R.S. Tjeerdema

## Section C

Omni San Diego Hotel  
Grand Ballroom D

### Advances in In Situ Pollutant Destruction by Nanoscale Zero Valent Iron & Other Engineered Nanoparticles

#### Applications of Nanoparticles to Pollutant Degradation: Inorganic Pollutants

A. Agrawal, S. R. Kanel, B. A. Manning, *Organizers, Presiding*

8:00 **ENVR 586.** Arsenic removal from water by nanoscaled zerovalent iron and iron oxides. **C. Su**

8:30 **ENVR 587.** Macroporous alginate substrate-bound growth of Fe<sup>0</sup> nanoparticles: Synthesis, structural characterization and application in nitrate reduction. **C. Lee**, Y. Chang, Y. Chang

8:50 **ENVR 588.** Imaging and spectroscopic studies of inorganic contaminant-treated nanoscale zerovalent particles. **B.A. Manning**, S.R. Kanel

9:10 **ENVR 589.** Novel magnetic sulfide modified nanoscale zerovalent iron with film-like structure for metal removal. **A.A. Keller**, Y. Su, A.S. Adeleye, Y. Huang, X. Zhou, Y. Zhang

9:30 Intermission.

9:50 **ENVR 590.** Surface reactions and modification of nanoscale zero-valent iron (nZVI) and iron oxide nanoparticles for environmental remediation. **B.E. Koel**

10:20 **ENVR 591.** Heavy metal remediation by nanoscale clay mineral. **H. Dong**

10:40 **ENVR 592.** Withdrawn.

11:00 **ENVR 593.** Stable bimetallic catalyst supported by nZSM-5 for selective nitrate reduction. **S. Hamid**, M.A. Kumar, W. Lee

11:20 **ENVR 594.** Reduction of decabromodiphenyl ether by organo-modified smectite clay-templated subnanoscale zero-valent iron. **K. Yu**, C. Gu, S. Boyd, W. Zhang, B.J. Teppen, C. Sun, H. Li

11:40 Concluding Remarks.

## Section D

Omni San Diego Hotel  
Gaslamp 4

### Membrane Technology for Water-Energy Sustainability

*Cosponsored by CEI*

D. Jassby, B. Mi, *Organizers, Presiding*

8:00 **ENVR 595.** Energy recovery from defective tomatoes (culls) using microbial electrochemical systems: Evaluating impedance characteristics of peel & seed to oxidation of culls. **A. Fogg**, N. Shrestha, D. Franco, V.R. Gadhamshetty

8:20 **ENVR 596.** Use of nanofiltration membranes for acid mine drainage treatment. **S. Wadekar**, R.D. Vidic

8:40 **ENVR 597.** Energy storage by reversible desalination: A concentration battery based on electro dialysis. **R.S. Kingsbury**, K. Chu, O. Coronell

9:00 **ENVR 598.** Hydrophobic microporous membranes for the recovery of insoluble oil from emulsions. **A. Mercelat**, L.E. Katz, K. Kinney, F. Seibert

9:20 Intermission.

9:40 **ENVR 599.** Adsorptive membranes for ammonia removal. **P. Ahmadiannamini**, S. Eswaranandam, R. Wickramasinghe, X. Qian

10:00 **ENVR 600.** Algal harvesting and destabilization by Ti<sub>4</sub>O<sub>7</sub> reactive electrochemical membrane. **L. Hua**, L. Guo, M. Thakkar, D. Wei, M. Agbakpe, L. Kuang, M. Magpile, B.P. Chaplin, Y. Tao, D. Shuai, X. Zhang, S. Mitra, W. Zhang

10:20 **ENVR 601.** Osmotic membrane electrochemical bioreactor for wastewater treatment and power production. **D.D. Hou**, L. Lu, Z. Ren

10:40 **ENVR 602.** Removal of surfactant-stabilized oil with γ-Fe<sub>2</sub>O<sub>3</sub> magnetic nanoparticles. **X. Zhu**, A. Dudchenko, D. Jassby

11:00 **ENVR 603.** Evaluating the use of metal dichalcogenide as corrosion-resistant coatings in aggressive microbial conditions. **K. Chilkoor Gopala**, N. Shrestha, V.R. Gadhamshetty

## Section F

Omni San Diego Hotel  
Gaslamp 3

### Chemistry & Application of Advanced Oxidation Processes for Water Purification, Treatment & Reuse

D. D. Dionysiou, G. Li Puma, D. Minakata, X. Quan, *Organizers*

K. E. O'Shea, *Organizer, Presiding*

M. Zanolli, *Presiding*

8:00 **ENVR 604.** Ti/TiO<sub>2</sub> nanotubes photoanodes applied on photoelectrocatalytic glucose oxidation. **R. Fabrao**, R.M. Fabrao, J.F. Brito, J. Silva, N.R. Stradiotto

8:35 **ENVR 605.** 4-chlorophenol removal by electro-Fenton-like process. **R. Natividad**, G. Santana-Martinez, G. Roa, R. Romero, E. Martin Del Campo, A. Ramirez-Serrano

9:00 **ENVR 606.** Development of a highly efficient, cost effective anode for chlorine evolution and wastewater electrolysis. **D. Ocasio**, Y. Yang, J. Naviaux, M.R. Hoffmann

9:25 **ENVR 607.** Enhancement in photoelectrocatalytic activity of TiO<sub>2</sub> nanotube arrays sensitized with CoFe<sub>2</sub>O<sub>4</sub>-graphene oxide composite for glycerol oxidation. **M. Niño**, N. Pico, Á. Meléndez

9:50 Intermission.

10:00 **ENVR 608.** Influence of electrode materials in the photoelectrocatalytic CO<sub>2</sub> reduction. **J.F. Brito**, M. Zanolli

10:25 **ENVR 609.** Abiotic and biotic catalysis of electrolytic 1,4-dioxane oxidation. **J. Blotvogel**, J. Jasmann, T.C. Sale, V. Glezakou, M. Myers, P. Gedalanga, S. Mahendra, T. Borch

10:50 **ENVR 610.** Photoelectrocatalytic oxidation of phenol by using TiO<sub>2</sub> anode. **J. Rodriguez**, J. Villota Zuleta

11:15 **ENVR 611.** Aggregation behavior of TiO<sub>2</sub> particles under UV light irradiation and its effects on photocatalytic hydrogen production. **B. Luo**, D. Jing

11:40 **ENVR 612.** Determination of the enthalpy of oxidation of soils using permanganate and persulfate. **N.A. Moulton**, S.P. Mezyk, M. Becker

### Greener Pathways to Organics & Nanomaterials: Sustainable Applications of Magnetic Nanocatalysts

*Sponsored by I&EC, Cosponsored by ENVR†*

#### Adsorption of Metals by Geomedia

#### Biosorption: Metal & Bacteria

*Sponsored by GEOC, Cosponsored by ENVR, MPPG† and NUGL*

#### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

## THURSDAY AFTERNOON

## Section A

Omni San Diego Hotel  
Grand Ballroom C

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Regulatory Aspects

*Cosponsored by CEI, ENFL and GEOC*

D. L. Drogos, R. Kleinberg, W. Orem, W. Stringfellow, *Organizers, Presiding*

1:30 **ENVR 613.** Assessment of hydraulic fracturing in California. **J.C. Long**, J. Birkholzer, L. Feinstein

2:10 **ENVR 614.** Potential shale oil production in California and its possible environmental consequences. **D. Gautier**, L. Feinstein, P. Dobson

2:30 **ENVR 615.** Groundwater monitoring for oil and gas development under California SB4. **B.K. Esser**, H.R. Beller, S.A. Carroll, J.A. Cherry, J. Gillespie, R.B. Jackson, P.D. Jordan, V. Madrid, J.P. Morris, B. Parker, W. Stringfellow, C. Varadharajan, A. Vengosh

2:50 **ENVR 616.** Regional monitoring of the effects of oil and gas development on groundwater resources in California. **M.K. Landon**, K.A. Taylor, P. McMahon, J.T. Kulongoski, M.S. Fram, L.B. Ball

3:10 Intermission.

3:30 **ENVR 617.** Unconventional oil and gas production: Studies by the consortium on health and energy research (CHER) group. **J. Zelikoff**, M. McCawley, W. Orem, T. Knuckles, B. Yan, L. Chen, G. Thurston, T. Gordon, M. Nye, M. Haley, J. Osborne, B. Stout, S. Chillrud, M. Howarth, J. Ross, J. Hause, L. Smith, M. Varonka, S. Poune, A. Kolker

**3:50 ENVR 618.** Improving public perception of environmental impacts for hydrofracking sites. **N. Duplan, M. Carr, J. Hawthorne**

**4:10 ENVR 619.** FracTracker abroad: Comparing international management of fossil fuel resources. **K. Ferrar, S.M. Rubright**

**4:30 ENVR 620.** Withdrawn.

**4:50** Panel Discussion.

## Section B

Omni San Diego Hotel  
Grand Ballroom E

### Aquatic Photochemistry

*Cosponsored by GEOC*

V. S. Lin, *Organizer*

K. P. McNeill, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 ENVR 621.** Photo-oxidation of dissolved organic carbon in natural waters: Insights from isotopic fractionation of DIC during initial stages of irradiation. **L. Powers, J. Brandes, A. Stubbins, W. Miller**

**1:55 ENVR 622.** Photochemical degradation of dissolved organic matter in natural waters: Characterizing the more labile constituents using gradient solid phase extraction. **B. Cottrell, M. Gonsior, S. Timko, I. Pinto, D.P. Soulsby, W.J. Cooper**

**2:15 ENVR 623.** Enhanced indirect photochemistry of dissolved free and combined histidine through association with chromophoric dissolved organic matter. **C. Chu, R. Lundeen, C.K. Remucal, M. Sander, K.P. McNeill**

**2:35 ENVR 624.** Mechanisms and factors controlling photochemical transformation of mercury and methylmercury in the aquatic environment. **B. Gu**

**2:55 ENVR 625.** Simulated sunlight-assisted fast oxidation of  $Mn^{2+}$  (aq) and formation of birnessite ( $\delta$ - $MnO_2$ ) nanosheets. **H. Jung, Y. Jun**

**3:15** Intermission.

**3:30 ENVR 626.** Estimation of the rate constants of photochemical generated dissolved gaseous mercury (DGM) in a lake using a simple mass balance model: A preliminary study. **L.S. Kocher, H. Zhang**

**3:50 ENVR 627.** Role of iron mediated photo-Fenton processes on the photofate of agrochemicals in wetlands. **C. Yuan, L. Weavers, Y. Chin**

**4:10 ENVR 628.** Removal of arsenic by UV photoreduction in the presence of dithionite. **B. Jung, A. Abdel-Wahab**

**4:30 ENVR 629.** Implications of iron(III) photoreduction in littoral sediments: A new look at the biogeochemical iron cycle. **C. Lockwood, U. Lueder, F. Schaedler, T. Himpel, C. Schmidt, A. Kappler**

**4:50 ENVR 630.** Impacts of tributaries on optical properties, singlet oxygen concentrations and contaminant photo-reactions in selected near-shore areas of the Great Lakes. **R.G. Zepp, G. Whelan, M. Molina, M. Cyterski, K. Wong, B. Acrey, A. Commodore**

## Section C

Omni San Diego Hotel  
Grand Ballroom D

### Advances in In Situ Pollutant Destruction by Nanoscale Zero Valent Iron & Other Engineered Nanoparticles

#### Applications of Nanoparticles to Pollutant Degradation: Organic Pollutants

A. Agrawal, S. R. Kanel, B. A. Manning, *Organizers, Presiding*

**1:30 ENVR 631.** Direct observation of interactive behavior for DNAPL-NZVI in porous media. **H. Choi**

**2:00 ENVR 632.** Evaluating the reactivities of nano zero-valent iron (nZVI) and Ni-modified nano zero-valent iron (Ni-nZVI) supported on clays, biochar and metal oxides towards groundwater pollutant. **R. Chowdhury, R. Ghose, A. Agrawal**

**2:30 ENVR 633.** Iron nanoparticle immobilized flat sheet and hollow fiber membranes for water remediation. **S. Hernández Sierra, D. Bhattacharyya, S. Lei, R. Wang, L. Ormsbee**

**2:50 ENVR 634.** Influence of natural organic matter on contaminant remediation by iron oxides with adsorbed Fe(II). **J.H. Strehlau, W. Arnold, R. Penn**

**3:10** Intermission.

**3:30 ENVR 635.** Surface conditioning of ZVI for enhanced dechlorination reactivity and material stability. **W. Yan, Y. Han**

**4:00 ENVR 636.** Withdrawn.

**4:20 ENVR 637.** Removal of reactive black 5 azo dye from water using nano MgO powder and immobilized MgO on cellulose fibre. **M. Chaubal, T. Ambawala, U.D. Patel, J. Ruparella**

**4:40 ENVR 638.** Reactivity of chemo-genic ferrous hydroxide and magnetite nanoparticles towards degradation of select chlorinated hydrocarbons. **A. Burdsall, A. Agrawal**

**5:00 ENVR 639.** Reductive photocatalysis of azo dyes using  $TiO_2$  nano-particles in the presence of some natural anti-oxidants as Hole scavengers. **B. Shah, M.A. Doshi, J. Ruparella, U.D. Patel**

**5:20** Concluding Remarks.

## Section D

Omni San Diego Hotel  
Gaslamp 4

### Membrane Technology for Water-Energy Sustainability

*Cosponsored by CEI*

D. Jassby, B. Mi, *Organizers, Presiding*

**1:30 ENVR 640.** Water-filled voids account for a significant volume fraction of the polyamide active layers of thin-film composite membranes and affect their water and solute transport properties. **L. Lin, R. Lopez, G. Ramon, O. Coronell**

**2:00 ENVR 641.** Modeling and minimization of dilutive ECP on support layer structure of forward osmosis membranes. **C. Morrow, A. Childress**

**2:20 ENVR 642.** Biofouling in-situ monitoring in spiral-wound membrane using optical coherence tomography (OCT). **L. Fortunato, R. Valladares Linares, H. Vrouwenvelder, T. Leiknes**

**2:40 ENVR 643.** Modeling and simulation of direct contact membrane distillation system for produced water treatment using Aspen Plus platform. **O.R. Lokare, R.D. Vedic**

**3:00 ENVR 644.** Development of innovative anti-biofouling polyamide thin film composite membranes with biofilm inhibiting 2-aminoimidazoles incorporated. **A. Atkinson, J. Wang, Z. Zhang, D. Zeng, A. Pollard, D. Jung, A. Gold, O. Coronell**

**3:20** Intermission.

**3:40 ENVR 645.** Partitioning of inorganic contaminants into the polyamide active layers of thin-film composite membranes for water purification. **J. Wang, L.A. Perry, O. Coronell**

**4:00 ENVR 646.** CLSM-compatible fluidic membrane biofilm flow cell as a novel tool to study membrane biofouling dynamics. **M. Mukherjee, N. Menon, Y. Kang, B. Cao**

**4:20 ENVR 647.** Electrochemical impedance spectroscopy study of membrane fouling and electrochemical regeneration at a sub-stoichiometric  $TiO_2$  reactive electrochemical membrane. **Y. Jing, L. Guo, B.P. Chaplin**

**4:40 ENVR 648.** Improving anti-biofouling property of the thin-film composite (TFC) reverse osmosis (RO) membrane by copper nanoparticles (CuNPs). **W. Ma, A. Soroush, T. Luong, S. Rahaman**

**5:00 ENVR 649.** Ultrafiltration membrane purification efficiency and mechanism with the synergistic effect of flocs. **B. Ma, C. Hu, H. Liu, J. Qu**

### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

## FLUO

## Division of Fluorine Chemistry

V. Petrov, *Program Chair*

### BUSINESS MEETINGS:

**FLUO Business Meeting, 8:00 AM: Tue**

## SUNDAY MORNING

### Section A

The Westin San Diego Gaslamp Quarter  
Harbor A/B

#### ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Steven H. Strauss

O. V. Boltalina, V. Petrov, N. Vasdev, *Organizers*

J. S. Thrasher, *Organizer, Presiding*

D. V. Peryshkov, *Presiding*

**8:00** Introductory Remarks.

**8:10 FLUO 1.** Creative design of experiments and equipment in service of fluorine chemistry. **I.V. Kuvychko**

**8:40 FLUO 2.** Novel metal-free B-H activation of icosahedral boron clusters. **D.V. Peryshkov, Y. Wong**

**9:10 FLUO 3.** Oxidation of fluorinated and other halogenated  $CB_{11}$  carborane anions. **F. Sembera, A. Wahab, Z. Janousek, J. Ludvik, J. Klima, R. Crespo, C. Piqueras, J. Michl**

**9:40** Intermission.

**10:00 FLUO 4.** Oxidation of fluorinated benzenes, dialkylchalcogenides, and perfluorophenyl-dichalcogenides. **M. Malischewski, H. Poleschner, M.A. Khanfar, K. Seppelt**

**10:30 FLUO 5.** Does the  $NF_4^+$  radical play a role in the synthesis of  $NF_4^+$  salts? **K.O. Christe, D.A. Dixon**

**11:00 FLUO 6.**  $[XeOXeOXe]_{[u-F(ReO_2F_3)_2]_2}$ ,  $F_6XeNCCH_3$ , and  $F_6Xe(NCCH_3)_2$ : Syntheses, structures and bonding. **M. Ivanova, J. Haner, K. Matsumoto, H. Mercier, G.J. Schrobilgen**

## SUNDAY AFTERNOON

### Section A

The Westin San Diego Gaslamp Quarter  
Harbor A/B

#### ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Steven H. Strauss

O. V. Boltalina, J. S. Thrasher, N. Vasdev, *Organizers*

V. Petrov, *Organizer, Presiding*

C. K. Chambliss, *Presiding*

**1:00 FLUO 7.** Chemistry of new refrigerant – 3,3,3,2-tetrafluoropropene-1 (HFO-1234yf). **V. Petrov, C. Junk, S. Shelyashenko, N. Pavlenko, Y. Yagupolskii, M. Nappa**

**1:30 FLUO 8.** Novel fluorinating reagents - fluorinated diazoalkanes. **P.K. Mykhailiuk**

**2:00 FLUO 9.** Reactions of nitriles with anhydrous HF: Synthesis of nitrilium and a-fluorinated alkylammonium salts. **R.M. Haiges, A.F. Baxter, K.O. Christe**

**2:30** Intermission.

**2:50 FLUO 10.** Advance in electrophilic trifluoromethylating agents. **T. Umemoto**

**3:20 FLUO 11.** Difluoromethylation and difluoromethylenation. **S.G. Prakash**

**3:50 FLUO 12.** New metal-mediated fluoroalkylation reactions. **D.A. Vicic, P.T. Kaplan, L. Xu, S. Yu**

**4:20 FLUO 13.** Withdrawn.

**4:50** Concluding Remarks.

## SUNDAY EVENING

### Section A

San Diego Convention Center  
Halls B/C

#### ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Steven H. Strauss

O. V. Boltalina, J. S. Thrasher, N. Vasdev, *Organizers*

V. Petrov, *Organizer, Presiding*

**6:00 - 8:00**

**FLUO 14.** Copper-catalyzed oxidative cyclization: Synthesis of 3-carbonyl-1-trifluoromethylpyrrolo[1,2-a]quinolines. **Z. Xu, F. Ni, J. Han, J. Chen, H. Zhang, W. Cao**

**FLUO 15.** Stereoselective synthesis of *trans*-perfluoroalkylated [1,3]oxazino[2,3-*a*]isoquinolines from aromatic aldehydes, methyl perfluoroalk-2-ynoates and isoquinolines. Z. Xu, T. Sun, Q. Cai, J. Han, J. Chen, H. Zhang, W. Cao

**FLUO 16.** Efficient one-pot two-step three-component process for the synthesis of perfluoroalkylated indolizines. D. He, Y. Xu, J. Han, J. Chen, H. Zhang, W. Cao

**FLUO 17.** Efficient one-pot two-step three-component process for the synthesis of trifluoromethylated chromenes. X. Yan, J. Han, G. Jiang, Y. Yang, J. Chen, H. Zhang, W. Cao

**FLUO 18.** Efficient process for the synthesis of fluorine and phosphorus containing 4*H*-pyrans. D. He, Y. Shen, J. Han, J. Chen, H. Zhang, W. Cao

**FLUO 19.** Efficient process for the synthesis of perfluoroalkylated benzazepines. X. Sun, J. Han, J. Chen, H. Zhang, W. Cao

**FLUO 20.** Crown ether nucleophilic catalysts (CENCs) for the ultrafast fluorination of silicon. S. Jana, M.H. Al-hunuti, S.D. Lepore

**FLUO 21.** Trifluoromethyl ether and trifluoromethyl thioether synthesis by silver catalyzed decarboxylative fluorination. S. Krishnamoorthy, S.D. Schnell, H. Dang, S.G. Prakash

**FLUO 22.** Computational study of the fluoro-substituent effect on cyclopropane acidity. J. Hinckley, G. Shelton

## MONDAY MORNING

### Section A

The Westin San Diego Gaslamp Quarter Harbor A/B

#### ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Steven H. Strauss

O. V. Boltalina, V. Petrov, J. S. Thrasher, N. Vasdev, *Organizers*

J. Rack, A. P. Sattelberger, *Presiding*

**8:30 FLUO 23.** Synthesis and characterization of novel metal polycyano compounds. P. Deokar, D. Leitz, R.M. Haiges, K.O. Christe

**9:00 FLUO 24.** Coordination modes of sterically hindered imidazolate ligands in metal complexes. S. Ivanov, W. Bailey, X. Lei, A. Derecskei-Kovacs, J. Norman

**9:30 FLUO 25.** Fullerene metal-organic frameworks. N.B. Shustova, D.E. Williams, E.A. Dolgoplova, A.M. Rice

**10:00** Intermission.

**10:20 FLUO 26.** Photoisomerization and photorefraction in ruthenium sulfoxide complexes. J. Rack

**10:50 FLUO 27.** Trifluoromethylfullerenes as model compounds for unraveling the photophysics of organic photovoltaics. N. Kopidakis

**11:20 FLUO 28.** Photoinduced electron transfer processes of trifluorinated molecules dispersed in conjugated polymer films. G. Rumbles

## MONDAY AFTERNOON

### Section A

The Westin San Diego Gaslamp Quarter Harbor A/B

#### ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Steven H. Strauss

V. Petrov, J. S. Thrasher, N. Vasdev, *Organizers*

O. V. Boltalina, *Organizer, Presiding*

N. B. Shustova, *Presiding*

**1:00 FLUO 29.** Perfluoroalkylated polyaromatic: Unique supramolecular synthons for functional organic materials. H. Sun

**1:30 FLUO 30.** Fluorine chemistry of carbon-rich and all-carbon substrates. O.V. Boltalina, S.H. Strauss, K.P. Castro, K. Rippey, N.J. DeWeerd, L. San, T. Cikeman, E.V. Bukovsky, C. Brook, B. Reeves

**2:00 FLUO 31.** Novel separations and analyses contributing to an improved molecular-level understanding of energy-relevant complex mixtures. C.K. Chambliss

**2:30** Intermission.

**2:45 FLUO 32.** Challenge to modern fluoro-chemists to recover fluoride from waste and depleted materials posing environmental threats. D.T. Meshri, S.D. Meshri, R. Adams, N.C. Mathur, H. Bhinhar, D. Pinnareddy, S. Bhagat

**3:15 FLUO 33.** Short F---F and F(Cl)---O contacts in fluoroorganic crystals, and short Ag---Ag and Ag---O contacts in silver polyfluoroacetate salts. X. Liu, A. Matsnev, S.P. Belina, C.D. McMillen, J.S. Thrasher

**3:45 FLUO 34.** Inorganic synthesis using salts of the bifluoride ion. A.P. Sattelberger

**4:15 FLUO 35.** Direct fluorination of B<sub>12</sub>H<sub>12</sub><sup>2-</sup>, B<sub>12</sub>H<sub>11</sub>(NH<sub>3</sub>)<sup>-</sup>, and isomers of B<sub>12</sub>H<sub>10</sub>(NH<sub>3</sub>)<sub>2</sub><sup>0</sup> in CH<sub>3</sub>CN: The effects of added KF, HF, or H<sub>2</sub>O. E.V. Bukovsky, A.M. Pluntze, D.V. Peryshkov, S.H. Strauss

**4:55** Concluding Remarks.

## MONDAY EVENING

### Section A

The Westin San Diego Gaslamp Quarter Harbor A/B

#### ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Steven H. Strauss

O. V. Boltalina, V. Petrov, J. S. Thrasher, N. Vasdev, *Organizers*

R. M. Haiges, *Presiding*

**6:00 FLUO 36. Award Address (ACS Award for Creative Work in Fluorine Chemistry sponsored by the Juhua Group Technology Center (China)).** From weak electron (pair) donors to strong electron acceptors. S.H. Strauss

## GEOC

### Division of Geochemistry

Y. Jun, *Program Chair*

#### OTHER SYMPOSIA OF INTEREST:

**New Challenges on Metals & Metalloids: Chemistry, Treatment & the Impacts on Water Quality** (see ENVR, Sun)

**Francis P. Garvan-John M. Olin Medal Award: Symposium in honor of Annie B. Kersting** (see NUCL, Mon)

**Carbonate & Sulfate Minerals: Nucleation, Growth and Control of Scale Formation** (see ENVR, Sun, Mon, Tue)

**Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing** (see ENVR, Mon, Tue, Wed, Thu)

**Aquatic Photochemistry** (see ENVR, Wed, Thu)

#### SOCIAL EVENTS:

**Reception, 5:30 PM:** Tue

#### BUSINESS MEETINGS:

**Business Meeting, 6:00 PM:** Sun

## SUNDAY MORNING

### Section A

Omni San Diego Hotel Grand Ballroom A

#### Closing the Human Phosphorus Cycle: Biogeochemistry, Sustainable Phosphorus Recovery, Speciation, Detection & Reuse

K. Ruttenberg, *Organizer*

L. E. Katz, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:10 GEOC 1.** Examples of the role of P in environmental chemistry: Lessons from density functional theory modeling. J.D. Kubicki

**8:40 GEOC 2.** Synchrotron-based techniques for determining phosphorus speciation in soils. A. Gamble, P. Northrup, D.L. Sparks

**9:05 GEOC 3.** Effects of Mg substitution on P K-edge XANES spectra of calcium phosphate minerals. D. Hilger, J. Hamilton, D. Peak

**9:25 GEOC 4.** Phosphorus speciation evolution during pedogenesis in a semi-arid environment. C. Gu, S.C. Hart, B.J. Cademenun, Y. Hu, L.C. Munn, M. Zhu

**9:50 GEOC 5.** Mineralogical controllers on phosphate bioaccessibility during subsurface PHC remediation. D. Peak, S. Siciliano, J. Hamilton, C. Phillips, D. Hilger, T. Carlson

**10:15** Intermission.

**10:30 GEOC 6.** Calcium phosphate-organic composites for a more sustainable P cycle: Learning from biomineralization. D. Kim, T.V. Wu, M. Cohen, Y. Jun

**10:55 GEOC 7.** Speciation dynamics of phosphorus during (hydro)thermal treatments of sewage sludge. R. Huang, Y. Tang

**11:20 GEOC 8.** Sorption, degradation and transformation of polyphosphates: Implications for understanding the biogeochemical cycling of polyphosphate. R. Huang, Y. Tang

**11:40 GEOC 9.** Effect of metal oxides on precipitation of struvite in synthetic livestock manure and human urine. J. Han, L.E. Katz

### Section B

Omni San Diego Hotel Grand Ballroom B

#### Geochemical Reactivity of Nanoparticles, Aggregates, Coatings & Organo-Nanoparticulate Flocculates

B. Gilbert, *Organizer*

C. S. Kim, *Organizer, Presiding*

**8:30 GEOC 10.** Role of Fe and Al-nanominerals on the contaminant mobility in Tinto and Odiel rivers. S. Carrero, A. Fernandez-Martinez, R. Pérez-López, J. Nieto

**8:50 GEOC 11.** Natural oxidized and reduced iron nanoparticles in the marine environment. G.W. Luther, S. Kato, A. Gartman, A. Findlay, C. Chan

**9:10 GEOC 12.** Electron mobility and trapping in ferrihydrite nanoparticles. J. Soltis, B. Gilbert, A. Schwartzberg, R. Penn

**9:30 GEOC 13.** Effects of aggregation, ligand complexation and time on metal adsorption/retention to iron oxyhydroxide nanoparticles. C. Kim

**9:50** Intermission.

**10:10 GEOC 14.** Cation effects on the reactions of birnessite with Mn(II). P. Yang, Q. Wang, K. Livi, M. Zhu

**10:30 GEOC 15.** Adsorption and oxidation of fulvic acid by birnessite. Q. Wang, P. Yang, M. Zhu

**10:50 GEOC 16.** Natural noble metals nanoparticles: Formation and fate in aquatic environment. V.K. Sharma

**11:10 GEOC 17.** Microbial reduction of U60 nanoclusters by *Shewanella oneidensis* MR-1. Q. Yu, J. Fein

### Section C

Omni San Diego Hotel Grand Ballroom D

#### Analytical & Computational Isotope Geochemistry

*Cosponsored by ENVR and MPPG†*

J. D. Kubicki, *Organizer*

A. Sessions, *Organizer, Presiding*

**8:30 GEOC 18.** Rolling revolution in analytical isotope geochemistry. J. Eiler

**9:10 GEOC 19.** Diverse origins of Arctic and subarctic methane point source emissions identified with multiple substituted isotopologues. P. Douglas, J. Eiler, D. Stolper, D. Smith, K. Walter Anthony, C. Paull, S. Dallimore, M. Wik, P. Crill, M. Winterdahl, A. Sessions

**9:35 GEOC 20.** Development and calibration of new natural gas  $\delta^{13}\text{C}$  and  $\delta^2\text{H}$  reference standards. R. Dias, G.S. Ellis, D.D. Coleman

**10:00** Intermission.

**10:20 GEOC 21.** H-D fractionation factors at individual sites on model petroleum compounds. J.D. Kubicki, M.V. LaCroce, C.C. Trout

**10:45 GEOC 22.** Path-integral methods for clumped and position-specific isotope studies. M. Webb, T.F. Miller

**11:10 GEOC 23.** Use of isotopes to elucidate mechanisms of nuclear waste glass corrosion. J. Neeway, J. Ryan, S.N. Kerisit

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## SUNDAY AFTERNOON

## Section A

Omni San Diego Hotel

Grand Ballroom A

## Environmental Interfaces

## Surface Structures

Cospponsored by COLL, ENVR and MPPG‡

A. M. Chaka, F. Geiger, A. Ilgen, *Organizers*Y. Jun, *Organizer, Presiding*

**1:30** GEOC 24. Spectroscopy and vibrational dynamics of strongly hydrogen bonded OH species at the  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (110)/H<sub>2</sub>O interface. A. Tuladhar, S. Dewan, E. Borguet

**2:10** GEOC 25. Direct comparison of DFT simulations with X-ray reflectivity data: The Al<sub>2</sub>O<sub>3</sub>(001)-water interface. P. Fenter, Y. Chen, E. Bylaska, J. Catalano, J. Weare

**2:50** GEOC 26. Structure and dynamics of water in natural organic matter: Variable temperature <sup>2</sup>H NMR results. V. Uddigiri, G.M. Bowers, J. Kirkpatrick

**3:10** GEOC 27. Ion-probe flow microcalorimetry and logistic modeling studies of the sorbent-water interface of (de)protonatable surfaces. O.R. Harvey

**3:30** Intermission.

**3:50** GEOC 28. Oxide/water interfaces probed by nonlinear optics. F. Geiger

**4:30** GEOC 29. Combining nonlinear optical methods to understand the interplay of water structure and surface potential at the silica/aqueous ion interface. J. Gibbs-Davis, A. Darlington, M. Azam

**4:50** GEOC 30. Connecting observations and simulations of the silica-water interface. J.D. Kubicki, J.D. Boettger, M. DelloStritto, J.O. Sofo

**5:10** GEOC 31. Modeled anionic stabilization of silica surface charge at low pH. J. Boettger, F. Tielens, M. DelloStritto, J.O. Sofo, J.D. Kubicki

## Section B

Omni San Diego Hotel

Grand Ballroom B

## Frontiers in Microscopic Techniques &amp; Applications to Geochemical Reactions

S. N. Kerisit, S. L. Riechers, *Organizers*J. Soltis, *Presiding*

**1:30** Introductory Remarks.

**1:35** GEOC 32. Using liquid-phase TEM to develop a unified framework to describe mineralization by particle attachment. J. De Yoreo

**2:10** GEOC 33. Influence of natural organic matter on relative reaction rates on different goethite crystal surfaces. R. Penn, J.H. Strehlau, A.M. Stemig, J. Tensfeldt, W. Arnold

**2:45** GEOC 34. Correlative cryo-TEM, cryo-SHXM and cryo-STXM study of selenium bioreduction in a contaminated aquifer. S. Fakra, B. Luef, T. Tyliczszak, C.J. Castelle, S.W. Mullin, L. Hug, M.A. Marcus, K. Williams, J.F. Banfield

**3:20** Intermission.

**3:40** GEOC 35. Toward predictive geochemistry: Time resolved, high resolution studies of atmospheric particle transformations. W. Harlow, M. Giordano, P.F. DeCarlo, M. Taheri

**4:15** GEOC 36. Selective preservation of organic carbon species in amended field soils using multi-edge STXM coupled with XANES spectroscopy. J. Yang, J. Wang, D.L. Sparks, C. Rumpel, N. Bolan

**4:35** GEOC 37. Atomic force microscopy measurements of layer heterogeneity in smectite swelling. D.S. Arndt, M.M. McGuire

## Section C

Omni San Diego Hotel

Grand Ballroom D

## Analytical &amp; Computational Isotope Geochemistry

Cospponsored by ENVR and MPPG‡

A. Sessions, *Organizer*J. D. Kubicki, *Organizer, Presiding*

**1:30** GEOC 38. Equilibrium mass-independent fractionation signatures. E. Schauble, E. Young

**2:10** GEOC 39. CO<sub>2</sub> hydration/hydroxylation and the origin of carbonate kinetic isotope effects. J. Boettger, J.D. Kubicki

**2:35** GEOC 40. Chromium incorporation and isotopic fractionation in different calcium carbonate phases: Implications for the Cr isotope paleoproxy. A. Brady, X. Wang, N. Planavsky, C. Reinhard, Y. Tang

**3:00** Intermission.

**3:20** GEOC 41. Isotope fractionation induced by ligand-promoted mobilization of Cr(III). E. Saad, X. Wang, C. Reinhard, N. Planavsky, Y. Tang

**3:45** GEOC 42. Zn isotope fractionation during sorption onto kaolinite. D. Guinoiseau, A. Gelabert, P. Louvat, M.F. Benedetti

**4:10** GEOC 43. Kinetic Monte Carlo study of interfacial Fe-isotope exchange in the redox transformation of iron(III) oxides. P. Zarzycki, K. Rosso

## Discussions with the President's Task Force on Employment

Sponsored by PRES, Cospponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## SUNDAY EVENING

## My Comments to the President's Task Force on Employment

Sponsored by PRES, Cospponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## My Experience with &amp; Advice for Improving Diversity in Chemistry

Sponsored by PRES, Cospponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

## My Experiences in &amp; Advice for Organic Chemistry Courses

Sponsored by PRES, Cospponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

## MONDAY MORNING

## Section A

Omni San Diego Hotel

Grand Ballroom A

## Environmental Interfaces

## Redox Reactions

Cospponsored by COLL, ENVR and MPPG‡

A. M. Chaka, F. Geiger, Y. Jun, *Organizers*A. Ilgen, *Organizer, Presiding*

**8:00** GEOC 44. Organic contaminant reduction at the clay mineral-water interface. A. Neumann, K.A. Rothwell, T.L. Olson, D. Latta, M. Scherer

**8:40** GEOC 45. Impacts of manganese oxides on the retention, speciation, and lability of soil organic carbon. J. Stuckey, D.L. Sparks

**9:00** GEOC 46. Impact of redox conditions on interfacial uranium chemistry in complex natural sediments. J.R. Bargar, S. Bone, J. Lezama-Pacheco, D. Alessi, J.M. Carrato, H. Veeramani, V. Noël, E. Suvorova, R. Bernier-Latmani, D. Giammar, P. Long, K. Williams

**9:40** GEOC 47. Regional importance of organic-rich sediments to uranium mobility in the upper Colorado River Basin. V. Noel, K. Boye, J.R. Bargar, P. Lefebvre, K. Maher, S.E. Bone, J. Lezama, E. Carderelli, W. Dam, R. Johnson

**10:00** Intermission.

**10:20** GEOC 48. Ab initio thermodynamics of how the oxidation of uranium dioxide's surface, subsurface, and bulk is determined by the chemical potentials of oxygen and water in the environment. A.M. Chaka, J. Stubbs, E. Ilton, E. Mark, P.J. Eng

**11:00** GEOC 49. Mineral-mediated processes of atmospheric importance: Semiconductor photocatalysis and transition metal ion catalysis. V.H. Grassian

**11:40** GEOC 50. First-principles investigation of Fe(II) adsorption and electron transfer at the goethite/water interfaces. V. Alexandrov, K. Rosso

## Section B

Omni San Diego Hotel

Grand Ballroom B

## Frontiers in Microscopic Techniques &amp; Applications to Geochemical Reactions

S. N. Kerisit, *Organizer*S. L. Riechers, *Organizer, Presiding*

**8:30** GEOC 51. Investigating the mineral-water interface using *in situ* high-resolution atomic force microscopy techniques. M. Nalbach, C. Marutschke, R. Momper, M. Schreiber, R. Bechstein, A. Kühnle

**9:05** GEOC 52. Chemical tip front atom characterization for high resolution and force distance measurements in ambient and liquid conditions. D.S. Wastl, M. Judmann, J.J. Weymouth, F.J. Giessibl

**9:40** GEOC 53. Surface morphology control versus molecular self-assembly: An *in situ* high-resolution atomic force microscopy study on calcite (10.4). M. Nalbach, S. Klassen, H. Söngen, R. Bechstein, A. Kühnle

**10:00** Intermission.

**10:20** GEOC 54. Microscopic observations of heterogeneous nucleation of manganese (hydr)oxide nanoparticles on geomedia. Y. Jun, H. Jung

**10:55** GEOC 55. Friction force microscopy in water: A powerful technique for mechanical-crystallographic investigations. E. Gneco, G. Vilhena, R. Perez, C. Pimentel, C. Pina

**11:30** GEOC 56. Probing dynamic heteroepitaxial nucleation processes of carbonates by atomic force microscopy. S.L. Riechers, S.N. Kerisit, K. Rosso

**11:50** GEOC 57. Microscopic pore-scale analysis of calcium carbonate precipitation and dissolution kinetics in microfluidic experiments. H. Yoon, C.J. Werth

## Environmental Aspects of Unconventional Oil &amp; Gas Production &amp; Hydraulic Fracturing

## Environmental Chemistry/Water Chemistry

Sponsored by ENVR, Cospponsored by CEI, ENFL and GEOC

## Is There a Crisis in Organic Chemistry Education?

Sponsored by PRES, Cospponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

## Carbonate &amp; Sulfate Minerals: Nucleation, Growth &amp; Control of Scale Formation

Sponsored by ENVR, Cospponsored by GEOC

## MONDAY AFTERNOON

## Section A

Omni San Diego Hotel

Grand Ballroom A

## Environmental Interfaces

## Nucleation, Growth &amp; Dissolution Processes

Cospponsored by COLL, ENVR and MPPG‡

F. Geiger, A. Ilgen, Y. Jun, *Organizers*A. M. Chaka, *Organizer, Presiding*

**1:30** GEOC 58. Molecular-scale mechanisms of heterogeneous nucleation and growth at mineral-water interfaces. S.N. Kerisit, S.L. Riechers, E.S. Ilton, M. Xu, M. Engelhard, K. Rosso

**2:10** GEOC 59. Growth of barite as a function of the aqueous cation:anion ratio. J. Bracco, A.G. Stack, S.R. Higgins

**2:30** GEOC 60. Nanoscale forces behind crystallization by oriented aggregation. K. Rosso, X. Zhang, M. Sushko, Z. Shen, S.N. Kerisit, D. Li, J. Chun, M. Bowden, M. Engelhard, J. Liu, C.J. Mundy, J. De Yoreo

**3:10** GEOC 61. Structure and morphology of the hematite-solution interface during electrochemical reductive dissolution. M.E. McBriarty, J. Stubbs, O. Qafoku, R. Comes, P.J. Eng, K. Rosso

**3:30** Intermission.

**3:40** GEOC 62. Natural organic matter and arsenic create different reactive interfaces of iron(III) (hydr)oxide nanoparticles. Y. Jun, C.W. Neil

## Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**4:20 GEOC 63.** Promotion of arsenopyrite dissolution and secondary mineral formation and phase transformation by aqueous  $\text{Fe}^{3+}$ . C.W. Neil, Y. Jun

**4:40 GEOC 64.** Effect of  $\text{Fe}^{2+}$  and  $\text{Cr(VI)}$  on redox-active  $\text{CeO}_2$  nanoparticle surface properties and transformation in aqueous systems. J. Ray, C.W. Neil, H. Jung, Z. Liu, Y. Jun

**5:00** Introduction of a GEOC Student Travel Awardee.

**5:05 GEOC 65.** Influence of biological interfaces on nucleation pathways and kinetics of calcium phosphate minerals. D. Kim, B. Lee, S. Thomopoulos, Y. Jun

## Section B

Omni San Diego Hotel  
Grand Ballroom B

### Adsorption of Metals by Geomedia

#### Theory & Modeling after Twenty Years

*Cosponsored by ENVR, MPPG† and NUCL*

J. Fein, Y. Yang, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 GEOC 66.** Dirac's dream: Understanding metal sorption by geomedia using density functional theory. K. Kwon, K. Refson, G. Sposito

**2:15 GEOC 67.** Theoretical modeling of adsorption at mineral-water interfaces: A predictive synthesis from protons to biomolecules. D.A. Sverjensky

**2:55 GEOC 68.** Modeling inorganic arsenic adsorption by oxides, clay minerals, and soils using surface complexation models. S.R. Goldberg, H.A. Al-Abadleh

**3:15 GEOC 69.** Use of DFT thermodynamics calculations to better understand how  $\text{Cd}^{2+}$  adsorbs to kaolinite (100) and gibbsite (100) surfaces. H. Watts, P.A. O'Day, J.D. Kubicki

**3:35** Intermission.

**3:55 GEOC 70.** Molecular dynamics simulations of cesium adsorption on illite. I.C. Bourg, L.N. Lammers, K. Kolluri, M. Okumura, G. Sposito, M. Machida

**4:35 GEOC 71.** Modeling  $\text{CrO}_4^{2-}$  adsorption onto ferrihydrite. J.D. Kubicki, E. Cerkez, D.R. Strongin

**4:55 GEOC 72.** Constrained surface complexation modeling:  $\text{Zn}_{2+}$ ,  $\text{CO}_{2+}$ , and  $\text{Ni}_{2+}$  adsorption onto rutile to 250°C. M.L. Machesky, D. Wesolowski, J.D. Kubicki

**5:15 GEOC 73.** Adsorption of divalent metals and oxyanions to goethite-water interfaces. L.J. Criscenti, K. Leung, L.E. Katz

### Diversity-Quantification-Success?

*Sponsored by PRES, Cosponsored by BIOL, GELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

Technical program information known at press time.

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## Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

### Environmental Chemistry/ Water Chemistry

*Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC*

### Carbonate & Sulfate Minerals: Nucleation, Growth & Control of Scale Formation

*Sponsored by ENVR, Cosponsored by GEOC*

### Undergraduate Research Posters

#### Geochemistry

*Sponsored by CHED, Cosponsored by GEOC and SOCED*

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

Y. Jun, *Organizer*

**8:00 - 10:00**

20. See previous listings.

157-158, 160-161, 163, 167, 171, 173-176, 180-184. See subsequent listings.

## TUESDAY MORNING

### Section A

Omni San Diego Hotel  
Grand Ballroom A

### Environmental Interfaces

#### Surface Adsorption

*Cosponsored by COLL, ENVR and MPPG†*

A. M. Chaka, A. Ilgen, Y. Jun, *Organizers*

F. Geiger, *Organizer, Presiding*

**8:00 GEOC 74.** Evaluating the adsorption of lead to hematite in the presence of naturally-occurring organic acids. M. Noerpel, S. Lee, J.J. Lenhart

**8:20 GEOC 75.** Multiple  $\text{Cd}_2^+$  surface complexes on gibbsite and kaolinite at low surface loading from combined experimental and computational methods. P.A. O'Day, N. Birkner, M. Small, H. Watts, J.D. Kubicki, J.J. Rehr

**8:40 GEOC 76.** Sorption of mercury to aged iron sulfides and the implications for Hg bioavailability. N.A. Rivera, C. Johnson, U. Ndu, H. Hsu-Kim

**9:00 GEOC 77.** Carbonate adsorption on ferrihydrite: A semi-quantitative ATR study. M. Chrysochoou

**9:20 GEOC 78.** Oxyanion adsorption on Al-substituted ferrihydrite. C. Johnston

**9:40 GEOC 79.** Chemical trends in cation adsorption at the quartz-solution interface from microcalorimetry and modeling experiments. N. Allen, L. Le, M.L. Machesky, D. Wesolowski, N. Kabengi

**10:00** Intermission.

**10:20 GEOC 80.** Impacts of surface site coordination on arsenate adsorption: Macroscopic uptake, competitive adsorption, and binding mechanisms on aluminum hydroxide surfaces. T. Xu, J.G. Catalano

**10:40 GEOC 81.** Adsorption of natural organic matter (NOM) onto environmental surfaces. W. Li, P. Liao, Y. Jiang, S. Yuan, D. Giammar, J. Fortner

**11:00 GEOC 82.** Influence of ionic size and charge on the interaction of natural organic matter with mineral surfaces: Molecular dynamics modeling results. N. Loganathan, O. Yazaydin, G.M. Bowers, A.G. Kalinichev, J. Kirkpatrick

**11:20 GEOC 83.** Effects of temperature and solution chemistry fluctuation on the sorption and desorption of NOM on oxides. R. Huang, Y. Tang

**11:40 GEOC 84.** Sulfate complexation on hematite surfaces. X. Wang, D. Peak, Y. Tang, M. Zhu

## Section B

Omni San Diego Hotel  
Grand Ballroom B

### Adsorption of Metals by Geomedia

#### Thermodynamics & Kinetics

#### Experimental Study

*Cosponsored by ENVR, MPPG† and NUCL*

J. Fein, *Organizer*

Y. Yang, *Organizer, Presiding*

H. Hsu-Kim, *Presiding*

**8:00 GEOC 85.** Kinetics and mechanisms of metal sorption at the mineral/water interface: What have we learned the past 20 years? D.L. Sparks

**8:40 GEOC 86.** Nanoscale mercury sulfide-organic matter interactions: Practical applications for environmental risk assessment. H. Hsu-Kim, A. Pham, C. Johnson, U. Ndu, N. Rivera, M.A. Deshusses

**9:00 GEOC 87.** Comparing the solubility products of layered  $\text{Me(II)-Al(III)-hydroxides}$  based on sorption studies with  $\text{Ni(II)}$ ,  $\text{Zn(II)}$ ,  $\text{Co(II)}$ ,  $\text{Fe(II)}$ , and  $\text{Mn(II)}$ . L. Bhattacharya

**9:20** Intermission.

**9:40 GEOC 88.**  $\text{Fe(II)}$ -catalyzed Fe oxide recrystallization: Effect of organic carbon. M. Scherer, A. Thompson, T. Borch, T. Pasakarnis, D. Latta, Z. Zhou

**10:20** Introduction of a GEOC Student Travel Awardee.

**10:25 GEOC 89.** Morphological and thermodynamic changes in goethite during  $\text{Fe(II)}$ -catalyzed recrystallization. P. Joshi, C.A. Gorski

**10:55 GEOC 90.** Resolving the fine-scale reactivity of chromate complexation on iron oxides surfaces. M. Chrysochoou, N. Kabengi, J.D. Kubicki

**11:15 GEOC 91.** Withdrawn.

## Section C

Omni San Diego Hotel  
Gaslamp 2

### General Geochemistry

Y. Jun, *Organizer, Presiding*

**8:30 GEOC 92.** Mechanistic investigation of the reduction and volatilisation of mercury in soil. E. Mann, R. Khushal, A. Carpi

**8:50 GEOC 93.** Characterization of KURT rock samples at various depths to understand the long-term uranium behaviors under the Korean geological environment of granites. T. Park, M. Baik, J. Ryu, K. Kim

**9:10 GEOC 94.** Withdrawn.

**9:30 GEOC 95.** Geochemical and microbiological dynamics in a diesel-contaminated subsurface environment during in situ soil flushing. M. Kwon, Y. Hwang, D. Lee, B. Ham, J. Lee, E.J. O'Loughlin

**9:50** Intermission.

**10:10 GEOC 96.** Geochemically feasible reactions assemble biomimetic microstructures from natural spring water. E. Nakouzi, O. Steinbock, J. García-Ruiz

**10:30 GEOC 97.** Rare earth element fingerprinting of northwestern Niger delta source rocks. A. Akinlua

**10:50 GEOC 98.** Critical activation time of cloud condensation nuclei for biogenic precursors. A.E. Vizenor, A. Asa-Awuoku

**11:10 GEOC 99.** Relationship between nitrogen isotope ratio delta  $15\text{N}/14\text{N}$  in nitrate ion in rainfall and nitrogen isotope ratio delta  $15\text{N}/14\text{N}$  in plants in Mt. Kinabalu, Borneo Island, Sabah, Malaysia. H. Katsura

## Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

### Microbial Processes & Treatment

*Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC*

### Carbonate & Sulfate Minerals: Nucleation, Growth & Control of Scale Formation

*Sponsored by ENVR, Cosponsored by GEOC*

## TUESDAY AFTERNOON

### Section A

Omni San Diego Hotel  
Grand Ballroom A

### Environmental Interfaces

#### Complex Surface Reactions

*Cosponsored by COLL, ENVR and MPPG†*

A. M. Chaka, F. Geiger, Y. Jun, *Organizers*

A. Ilgen, *Organizer, Presiding*

**1:30 GEOC 100.** Stunning complexity of the water-soil-atmospheric interface driven by both natural and anthropogenic forcing, as directly observed at the nanoscale in real soils. M.F. Hochella, M. Schindler

**2:10 GEOC 101.** Structure and reactivity of biogenic manganese and iron minerals. O. Duckworth, M. Andrews, E. Mitchell, T. Sowers, A. Whitaker, M. Polizzotto, L.A. Sombers, C. Santelli

**2:50 GEOC 102.** Nanophase thermodynamics influence redox at the surface-water interface. N.R. Birkner, A. Navrotsky

**3:10 GEOC 103.** Thermodynamically characterizing interfacial iron redox couples using mediated potentiometry. C. Gorski, R. Edwards, S. Stewart, A. Costa

**3:30** Intermission.

**3:50 GEOC 104.** Ice grain boundary interface as a non-conventional reaction medium of environmental chemical processes. W. Choi, K. Kim, D. Jeong

**4:30 GEOC 105.** Microbial exudate promoted dissolution and transformation of chromium containing minerals. E. Saad, J. Sun, S. Chen, Y. Tang

**4:50 GEOC 106.** Accelerated free radical chemistry in the heterogeneous oxidation of semisolid organic aerosol. A.A. Wiegell, M. Liu, K.R. Wilson, W.D. Hinsberg, F.A. Houle

**5:10 GEOC 107.** Ferrihydrite: Structure possibilities, thermodynamics, and particle size effects from first principles calculations. M. Sassi, A.M. Chaka, K. Rosso

## Section B

Omni San Diego Hotel  
Grand Ballroom B

## Adsorption of Metals by Geomedial

Thermodynamics & Kinetics  
Experimental Study

*Cosponsored by ENVR, MPPG‡ and NUCL*

J. Fein, Y. Yang, *Organizers*

Y. Hu, Y. Tang, *Presiding*

**1:30 GEOC 108.** Transition from adsorption to precipitation for uranium uptake on geomedial. **D. Giammar, Z. Wang, Z. Wang, L. Troyer, J.G. Catalano**

**2:10 GEOC 109.** Influence of sea level rise on arsenic mobility in coastal soils. **J.J. LeMonte, J. Stuckey, X. Yu, J. Rinklebe, R. Tappero, H.A. Michael, D.L. Sparks**

**2:30 GEOC 110.** Superfund cycling: The fate of hexavalent chromium in the subsurface environment. **J. Fischel, D.L. Sparks**

**2:50 GEOC 111.** Impact of sea level rise on arsenic speciation in *Phragmites australis* and *Spartina alterniflora*. **M. Fischel, D.L. Sparks**

**3:10** Intermission.

**3:30 GEOC 112.** Selective sorption of humic substances on mineral surfaces. **S.C. Myneri, A. Habermann, A. Raghu, P. Hatcher**

**4:10** Introduction of a GEOC Student Travel Awardee.

**4:15 GEOC 113.** Asynchronous mobilization of iron and organic carbon from hematite-humic acid complexes during abiotic iron reduction. **D. Adhikari, S.R. Poulson, S. Sumaila, J.J. Dynes, J.M. McBeth, Y. Yang**

**4:45 GEOC 114.** Phosphate, arsenate, and arsenite oxyanion adsorption to CeO<sub>2</sub> affects nanoparticle reactivity and colloidal stability. **C.W. Neil, S. Jung, D. Kim, Y. Zhu, J. Ray, Y. Jun**

**5:05 GEOC 115.** Comparison of tungstate and thiotungstate adsorption to iron sulfide and iron oxides minerals under anoxic condition. **M. Cui, K.H. Johannesson**

Environmental Aspects of  
Unconventional Oil & Gas Production  
& Hydraulic Fracturing

## Geochemistry

*Sponsored by ENVR, Cosponsored by CEI and GEOC*

## WEDNESDAY MORNING

## Section A

Omni San Diego Hotel  
Grand Ballroom A

## Environmental Interfaces

## Complex Surface Reactions

*Cosponsored by COLL, ENVR and MPPG‡*

A. M. Chaka, A. Ilgen, Y. Jun, *Organizers*

F. Geiger, *Organizer, Presiding*

**8:00 GEOC 116.** Investigation of Wyoming bentonite hydration in dry to water-saturated supercritical CH<sub>4</sub> and CH<sub>4</sub>/CO<sub>2</sub> mixtures: Implications for CO<sub>2</sub>-enhanced gas production. **J. Loring, D.W. Hoyt, D.A. Dixon, E.S. Ilton, C.J. Thompson, O. Qafoku, K. Rosso, P. McGrail, T. Schaefer**

**8:40 GEOC 117.** Water dynamics in 2-dimensional nano-confinement: <sup>2</sup>H NMR and molecular dynamics modeling of smectite interlayers. **R.J. Kirkpatrick, U. Reddy, N. Loganathan, G.M. Bowers, A.O. Yazaydin, M. Bowden, A.G. Kalinichev**

**9:00 GEOC 118.** Electrolytes at the muscovite (001) interface: A molecular dynamics study. **A. Prakash, C.J. Mundy, M.D. Baer, J. Pfandtner**

**9:20 GEOC 119.** Prediction of alkaline earth metal ion adsorption on goethite for various background electrolytes. **J. Han, L.E. Katz**

**9:40** Introduction of a GEOC Student Travel Awardee.

**9:45 GEOC 120.** Interfacial interactions between cations and plagioclase under conditions relevant to subsurface CO<sub>2</sub> injection. **Y. Min, Y. Jun**

**10:15** Intermission.

**10:35 GEOC 121.** Mancos shale-brine-CO<sub>2</sub> interactions and the long-term stability of shale caprock. **A. Ilgen, T. Stewart, J. Griego, M. Rodriguez, J. Feldman, M. Aman, N. Ezpinoza, T. Dewers**

**10:55 GEOC 122.** Effect of surfactant adsorption on shale wettability. **S. Das, L. Zhou, B. Ellis**

**11:15 GEOC 123.** Biotite wettability changes under geologic CO<sub>2</sub> sequestration conditions: Influences of salinity-induced chemical reactions. **L. Zhang, Y. Kim, J. Wan, Y. Jun**

**11:35 GEOC 124.** How the route of magnetite synthesis influences magnetite redox reactions with humic substances. **A. Kappler, J. Byrne, A. Sundman**

**11:55 GEOC 125.** Molecular modeling of the adsorption and transport of methane within overmature kerogen. **T.A. Ho, L.J. Criscenti, Y. Wang, Y. Akkutlu**

## Section B

Omni San Diego Hotel  
Grand Ballroom B

## Adsorption of Metals by Geomedial

Radionuclides: Uranium &  
Transuranium - Extension of ACS  
Garvan-Olin Medal Session

*Cosponsored by ENVR, MPPG‡ and NUCL*

J. Fein, Y. Yang, *Organizers, Presiding*

**8:00 GEOC 126.** Role of organic matter and microbes in plutonium redox transformations and sorption reactions. **A. Kersting**

**8:40 GEOC 127.** Diffusion of Np(V) through a compact engineered clay barrier under repository conditions. **R. Pope, B.A. Powell**

**9:00 GEOC 128.** Influence of mineral surfaces on the speciation of uranium under reducing conditions. **M. Boyanov, D. Latta, B. Mishra, M. Scherer, E.J. O'Loughlin, K.M. Kemner**

**9:20** Intermission.

**9:40 GEOC 129.** Surface complexation from the grain to plume scale in a gravel aquifer: Considerations and challenges for predictability. **J. Zachara, C. Liu, X. Chen, G. Hammond, D.B. Kent, D. Stoliker**

**10:20 GEOC 130.** Bioassociation of actinides towards halophilic bacteria and archaea. **D.T. Reed, J. Swanson, T. Dittirich, M. Richmann**

**10:40 GEOC 131.** Impact of phosphate on immobilization of U(VI) in sediments. **Z. Pan, D. Giammar, L. Troyer, J.G. Catalano, Z. Wang**

**11:00 GEOC 132.** Effect of oxidation state and ionic strength on sorption of actinides (Th, U, Np, Am) to geologic media. **T.M. Dittirich, M. Richmann, D.T. Reed**

## Section C

Omni San Diego Hotel  
Grand Ballroom D

Environmental Consequences  
of Resource Development

E. Herndon, D. Singer, *Organizers, Presiding*

**8:00 GEOC 133.** Enhanced distribution and bioavailability of arsenic as an outcome of gold mining processes. **C.S. Kim**

**8:30 GEOC 134.** Surficial geochemistry of tellurium in a semi-arid environment: Implications for transport and environmental health. **S.M. Hayes, N. Knight**

**8:50 GEOC 135.** Understanding Se biogeochemistry in seleniferous reclaimed mine soils. **C. Rosenfeld, B.R. James, C.M. Santelli**

**9:10 GEOC 136.** Metal(loid) leaching from soils developed on coal mine waste. **E. Herndon, D. Singer, L. Zemanek, B. Yarger, S. Morrison**

**9:30 GEOC 137.** Effects of mineralogical transformations on the mobility of trace metals in an area affected by acid mine drainage, Huff Run, Ohio. **E. Traub, A. Jefferson, D. Singer**

**9:50 GEOC 138.** Investigation of the Gold King mine spill impact in water and sediments downstream of the Animas river. **L. Rodriguez Freire, S. Avasarala, A. Ali, K. Artyushkova, E. Peterson, L. Crossley, A. Brearley, J.M. Cerrato**

**10:10 GEOC 139.** Challenges and potential benefits of managing acidic mining influenced water. **K. Campbell, C. Alpers, K. Nordstrom**

**10:30 GEOC 140.** Using noble gas geochemistry to determine the source and mechanism of natural gas leakage into shallow aquifers near unconventional drilling. **T.H. Darrah, R. Jackson, R.J. Poreda, K. Muehlenbachs, N.R. Warner, C.J. Whyte, A. Vengosh**

**10:50 GEOC 141.** Characterization of flow-back of fracturing fluids with upgraded visualization of hydraulic fracturing treatment & its implications on overall well performance. **K. Desai, F. Aminzadeh**

**11:10 GEOC 142.** Incidental nanoparticles, from quantum confinement to global issues: An unintended and hidden consequence of resource development and use. **M.F. Hochella**

Environmental Aspects of  
Unconventional Oil & Gas Production  
& Hydraulic Fracturing

## Water Use &amp; Reuse

*Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC*

## Aquatic Photochemistry

*Sponsored by ENVR, Cosponsored by GEOC*

## WEDNESDAY AFTERNOON

## Section A

Omni San Diego Hotel  
Grand Ballroom A

## Environmental Interfaces

## Complex Surface Reactions

*Cosponsored by COLL, ENVR and MPPG‡*

F. Geiger, A. Ilgen, Y. Jun, *Organizers*

A. M. Chaka, *Organizer, Presiding*

**1:30 GEOC 143.** Reactivity of metals from wildfire ash and effects on water quality. **J.M. Cerrato, A. Clark, N. Correa, C. Hirani, J. Blake, A. Ali, R. Bixby**

**1:50 GEOC 144.** Charcoal quenching of cell-cell communication can arise from a combination of signaling molecule hydrolysis and sorption. **X. Gao, H. Cheng, S. Liu, C.A. Masiello, J.J. Silberg**

**2:10 GEOC 145.** Toward a comprehensive picture of amine uptake and solvation on the surface of liquid aerosols: A computational study. **I. Gladich, R. Hoehn, M. Carignano, J.S. Francisco**

**2:30 GEOC 146.** Microbially induced redox reaction of Fe/As in extreme environment, Norris Geyser Basin, Yellowstone National Park, USA. **T. Koo, J. Kim, K. Park, D. Jung, G. Geesey, J. Kim**

**2:50 GEOC 147.** Reduction of lepidocrocite by polysulfides: Kinetics and mechanism. **M. Shi, J.S. Zheng, B. Deng**

## Section B

Omni San Diego Hotel  
Grand Ballroom B

## Adsorption of Metals by Geomedial

## X-ray Spectroscopy

*Cosponsored by ENVR, MPPG‡ and NUCL*

J. Fein, Y. Yang, *Organizers*

J. Catalano, M. A. Ginder-Vogel, *Presiding*

**1:30 GEOC 148.** Metal ion sorption at mineral/aqueous solution interfaces: Effects of complex coatings and particle/pore sizes. **G.E. Brown, Y. Wang, C. Cismasu, P.J. Eng, A. Spormann, Y. Wang, G. Dublet, A.D. Jew, J. Jung, J. Wilcox, J.R. Barqar**

**2:10 GEOC 149.** Response of interfacial water to arsenate adsorption: Effects of surface coverage and pH. **J.G. Catalano, T. Xu**

**2:30 GEOC 150.** Surface reconstruction and electronic bonding states of Cd sorbed to gibbsite from experimental and theoretical XANES spectra and DFT computations. **N.R. Birkner, M. Small, H. Watts, J.D. Kubicki, P.A. O'Day**

**2:50** Intermission.

**3:10 GEOC 151.** Heteroepitaxial growth of (Cd,Ca)CO<sub>3</sub> solid solution at the dolomite (104)-water interface. **N.C. Sturchio, E. Callagon, S. Lee, K.L. Nagy, P. Fenter**

**3:50 GEOC 152.** Impact of Fe (hydr) oxide redox cycling on Cr(VI) reduction. **M.A. Ginder-Vogel, E. Tomaszewski**

**4:10 GEOC 153.** Impure ferrihydrite nucleation and growth: Interactions among metal ions, Fe hydroxide nanoparticles, and mineral surfaces. **Y. Hu, C. Dai, X. Zuo, B. Cao, D. Brewe**

**4:30** Introduction of a GEOC Student Travel Awardee.

**4:35 GEOC 154.** Effects of oxalate on Ni adsorption and repartitioning during Fe(II)-promoted iron oxide recrystallization. **E.D. Flynn, J.G. Catalano, H.J. Gadol**

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Water Use & Reuse/Water Treatment

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Aquatic Photochemistry

Sponsored by ENVR, Cosponsored by GEOC

## WEDNESDAY EVENING

### Section A

San Diego Convention Center  
Hall D

#### Adsorption of Metals by Geomedia

Cosponsored by ENVR and NUCL

J. Fein, Y. Yang, *Organizers*

#### 8:00 - 10:00

**GEOC 155.** Cu(II) and Zn(II) adsorption and retention to iron oxyhydroxide nanoparticles: Effects of aggregation state and sulfate concentration. L. Smith

**GEOC 156.** Hematite modified cementitious material for uranium (VI) immobilization. B. Cao, S. Fan, Z. Han, M. Li, Y. Hu

**GEOC 157.** Withdrawn.

**GEOC 158.** Complex interactions between mercury (Hg) and bacterial cells on Hg sorption, reduction, oxidation, and methylation. X. Lu, H. Lin, B. Gu

**GEOC 159.** Comparison of zinc sorption affinity to synthetic and biogenic manganese oxides. M. Jones, T. Sowers, M. Andrews, O. Duckworth

**GEOC 160.** Remediation of As(V) contaminated groundwater through enhanced natural attenuation: Batch and column studies. S. Hafeznezami, J. Jay

### Section A

San Diego Convention Center  
Hall D

#### Applied Geochemical Modeling

E. Chiang, R. M. Santos, *Organizers*

#### 8:00 - 10:00

**GEOC 161.** Geochemical modeling applied to research on waste valorization, carbon sequestration and environmental remediation: A review of SMaRT-Pro<sup>2</sup> cases. R.M. Santos, E. Chiang

### Section A

San Diego Convention Center  
Hall D

#### Closing the Human Phosphorus Cycle: Biogeochemistry, Sustainable Phosphorus Recovery, Speciation, Detection & Reuse

L. E. Katz, K. Ruttenberg, *Organizers*

#### 8:00 - 10:00

**GEOC 162.** Phosphorus speciation changes in semi-arid grassland soils along a climate gradient in Inner Mongolia, China. C. Gu, S.E. Evans, I.C. Burke, M. Zhu

### Section A

San Diego Convention Center  
Hall D

#### Environmental Consequences of Resource Development

E. Herndon, D. Singer, *Organizers*

#### 8:00 - 10:00

**GEOC 163.** Mineralogical characterization of colloids and macroscopic precipitates in abandoned mine drainage (AMD). S.L. Bradley, E.K. Herman, M.M. McGuire

**GEOC 164.** Examination of tellurium oxyanion sorption to ferrihydrite and characterization of sorption complex geometry. N. Knight, L. Balistrieri, S.M. Hayes

### Section A

San Diego Convention Center  
Hall D

#### Environmental Interfaces

Cosponsored by COLL and ENVR

A. M. Chaka, F. Geiger, A. Ilgen, Y. Jun, *Organizers*

#### 8:00 - 10:00

**GEOC 165.** Structural characterization of phosphate and silicate surface species on metal oxides. X. Wang, M. Zhu

**GEOC 166.** Manganese oxide amendments for *in situ* remediation of mercury contaminated sediments. A.M. Leven, D. Vlassopoulos, J. Goin, M. Kanematsu, P.A. O'Day

**GEOC 167.** Evidence for the formation of Fe-layered hydroxides using spectroscopic techniques. A. Starcher, E. Elzinga, R. Kukkadapu, D.L. Sparks

**GEOC 168.** Reactivity at the mineral-water interface of corundum ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>): Surface protonation, surface charging, and dissolution. M.K. Ridley, D. Tunega

**GEOC 169.** Effects of suspended particulates on *Acidovorax* sp. 2AN growth and proposed mechanisms. F.W. Picardal, T. An

**GEOC 170.** Iron sulfide surface products formed during dechlorination of tetrachloroethylene and trichloroethylene. Y. Lan, E.C. Butler

**GEOC 171.** Role of iron minerals in preserving organic carbon during aerobic degradation. S. Cronk, C.A. Gorski

**GEOC 172.** Arsenic bioaccessibility as a function of rainfall exposure and time in mining-impacted sediments. K. Whiteman, C. Kim

**GEOC 173.** Debris plastics as the sources of chemicals surrounding Japan and open sea in the North Pacific Ocean. K. Amamiya, K. Takatama, K. Koizumi, N. Maximenko, A. Okabe, D.M. Karl, K. Saido

### Section A

San Diego Convention Center  
Hall D

#### General Geochemistry

Y. Jun, *Organizer*

#### 8:00 - 10:00

**GEOC 174.** Effects of adsorbed Cd(II) on the Mn(II)-catalyzed transformation of hexagonal birnessite. H. Cui, D.L. Sparks

**GEOC 175.** Preliminary study on Korean bentonite: Supporting safety cases for radioactive waste disposal by means of providing the basis for use of natural analogues study. T. Park, M. Baik, S. Lee, G. Kim

**GEOC 176.** Effects of soluble electron shuttles on microbial Fe(III) reduction and methanogenesis in wetland sediments. E.J. O'Loughlin, M.F. Sladek, D.A. Antonopoulos, T. Flynn, J.C. Koval, C. Marshall, K.M. Kemner

**GEOC 177.** Withdrawn.

**GEOC 178.** Mechanisms of stabilization of heavy metals in mine tailings through carbonation process. S. Jeong, S. Kim, K. Nam

**GEOC 179.** Withdrawn.

**GEOC 180.** Toward a better understanding of Mo burial in anoxic sediments: Roles of Fe<sup>II</sup>-Mo<sup>V</sup>-S cubane clusters, sol stability, and ionic strength. P. Vue, W.G. Hunter, A. Chappaz, T.P. Vorlicek

**GEOC 181.** Effect of methylmercury (MeHg) speciation on MeHg degradation by an anaerobic bacterium. E. Leverich, X. Yang, A. Graham

**GEOC 182.** DOM sulfidization increases Hg bioavailability for microbial methylation in Hg-sulfide-DOM solutions. D. Msekela, H. Hajic, C. Lee, K. Cameron-Burr, C.C. Gilmour, A. Graham

**GEOC 183.** Geochemical characterization of well-cuttings from an oil producing well in the central Kansas uplift using flame atomic absorption spectrometry. A.J. Cruz, S. Markham, H. Ali, A. Christiano

### Section A

San Diego Convention Center  
Hall D

#### Geochemical Reactivity of Nanoparticles, Aggregates, Coatings & Organo-Nanoparticulate Flocculants

B. Gilbert, C. S. Kim, *Organizers*

#### 8:00 - 10:00

**GEOC 184.** Influence of humic acid, light exposure, and pH on silver nanoparticle properties. W. Zhou, Y. Liu, A.M. Stallworth, J.J. Lenhart

**GEOC 185.** Effects of pH on the aggregation and Cu(II) adsorption behavior of iron oxyhydroxide nanoparticles. B. Lamb, A. Torossian, C. Kim

**GEOC 186.** Single approach to synthesize birnessite of various sizes. Q. Wang, X. Liao, W. Xu, K. Livi, Y. Ren, M. Zhu

#### Aquatic Photochemistry

Sponsored by ENVR, Cosponsored by GEOC

## THURSDAY MORNING

### Section A

Omni San Diego Hotel  
Grand Ballroom A

#### Applied Geochemical Modeling

#### Carbon Storage & Environmental Protection

Cosponsored by MPPG†

E. Chiang, *Organizer*

R. M. Santos, *Organizer, Presiding*

#### 8:30 Introductory Remarks.

**8:35 GEOC 187.** Integrated geochemical modeling approaches for CO<sub>2</sub> capture utilization and storage (CCUS). A. Ji Whan, T. Thenepalli

**9:05 GEOC 188.** Reactive transport modeling of CO<sub>2</sub> sequestration in mine tailings. A. Harrison, D. Su, S.A. Wilson, I.M. Power, G.M. Dipple, K. Mayer

**9:35 GEOC 189.** Experimental and modeling investigations of Portland cement deterioration under geologic CO<sub>2</sub> sequestration conditions. Q. Li, C. Steefel, Y. Lim, Y. Jun

**9:55 Intermission.**

**10:15 GEOC 190.** Arsenic potential migration in carbon storage environments upon contact with anoxic brines. A. Karamalidis, H. Parthasarathy, L. Zhang, D.A. Dzombak, A. Namhata

**10:45 GEOC 191.** Analytical solution of multicomponent ion exchange during surfactant floods in porous media. H. Sharma, A. Venkatraman, M. Wheeler, K. Mohanty

**11:05 GEOC 192.** Comparing exothermic reaction rates using geochemical and heat-flow modeling of a contaminated aquifer. E. Warren, B.A. Bekins, G. Ng, I.M. Cozzarelli

### Section B

Omni San Diego Hotel  
Grand Ballroom B

#### Adsorption of Metals by Geomedia

#### Biosorption: Metal & Bacteria

Cosponsored by ENVR, MPPG† and NUCL

J. Fein, Y. Yang, *Organizers*

B. Mishra, A. Vazquez-Ortega, *Presiding*

**8:00 GEOC 193.** Modeling metal bioavailability to bacteria using surface complexation modeling. J. Fein, D. Borrok, S. Flynn

**8:20 GEOC 194.** Effect of cysteine and cell metabolism on Hg(II) sorption and coordination to *Escherichia coli*. S. Thomas, J. Gaillard

**8:40 GEOC 195.** Thermodynamic modeling of Mn(II) adsorption onto manganese oxidizing bacteria. A. Vázquez-Ortega, J. Fein

**9:00 Intermission.**

**9:20 GEOC 196.** Abiotic reduction of Ag<sup>+</sup>, Au<sup>3+</sup> and AsO<sub>4</sub><sup>3-</sup> by extracellular polymeric substances (EPS) excreted by microorganisms: Mechanisms and environmental implication. F. Kang, X. Zhou, D. Zhu

**9:40 GEOC 197.** Biogeochemistry of the molecular scale interactions of metals with bacteria. B. Mishra

**10:00 GEOC 198.** Role of flavin as redox mediator for efficient inorganic Hg(II) reduction by *Shewanella oneidensis* MR-1. G.H. Qasim, S. Han

**10:20 GEOC 199.** Influence of sulfhydryl sites on gold binding by bacteria. R. Nell, J. Fein

### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Modeling

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Aquatic Photochemistry

Sponsored by ENVR, Cosponsored by GEOC



## THURSDAY AFTERNOON

## Section A

Omni San Diego Hotel  
Grand Ballroom A

## Applied Geochemical Modeling

Energy Exploration,  
Metals & Metalloids

*Cosponsored by MPPG‡*

R. M. Santos, *Organizer*

E. Chiang, *Organizer, Presiding*

**1:30 GEOC 200.** From diagenetic models to spectroscopic data. J. Gaillard

**2:00 GEOC 201.** Precipitation and kinetics of mixed-metal solids in soils, sediments, and mineral systems: Implications for equilibrium speciation calculations. M. Siebecker, G.W. Luther, D.L. Sparks

**2:30 GEOC 202.** Metals in the aquatic environment: interactions and implications for the speciation and bioavailability. R. Domingos, A. Gelabert, S. Carreira, A. Cordeiro, Y. Sivry, M.F. Benedetti

**3:00** Intermission.

**3:20 GEOC 203.** Modelling speciation and uptake of trace metal as influenced by metallophores. W. Schenkeveld, S.M. Kraemer

**3:50 GEOC 204.** Surface complexation modelling of chromate adsorption on iron oxides. N. Bompoti, M. Chrysochoou, M.L. Machesky

**4:10 GEOC 205.** Molecular dynamics simulation approach in estimating organic-rich shale permeability. R. Kou, Y. Akkutlu

**4:30 GEOC 206.** Gas storage in model kerogen pores with surface heterogeneities. D. Cristancho

**4:50** Concluding Remarks.

Environmental Aspects of  
Unconventional Oil & Gas Production  
& Hydraulic Fracturing

## Regulatory Aspects

*Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC*

## Aquatic Photochemistry

*Sponsored by ENVR, Cosponsored by GEOC*

## HIST

Division of the History  
of Chemistry

S. Rasmussen, *Program Chair*

## BUSINESS MEETINGS:

Executive Committee Meeting,  
5:00 PM: Sun

## SUNDAY MORNING

## Section A

Hilton San Diego Bayfront  
Aqua 311A/B

## HIST Tutorial &amp; General Papers

S. C. Rasmussen, *Organizer, Presiding*

**8:30 HIST 1.** Intersection of art and science in the discovery of molecular chirality by Louis Pasteur (1822-1895) in 1848. J. Gal

**9:00 HIST 2.** The Royal Society of Chemistry: History now online. S. Dabb

**9:30 HIST 3.** Butlerov Museum of the Kazan School of Chemistry. A.R. Davis, E.T. Walsh, D.E. Lewis

**10:00** Intermission.

**10:15 HIST 4.** Philatelic history of vitamin C. D. Rabinovich

**10:45 HIST 5.** Astatine: The elusive one. K. Kostecka

**11:15 HIST 6.** Robert Boyle and Urban Hjarne: At the crossroads. S. Mitra, S.B. Mitra

## SUNDAY AFTERNOON

## Section A

Hilton San Diego Bayfront  
Aqua 311A/B

## Preceptors of Chemistry

*Cosponsored by CHED*

G. D. Patterson, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 HIST 7.** Ghost of Libau and problems with teaching "chemistry". B.T. Moran

**1:35 HIST 8.** Herman Boerhaave and the use of demonstration-experiments in chemistry courses. J.C. Powers

**2:05 HIST 9.** Teaching chemistry in eighteenth-century France. B. Bensaude-Vincent

**2:35 HIST 10.** Withdrawn.

**3:05** Intermission.

**3:15 HIST 11.** Mendeleev and the chemistry textbook in Russia. V.V. Mainz

**3:45 HIST 12.** Fred Basolo and the (re)naissance of American inorganic chemistry. J.A. Labinger, H.B. Gray

**4:10 HIST 13.** Paul Doughty Bartlett: Evangelist for mechanistic organic chemistry. S.J. Weininger

**4:35 HIST 14.** Linus Pauling: The right to be wrong. G.D. Patterson

## MONDAY MORNING

## Section A

Hilton San Diego Bayfront  
Aqua 311A/B

The Posthumous Nobel Prize  
in Chemistry: Correcting the  
Errors & Oversights of the  
Nobel Prize Committee

T. Strom, *Organizer, Presiding*

**8:40** Introductory Remarks.

**8:45 HIST 15.** The Nobel prize: A brief overview. W. Jensen, T. Strom

**9:15 HIST 16.** Dmitri Mendeleev's Nobel prize-losing research. C.J. Giunta

**9:45 HIST 17.** Who got Moseley's prize? V.L. Trimble

**10:15** Intermission.

**10:30 HIST 18.** Herman Mark's claim to fame. G.D. Patterson

**11:00 HIST 19.** Wallace Carothers and polymer chemistry: A partnership ended far too soon. E.T. Strom

**11:30 HIST 20.** BET equation: Nominated, but not selected. B.H. Davis

## MONDAY AFTERNOON

## Section A

Hilton San Diego Bayfront  
Aqua 311A/B

The Posthumous Nobel Prize  
in Chemistry: Correcting the  
Errors & Oversights of the  
Nobel Prize Committee

T. Strom, *Organizer, Presiding*

**1:30 HIST 21.** Yevgenii Konstantinovich Zavoiskii (1907-1976): Overlooked pioneer in magnetic resonance. D.E. Lewis

**2:00 HIST 22.** Between two stools: Pauling, Mulliken, and Michael J. S. Dewar. E. Healy

**2:30 HIST 23.** Hammett deserved a Nobel prize. C. Perrin

**3:00** Intermission.

**3:15 HIST 24.** R. B. Woodward: One was just not enough. J. Seeman

**3:45 HIST 25.** Neil Bartlett: No Nobel for noble gases: Some guesses why. J.F. Liebman

**4:15 HIST 26.** Proposing Howard E. Simmons, Jr. P. Laszlo

## MONDAY EVENING

## Section A

San Diego Convention Center  
Halls D/E

## Sci-Mix

S. C. Rasmussen, *Organizer*

**8:00 - 10:00**

1, 11, 16. See previous listings.

**HIST 27.** Translation of Markivcnikov's Magistr Khimii dissertation: A progress report. A.R. Davis, E.T. Walsh, D.E. Lewis

## TUESDAY MORNING

## Section A

Hilton San Diego Bayfront  
Aqua 311A/B

## HIST Tutorial &amp; General Papers

S. C. Rasmussen, *Organizer*

N. V. Tsarevsky, *Presiding*

**9:00 HIST 28.** Oldest planetary, astrochemical mystery: Jupiter's great (but shrinking) red spot. R.L. Hudson

**9:30 HIST 29.** Eponym's curse. V.L. Trimble

**10:00** Intermission.

**10:15 HIST 30.** Gilbert Lewis and the conceptual evolution of the chemical bond. S. Mitra

**10:45 HIST 31.** R.J.P. Williams and the chemical sequence of natural history. B.J. McFarland

Memorial Symposium  
Honoring Karen J. Brewer

*Sponsored by INOR, Cosponsored by HIST‡*

## TUESDAY AFTERNOON

Memorial Symposium  
Honoring Karen J. Brewer

*Sponsored by INOR, Cosponsored by HIST‡*

## WEDNESDAY MORNING

## The History of Chemistry &amp; Computing

*Sponsored by MPPG, Cosponsored by COMP, HIST and PHYS‡*

Memorial Symposium  
Honoring Karen J. Brewer

*Sponsored by INOR, Cosponsored by HIST‡*

## WEDNESDAY AFTERNOON

Memorial Symposium  
Honoring Karen J. Brewer

*Sponsored by INOR, Cosponsored by HIST‡*

## I&amp;EC

Division of Industrial  
and Engineering  
Chemistry

P. Smith and E. Rosenberg, *Program Chairs*

## OTHER SYMPOSIA OF INTEREST:

Industrial Research at the Interface  
of Inorganic Chemistry & Polymer  
Science (see POLY, Sun)

Sustainable Polymers, Processes &  
Applications (see POLY, Sun, Mon, Tue)

Downstream Processes:  
Advances in Chromatographic  
Separations (see BIOT, Mon)

Industrial Innovation in Polymer  
Chemistry: Sustainable  
Polymerization Feedstocks & Process  
Technology (see POLY, Mon)

Upstream Processes: Metabolic  
Engineering & Synthetic Biology:  
Pathways/Products (see BIOT, Tue)

Upstream Processes: Engineering Natural  
Products Biosynthesis (see BIOT, Thu)

## BUSINESS MEETINGS:

Business Meeting, 4:30 PM: Sun

## SUNDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Temecula 1&2

Alpha Olefin Catalysis: Production  
& Transformations

## Catalytic Production

*Cosponsored by CATL and INOR‡  
Financially supported by Chevron  
Phillips Chemical*

G. G. Stanley, *Organizer*

O. L. Sydora, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 I&EC 1.** Ethylene oligomerization catalyst development and process improvements. S.M. Bischof

**8:35 I&EC 2.** Shell higher olefin process: Growing the worldwide supply of alpha-olefins. M. Bolinger

**9:05 I&EC 3.** Adventures in selective ethylene oligomerisation at Sasol Technology. K. Blann

**9:35** Intermission.

**9:50 I&EC 4.** Ethylene and alpha olefin trimerization and tandem trimerization/polymerization of ethylene. **J.E. Bercaw**, L. Do, A. Sattler, D. Aluthge, J.A. Labinger, M. Al Harthi

**10:20 I&EC 5.** Potential catalytic system for selective ethylene trimerization of ethylene shifting from full range to selectivity of 1-hexene. **M.H. Al-Hazmi**, A. Alqahtani, N. Peulecke, B. Müller, U. Rosenthal, A. Wöhl, W. Müller

**10:50 I&EC 6.** Vinyl terminated atactic polypropylene oligomers: Characterization and reactions of distilled narrow molecular weight distribution fractions. **P. Brant**

## Section B

Marriott Marquis San Diego Marina  
Temecula 3&4

### ACS Award in Separations Science & Technology: Symposium in honor of Steven M. Cramer

*Cosponsored by BIOT*

A. M. Lenhoff, *Organizer, Presiding*

**8:30 I&EC 7.** Process development strategies for production of protein therapeutics. **N. Tugcu**, H. Chen, J. Pollard, D.J. Roush, F.K. Insaiddo, H. Li

**8:50 I&EC 8.** Downstream processing: Standing on the shoulders of giants. **A.A. Shukla**

**9:10 I&EC 9.** Downstream manufacturing technologies to enable process intensification. **M.W. Phillips**

**9:30 I&EC 10.** The shrinking footprint: Next generation technologies in biomanufacturing. **S. Guhan**

**9:50** Intermission.

**10:10 I&EC 11.** Nevermind chromatography, here's precipitation. **T.M. Przybycien**

**10:30 I&EC 12.** Chromatography for clinical diagnostics. **R.C. Willson**

**10:50 I&EC 13. Award Address** (ACS Award in Separations Science and Technology sponsored by Waters Corporation). Protein selectivity in chromatographic systems: Fundamental understanding and predictive tools. **S.M. Cramer**

## SUNDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Temecula 1&2

### Alpha Olefin Catalysis: Production & Transformations

#### Alpha Olefin Transformations

*Cosponsored by CATL and INOR; Financially supported by Chevron Phillips Chemical*

O. L. Sydora, *Organizer*

G. G. Stanley, *Organizer, Presiding*

**1:00** Introductory Remarks.

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**1:05 I&EC 14.** Transformations of alpha olefins using homogeneous dinuclear nickel catalysts. **C. Uyeda**, T. Steiman, Y. Zhou

**1:35 I&EC 15.** Green chemical products from olefin metathesis of renewal seed oils. **R.L. Pederson**

**2:05 I&EC 16.** Kinetics of metal-dependent insertion polymerization of 1-hexene. **M.M. Abu-Omar**, J. Caruthers, N. Delgass, G. Medvedev, K. Steelman, P. Pletcher, J. Switzer

**2:35** Intermission.

**2:50 I&EC 17.** Rapid, regioconvergent alkene hydrosilylation with cobalt catalysts. **C. Chen**, B.Q. Mercado, D.J. Weix, **P.L. Holland**

**3:20 I&EC 18.** New esters derived from linear olefins. **J.C. Gee**, S. Fisher

**3:50 I&EC 19.** Bimetallic hydroformylation: Twice the fun? **G.G. Stanley**, R.G. Fernando, M.D. Moulis, C.V. Duronslet

## Section B

Marriott Marquis San Diego Marina  
Temecula 3&4

### Industrial & Engineering Fellow: Symposium in honor of Bala Subramaniam

#### Development of Sustainable Chemical Processes

R. Chaudhari, *Organizer, Presiding*

K. W. Hutchenson, *Presiding*

**1:00** Introductory Remarks.

**1:05 I&EC 20.** Rate limiting steps in polyolefin fiber sulfonation. **D. Hickman**, E. Hukkanen, H. Wang, M. Behr, L. Brehm, B. Haskins, M. Ferries

**1:25 I&EC 21.** Study on dry reforming of methane using isotopic  $^{13}\text{C}$  switching. **N. Kumar**, S. Kanitkar, J.J. Spivey

**1:45 I&EC 22.** Production of furfural, a platform bio-based intermediate. **K.W. Hutchenson**

**2:05 I&EC 23.** Impact of new technologies and chemical manufacturing routes on the petrochemical industry in the United States. **S. DeRosa**, D.T. Allen

**2:25 I&EC 24.** Stabilizing gold nanoparticles in a gaseous HCl environment using high surface free energy core anchoring. **K. O'Connell**, J.R. Regalbuto, J.R. Monnier

**2:45** Intermission.

**3:00 I&EC 25.** Rational design of  $\text{Zn}_2\text{Zr}_2\text{O}_7$  catalysts for the conversion of ethanol to isobutene with improved selectivity and stability. **R.A. Baylon**, C. Smith, J. Sun, C. Liu, Y. Wang

**3:20 I&EC 26.** Volarization of lignin first as a new biorefinery concept for making fuels and chemicals. **M.M. Abu-Omar**, T. Parsell, I. Klein, H. Luo, F. Ribeiro

**3:40 I&EC 27.** Phase equilibrium, structure and transport of ethylene-expanded methanol and methanol/water mixtures in bulk and under confinement in silica nanopores. **B.B. Laird**, J. Kern, K. Steenbergen, W. Thompson, Z. Wang

**4:00 I&EC 28.** Design of bimetallic nano-catalysts for biomass conversion to chemicals. **R.V. Chaudhari**, X. Jin

**4:20 I&EC 29.** Application of life cycle assessment in the oil and gas industry: Challenges and opportunities. **H. Jin**

**4:40** Remarks by Prof. Subramaniam.

**4:45** Concluding Remarks.

### Discussions with the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

## SUNDAY EVENING

### My Comments to the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

### My Experience with & Advice for Improving Diversity in Chemistry

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### My Experiences in & Advice for Organic Chemistry Courses

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## MONDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Coronado Room

### New Reality of the Chemical Enterprise: Traditional & Non-traditional Career Paths

#### Chemistry Professionals Working "Outside the Box"

*Cosponsored by CTA, PRES and SOCED Financially supported by ACS Graduate and Postdoctoral Scholars Office*

M. K. Engelman, J. M. Smith, *Organizers*

J. Engelman, M. A. Thomson, *Presiding*

**8:15** Introductory Remarks.

**8:30 I&EC 30.** Keynote Sandra Flank: Think "outside the box" for chemistry careers. **S. Flank**

**8:55 I&EC 31.** Discovering chemistry outside the lab. **S. Large**

**9:20 I&EC 32.** Challenging career in the changing regulatory climate. **T.M. Leaym**

**9:45 I&EC 33.** All in the title: Modern baccalaureate level chemist. **B. Maye**

**10:10 I&EC 34.** Career transitions: A personal story. **K.M. Allen**

**10:35 I&EC 35.** Food and pharma: Options for chemical undergraduate students. **C.J. Archambault**

**11:00 I&EC 36.** From working the lab to saving the lab. **J. Taylor**

### Section B

Marriott Marquis San Diego Marina  
Temecula 3&4

### Industrial & Engineering Fellow: Symposium in honor of Mark B. Shiflett

A. M. Scurto, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 I&EC 37.** Ionic liquid-liquid chromatography (ILLC™). **K.R. Seddon**, M.A. Gilea, M. Earle, N.V. Plechkova, L. Brown

**8:55 I&EC 38.** Insights into the molecular dynamics at the cathode/electrolyte interface of electrocatalyst materials for  $\text{CO}_2$  reduction in the presence of room temperature ionic liquids. **J. Rosenthal**, J.L. DiMeglio, J. Medina-Famos

**9:15 I&EC 39.** Photopolymerization behaviors of ionic liquid-based monomers. **J. Bara**, J.W. Whitley

**9:35 I&EC 40.** Water at ionic liquid-vapor interfaces. **J.T. Newberg**, Y. Khalifa, A. Broderick

**9:55 I&EC 41.** Ion diffusion in ionic liquids: Single molecule fluorescence spectroscopy. **T. Welton**, J.B. Ediel, A.J. McIntosh

**10:15 I&EC 42.** Structure and tensile properties of cross-linked Pluronic-diacrylate copolymers /ethylammonium nitrate iono-elastomers. **C. Lopez-Barron**, R. Chen, N.J. Wagner

**10:35 I&EC 43.** Radiation and radical chemistry of ionic liquids for energy applications. **J.F. Wishart**, I.A. Shkrob, S. Dhiman, D.C. Grills, A.R. Cook

**10:55 I&EC 44.** Ionic liquids as 'liquid solids' and their design for separations, catalysis, and more. **J.H. Davis**

**11:15 I&EC 45.** Ionic liquids for controlled synthesis of functional materials for energy-related applications. **S. Dai**

**11:35 I&EC 46.** Poly(ionic liquid)/ionic liquid composite membranes for high temperature ion ConductancePoly(ionic liquid)/ionic liquid composite membranes for high temperature ion conductance. **A. Lopez**, M. Cowan, M. Masuda, Y. Kohno, D.L. Gin, **R.D. Noble**

### Is There a Crisis in Organic Chemistry Education?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## MONDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Coronado Room

### New Reality of the Chemical Enterprise: Traditional & Non-traditional Career Paths

#### Chemistry Professionals Working "Outside the Box"

*Cosponsored by CTA, PRES and SOCED Financially supported by ACS Graduate and Postdoctoral Scholars Office*

M. K. Engelman, J. M. Smith, *Organizers*

M. A. Thomson, *Presiding*

**1:00 I&EC 47.** Fun working for BioSolutions. **J. Saviano**

**1:25 I&EC 48.** Keys to career advancement using your bachelor's degree. **J. Barcus**

**1:50 I&EC 49.** Withdrawn.

**2:15 I&EC 50.** Embracing change. **A. Graf**

**2:40 I&EC 51.** My employees are me, myself, and I...maybe a few others. **R.A. Hathaway**

**3:05 I&EC 52.** Good fellows: Getting paid to gain experience doing cutting-edge science. **J. Fleming**

**3:30 I&EC 53.** Building a distillery from scratch. **S. Callahan**

## Section B

Marriott Marquis San Diego Marina  
Temecula 3&4

### Industrial & Engineering Fellow: Symposium in honor of Mark B. Shiflett

A. M. Scurto, *Organizer, Presiding*

- 1:00 I&EC 54.** Translational research: From academia to industry. Following the pathway of George Washington Carver. J.L. Shamshina, G. Gurau, R.D. Rogers
- 1:20 I&EC 55.** Interactions of ionic liquids with polyaromatic hydrocarbons and fullerenes. M.F. Costa Gomes, E. Bordes, J. Szala-Bilnik, J. Andanson, A. Padua
- 1:40 I&EC 56.** Ionic liquids: From lab curiosities to industrial demands & applications: A short overview. F.M. Stiemke, P. von Czarniecki, T. Schubert
- 2:00 I&EC 57.** Low-cost ionic liquids for lignocellulose deconstruction. J.P. Hallett, A. Brandt
- 2:20 I&EC 58.** Extraction, recovery, and identification of contaminants from water. R.E. Del Sesto, A.T. Koppisch, M. Jones
- 2:40 I&EC 59.** Advances in surface and interface science of ionic liquids. F. Maier, H. Steinruck
- 3:00 I&EC 60.** Multipurpose cellulosic ionogels. G.A. Baker
- 3:20 I&EC 61.** Cosolvent and anti-solvent effects for cellulose processing in ionic liquids. D. Minnick, A.M. Scurto
- 3:40 I&EC 62.** Vapor + liquid phase equilibrium for [C6mim][Tf2N]: For session honoring I&EC fellow Dr. Mark Shiflett. J. Magee
- 4:00 I&EC 63.** Human gut microbiome and health: Insights from system-level models. P. Dhurjati
- 4:20** Concluding Remarks.

### Diversity-Quantification-Success?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, GINF, COLL, COMSCI, DAC, GECC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### Undergraduate Research Posters

#### Green Chemistry & Sustainability

*Sponsored by CHED, Cosponsored by CEI, I&EC and SOCED*

## MONDAY EVENING

## Section A

San Diego Convention Center  
Halls D/E

### Sci-Mix

P. M. Smith, *Organizer*

8:00 - 10:00

25. See previous listings.

83-84, 87, 91, 98, 113, 118, 120, 129, 144-145, 149, 153-154, 156-157, 161, 164-165. See subsequent listings.

## TUESDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Coronado Room

### New Reality of the Chemical Enterprise: Traditional & Non- traditional Career Paths

#### Chemistry Professionals Working in the Government

*Cosponsored by CTA, PRES and SOCED  
Financially supported by ACS Graduate  
and Postdoctoral Scholars Office*

J. M. Smith, *Organizer*

M. K. Engelman, *Organizer, Presiding*

**8:15** Introductory Remarks.

**8:30 I&EC 64.** David McCollam forensic chemist explosives unit FBI laboratory. D. Mccollam

**9:30 I&EC 65.** Chemistry of space exploration. L.B. Roberson

**10:00 I&EC 66.** Alternative careers in chemistry: Failure investigations in the aerospace industry. E. Barrios

**10:25 I&EC 67.** My journey from laboratory chemist to FDA interdisciplinary scientist. J. Doran

**10:50 I&EC 68.** Chemist as a project management professional at the FDA. R. Frey-Cooper

**11:15 I&EC 69.** Things I wish I had known or you can learn from my mistakes. L.M. Balbes

## Section B

Marriott Marquis San Diego Marina  
Temecula 1&2

### ACS Award in Industrial Chemistry: Symposium in honor of Ted C. Germroth

*Cosponsored by POLY*

D. Mason, *Organizer*

C. Killian, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:10 I&EC 70.** Controlling sequence in step-growth polymerization: From random liquid crystalline copolyesters to segmented polyester ionomers. T.E. Long, M. Zhang, A.M. Nelson, J.M. Dennis

**8:45 I&EC 71.** Unlikely commercialization story. B. Duckworth

**9:20 I&EC 72.** Levering networks and legacy research for enabling new polymer products. S.R. Turner

**9:55 I&EC 73.** Eastman Tritan™ copolyester. E. Crawford

**10:30 I&EC 74.** Polymer films that improve the viewability of liquid crystal displays. F.W. Harris, X. Zheng, D. Zhang, J. Jing, T.C. Germroth, B. King, T. Kuo

**11:05 I&EC 75. Award Address** (ACS Award in Industrial Chemistry sponsored by the ACS Division of Industrial and Engineering Chemistry). Industrial discovery: Process and product. T.C. Germroth

### Green Chemistry: Theory & Practice

*Sponsored by CHED, Cosponsored by CEI, I&EC and SOCED*

## TUESDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
Coronado Room

### New Reality of the Chemical Enterprise: Traditional & Non- traditional Career Paths

#### Chemistry Professionals are Entrepreneurs & More

*Cosponsored by CTA+, PRES and SOCED  
Financially supported by ACS Graduate  
and Postdoctoral Scholars Office*

J. M. Smith, *Organizer*

M. K. Engelman, *Organizer, Presiding*

**1:30 I&EC 76.** Panel discussion. M.K. Engelman

## Section B

Marriott Marquis San Diego Marina  
Temecula 1&2

### Separations for the Nuclear Fuel Cycle in the 21st Century Revisited

*Cosponsored by NUCL*

G. J. Lumetta, *Organizer*

K. L. Nash, *Organizer, Presiding*

M. L. Dietz, *Presiding*

**1:00** Introductory Remarks.

**1:15 I&EC 77.** Fission product performance in the co-decontamination process. L.R. Martin, C. Riddle

**1:45 I&EC 78.** Lab-scale testing of a co-decontamination process. C. Pereira, C. Launier, J. Krebs

**2:15 I&EC 79.** Alternative approach to TALSPEAK chemistry using SO<sub>3</sub>-Ph-BTP. A. Geist

**2:45** Intermission.

**3:00 I&EC 80.** Use of 2-ethylhexylphosphonic acid mono-2-ethylhexyl ester as an extractant for minor actinide separations. G.J. Lumetta, A.J. Casella, T.G. Levitskaia, L. Lin, S.I. Sinkov, J.C. Carter, A. Gelis

**3:30 I&EC 81.** Spectroscopic studies of neodymium in the ALSEP extraction process. G.B. Hall, F.N. Smith, T.G. Levitskaia, G.J. Lumetta

**4:00 I&EC 82.** Enhancing the lability of f-element / aminopolycarboxylate complex for efficient differentiation of trivalent actinides from trivalent actinides. P.R. Zalupski, C.R. Heathman, T.S. Grimes

### Green Chemistry: Theory & Practice

*Sponsored by CHED, Cosponsored by CEI, I&EC and SOCED*

## TUESDAY EVENING

## Section A

San Diego Convention Center  
Hall D

### General Posters

P. M. Smith, *Organizer*

5:00 - 7:00

**I&EC 83.** Morphological control of samarium oxide particles produced via precipitation stripping. B. Gibbons, P.M. Smith

**I&EC 84.** Micro crystalline cellulose based amidoxime functionalized mesoporous silica for high temperature carbon dioxide sorption. C. Gunathilake, R. Dassanayake, N. Abidi, M. Jaroniec

**I&EC 85.** Extraction and recovery of rare earth elements from phosphate ore and phosphate mining waste products using 1-octadecene, polymer with 2,5-furandione, sodium salt. J.P. Laurino, J. Mustacato

**I&EC 86.** Multi-functional gel materials for malodor remediation in sewer systems. L. Luk, W. Han, K. Cheung, J. Lee, K. Yeung

**I&EC 87.** Amine modified silica nanotubes and nanospheres for CO<sub>2</sub> adsorption. A. Manchanda, C. Gunathilake, P. Ghimire, M. Jaroniec, M. Kruk

**I&EC 88.** Novel synthesis and characterization of electron donor-sigma-acceptor molecules functioned as molecular rectification. Y. Lo, H. Honda, T. Wei, M. Hsiao

**I&EC 89.** Novel approaches to the chemical synthesis of cholest-8-en-7-one a potent inhibitor of sterol biosynthesis. Y. Lo, H. Shyu, H. Honda, T. Wei, M. Dai

**I&EC 90.** Novel approaches to the chemical synthesis and characterization of alkyl phenols derivatives with various side chains. Y. Lo, M. Hsiao, H. Honda, T. Wei

**I&EC 91.** Heat treatment intensity on rutile pigment production from unenriched industrial TiOSO<sub>4</sub> solution via short sulfate process. C. Tian

**I&EC 92.** Flash drying characteristics of low grade coal in a pressurized micro-riser. S. Lee, I. Gwak

**I&EC 93.** CO<sub>2</sub> gasification kinetics of petroleum coke mixture. S. Lee, J. Kook, J. Sohn

**I&EC 94.** Entrained-flow gasification of coal and industrial waste water mixture. S. Yoon, H. Ra, G. Oh, M. Seo, S. Yoon, J. Lee

**I&EC 95.** Fabrication of magnetically responsive core-shell adsorbents for desulfurization. P. Tan, X. Liu, L. Sun

**I&EC 96.** Low-temperature fabrication of strong basicity on mesoporous silica through a redox strategy. L. Zhu, N. Yan, L. Cheng, J. Ding, L. Sun

**I&EC 97.** Increased reducibility of rare earth oxides in pyro-electrochemical fuel processing. M. Lee, S. Jeong

**I&EC 98.** Responsive nanoporous membranes by selective swelling of triblock terpolymers. Y. Wang, Z. Wang

**I&EC 99.** Ammonia activated carbons using 2,2-biphenol and their application for carbon capture. S. Park, J. Lee

**I&EC 100.** Effects of LiCl on the dissolution of cellulose in imidazolium based ionic liquids. S. Park, J. Lee, M. Cheong

**I&EC 101.** Ammonia activation of porous carbons derived from biomass for carbon capture. S. Park, J. Lee

**I&EC 102.** CO<sub>2</sub> activated carbons using 2,2-biphenol and their application for carbon capture. S. Park, J. Lee

**I&EC 103.** Preparation of antibacterial inorganic particles through polyelectrolyte multilayering technique and its application to paper. H. Youn, J. Lee, K. Sim, H. Lee

**I&EC 104.** Resource recovery and reuse: Recycled magnetically separable iron-based catalysts for phosphate recovery and arsenic removal. C. Han, G. Varshney, N. Kesav, M. Nadagouda

**I&EC 105.** Kinetic promotion effect of ionic liquid on CH<sub>4</sub> hydrate formation. S. Kang, J. Shin, K. Kim

**1&EC 106.** Aqueous complexation of actinyl ions by Schiff base ligands: Effects on solvent extraction. C.A. Hawkins, C.G. Bustillos, R. Copping, I. May, M. Nilsson

**1&EC 107.** Survey of the chromotropic dyes arsenazo-iii, chlorophosphonazo-iii, and xlenol orange for use in lanthanum binding kinetic determinations with 1,2-cyclohexanediaminetetraacetic acid (CDTA). R.G. McDowell, N. Hibert, S.P. Mezyk, L.R. Martin

**1&EC 108.** Unattended, representative sampling for a wide range of chemical reactions. J. Riley

## WEDNESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Temecula 1&2

#### Greener Pathways to Organics & Nanomaterials: Sustainable Applications of Magnetic Nanocatalysts

*Cosponsored by ENVR†*

V. K. Sharma, *Organizer*

L. Sun, *Presiding*

**8:30** Introductory Remarks.

**8:40 1&EC 109.** In search of green chemistry and sustainable: Polymeric materials based on renewable polymers. P. Berton, G. Gurau, J.L. Shamshina, R.D. Rogers

**9:05 1&EC 110.** Greener synthesis and applications of responsive and catalytic nanostructured membranes. D. Bhattacharyya, S. Hernandez, A. Saad, H. Wan, D. Davenport, L. Ormsbee

**9:30 1&EC 111.** Synthesis of novel magnetic nanoparticles with mesoporous surfaces and their application in catalysis. J. Zhi, B. Kastl, S. Ranjbar, O. Reiser

**9:55** Intermission.

**10:10 1&EC 112.** Reduced iron nanoparticles as magnetically retrievable catalysts for alkene hydrogenation and as galvanic reducers to access Cu and Ru-based catalysts for azide-alkyne condensation and transfer hydrogenation. A.H. Moores, R. Hudson, C. Li, M. Masnadi, M. Bateman

**10:35 1&EC 113.** Newly eco-designed magnetically separable catalysts for environmental applications. D. Hermosilla, B. Ren, M. Nadagouda, C. Han, A. Gascó, P. Campo Moreno, D.D. Dionysiou

**11:00 1&EC 114.** Magnetic nanocatalysts for benign organic transformations. A. Rathi, M. Gawande, J. Filip, R.S. Varma, R. Zboril

### Section B

Marriott Marquis San Diego Marina  
Coronado Room

#### Separations for the Nuclear Fuel Cycle in the 21st Century Revisited

*Cosponsored by NUCL*

K. L. Nash, *Organizer*

G. J. Lumetta, *Organizer, Presiding*

P. R. Zalupski, *Presiding*

**8:00 1&EC 115.** Investigating  $\text{Ca}_2[\text{UO}_2(\text{CO}_3)_2]$  (aq.) from the perspective of DFT. C. Priest, D. Jiang

**8:30 1&EC 116.** Solid state inorganic ion exchanger for isolation of uranium from ocean water and ground water. A.W. Apblett, C.K. Perkins

**9:00 1&EC 117.** Bifunctional amidoxime fibers for the recovery of uranium from seawater. S. Alexandratos, X. Zhu

**9:30 1&EC 118.** Selective removal of uranium from high sulfate, high nitrate streams using hybrid organic inorganic materials. E. Rosenberg, R. Tsosie

**10:00** Intermission.

**10:15 1&EC 119.** Progress in ionic liquids for advanced nuclear separations. J.F. Wishart, S. Dai, M.L. Dietz, H. Luo, I.A. Shkrob

**10:45 1&EC 120.** Chemistry and electrochemistry of selected radionuclides in several groups of room temperature ionic liquids. M. Straka, L. Szatmary

**11:15 1&EC 121.** Process development in Japan of supercritical fluid extraction of heavy metals from actual used nuclear fuel in the past decade, light and shadow parts. Y. Enokida

## WEDNESDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Temecula 1&2

#### Greener Pathways to Organics & Nanomaterials: Sustainable Applications of Magnetic Nanocatalysts

*Cosponsored by ENVR†*

V. K. Sharma, *Organizer*

P. Kajitvichyanukul, *Presiding*

**1:00 1&EC 122.** Developing sustainable reaction conditions via mechanochemistry. L. Chen, K. Leahy, R. Haley, H. Hoppogod, J. Mack

**1:25 1&EC 123.** Withdrawn.

**1:50 1&EC 124.** Green chemical processes under ultrasound and microwave irradiation: From batch to flow technology. G. Cravotto, E. Calcio Gaudino, A. Barge, K. Martina

**2:15 1&EC 125.** Copper-containing rod-shaped nano-sized silica particles for microwave assisted synthesis of triazoles in aqueous solutions. E. Colacino, C. Charnay

**2:40** Intermission.

**2:55 1&EC 126.** Formation of active sites within nano-confined space. Y. Jiang, Y. Kang, X. Liu, L. Sun

**3:20 1&EC 127.** Withdrawn

**3:45 1&EC 128.** Graphitic carbon nitride ( $\text{g-C}_3\text{N}_4$ ): A promising support for photo-active heterogeneous catalysis. S. Verma, N.R. Baig, M. Nadagouda, R.S. Varma

**4:10 1&EC 129.** Ferrite-titania nanocomposites with core-shell structure for environmental remediation. B. Ren, C. Han, M. Nadagouda, V. Sharma, K.E. O'Shea, D.D. Dionysiou

### Section B

Marriott Marquis San Diego Marina  
Coronado Room

#### Separations for the Nuclear Fuel Cycle in the 21st Century Revisited

*Cosponsored by NUCL*

G. J. Lumetta, K. L. Nash, *Organizers, Presiding*

**1:00 1&EC 130.** Experimental and modelling investigation into the radiolysis of the Purex solvent system. G.P. Horne, H.E. Sims, R.J. Taylor, S.M. Pimblott

**1:30 1&EC 131.** Development of a long term partitioning processes for minor actinides: Influence of gamma radiation on extraction systems based on diglycolamides such Euro-GANEX process. M. Galan, A. Nuñez, D. Munzel, U. Müllich, J. Cobos, A. GEIST

**2:00 1&EC 132.** Investigation of the impacts of gamma radiolysis on a SANEX process solvent. D.R. Peterman, B.J. Mincher

**2:30** Intermission.

**2:45 1&EC 133.** Hexavalent actinide co-crystallization: New approach to group actinide separation. J. Burns, B.A. Moyer

**3:15 1&EC 134.** Managing molybdenum in ALSEP and the Mo-acetohydroxamic acid complex. M. Brown, A.T. Breshears, J.R. Walensky, A.V. Gelis

**3:45 1&EC 135.** Design of Mo-99 recovery and concentration processes from irradiated uranyl sulfate target solution. D. Stepinski, A. Youker, D. Rotsch, P. Tkac, S. Chmerisov, G.F. Vandegriff

**4:15** Concluding Remarks.

## THURSDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Temecula 1&2

#### Greener Pathways to Organics & Nanomaterials: Sustainable Applications of Magnetic Nanocatalysts

*Cosponsored by ENVR†*

V. K. Sharma, *Organizer, Presiding*

**8:30 1&EC 136.** Synthesis and surface properties of catanionic fluorosurfactants. K.R. Seddon

**8:55 1&EC 137.** Designer bionanocomposite for biomedical applications. R. Luque

**9:20 1&EC 138.** Withdrawn.

**9:45 1&EC 139.** Glycerol: A solvent and building block of choice for alternative technologies. C. Len

**10:10** Intermission.

**10:25 1&EC 140.** Fabrication of titanate nanotube-supported carbon-zerovalent iron nanocomposites for enhanced dechlorination of trichloroethylene. R. Doong, F. Tsou

**10:50 1&EC 141.** Withdrawn.

**11:15 1&EC 142.** Removal of arsenite from water by adsorption onto humic acid coated magnetite nanoparticles. M. Rashid, Y. Cai, K.E. O'Shea

**11:40 1&EC 143.** Ferrate ( $\text{Fe}^{\text{VI}}$ ) as a sustainable green oxidant: Selectivity and transformation of pharmaceuticals. V.K. Sharma

### Section B

Marriott Marquis San Diego Marina  
Temecula 3

#### General Papers

L. R. Martin, *Organizer, Presiding*

**8:00 1&EC 144.** Synthesis of mesoporous alumina with amidoxime groups for ambient and elevated temperature  $\text{CO}_2$  sorption. C. Gunathilake, M. Jaroniec

**8:20 1&EC 145.** Using aluminum acetylacetonate as an electrolyte additive to mitigate thermal runaway in lithium-ion batteries. Y. Shi, D. Noelle, M. Wang, A. Le, Y. Qiao

**8:40 1&EC 146.** Functionalized mesoporous silica membranes on polymeric hollow fibers for separation applications. H. Kim, W. Koros, S. Nair, C.W. Jones

**9:00 1&EC 147.** Optimization of separations of rare earths and actinides through computational approaches. D.A. Penchoff, C. Peterson, G.K. Schweitzer, A.K. Wilson

**9:20 1&EC 148.** Effect of rapid pressurization on the solubility of small organic molecules. N.T. Morgan, T.C. Frank, R.J. Holmes, E.L. Cussler

**9:40 1&EC 149.** Role of n-alkane solvent carbon number on the gelation of long-chained n-alkanes in solution. M. Senra, M. Grewal, J.H. Jarboe

**10:00** Intermission.

**10:10 1&EC 150.** Development of flexible power sources using nanomaterials and polymers. X. Meng, Z. Wang, Z. Wu, S. Mitra

**10:30 1&EC 151.** Atomic layer deposition enabled advanced membranes. Y. Wang

**10:50 1&EC 152.** Developing green and recyclable sulfonolene systems. Y. Huang

**11:10 1&EC 153.** Study and removal of ppb level lead (II) from after wash glass bottles in beverage industry. A. Altaf, M. Ayub, A. Badshah

**11:30 1&EC 154.** Withdrawn.

**11:50 1&EC 155.** Highly sensitive and specific detection of toxic metals by biosensors. S.F. Li

## THURSDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Temecula 1&2

#### General Papers

L. R. Martin, *Organizer, Presiding*

**1:00 1&EC 156.** Supramolecular materials for trace collection of small molecule organics from water. K.M. Nell, S.A. Fontenot, D.W. Johnson

**1:20 1&EC 157.** New application of dividing-wall columns for the separation of coal based light olefins. J. Li

**1:40 1&EC 158.** Sustainable  $\text{CO}_2$ -based processes through methanol and DME production. U. Suriyapraphadilok, T. Nguyen, W. Prasertsri, R. Gani

**2:00 1&EC 159.** Ion transport behavior in self-assembled ionogel. S. Park, J. Lee

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- 2:20 I&EC 160.** Optimizing high-pressure chemical vapor deposition processes for void-free filling of silica optical fiber microcapillaries with hydrogenated amorphous silicon. **S. Motevalian, S. Aro, H.Y. Cheng, J.V. Badding, A. Borhan**
- 2:40 I&EC 161.** High silica zeolite-Y membranes: Motivation, development, characterization, and application. **S. Chakraborty, P. Dutta, S.J. Singer**
- 3:00 I&EC 162.** Sustainable production of chemicals using continuous flow technology. **Y. Huang**
- 3:20 I&EC 163.** Assessment of advanced easy-clean durable coatings. **A. Wojdyła-Cieslak, G.G. Durand, A. Taylor, I. Boyd**
- 3:40 I&EC 164.** Isomerization and self-metathesis of raffinate butenes to propylene on a W/Si-Al catalyst. **F. Alshafei, N. Sulais, M. Khokhar, R. Daadoush, R. Abudawoud, S. Shaikh**
- 4:00 I&EC 165.** Intensification of capture CO<sub>2</sub> from IGCC flue gas by hydrate formation under direct heat removal by phase change of n-tetradecane. **Y. Luo, X. Guo**
- 4:20 I&EC 166.** Encapsulated ferrate for air purification application. **W. Den, R. Wu, E. Kanchanatip**
- 4:40 I&EC 167.** Resistive response of carbon nanotube membrane for the detection of chlorophenols. **W. Den, N. Grisdanurak, E. Kanchanatip**
- 5:00 I&EC 168.** Synthesis of poly(vinyl butyral) based on a new micro-structured chemical system for process intensification. **X. Lin, K. Wang, J. Zhang, G. Luo**

## INOR

### Division of Inorganic Chemistry

**N. Radu and S. Koch, Program Chairs**

#### OTHER SYMPOSIA OF INTEREST:

**Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Matthew J. Polinski & Thomas E. Albrecht-Schmitt** (see NUCL, Sun)

**ACS Award for Creative Work in Fluorine Chemistry** (see FLUO, Sun, Mon)

**Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger** (see NUCL, Wed, Thu)

### SUNDAY MORNING

#### Section A

San Diego Convention Center  
Room 30B

#### Undergraduate Teaching at the Frontiers of Inorganic Chemistry

##### Framing the Future

*Cosponsored by CHED*

**B. A. Reisner, Organizer**

**J. L. Stewart, Organizer, Presiding**

**8:30** Introductory Remarks.

**8:35 INOR 1.** One eye on the past, one eye on the future: A reflection on the undergraduate inorganic chemistry curriculum. **B.A. Reisner**

**8:55 INOR 2.** Weaving the fundamentals of inorganic chemistry through upper level elective courses that touch on diverse topics such as nanoscale science and energy storage and conversion. **A.L. Prieto**

**9:15 INOR 3.** Beyond workshops: Partnering with R1-research groups to develop materials to post on VIPER. **M. Cass**

**9:35 INOR 4.** Development of a comprehensive multistep advanced laboratory experiment: Synthesis and characterization of Re(V)-oxo complexes with study of catalysis and reaction kinetics. **E.A. Ison, A. Ison**

**9:55** Intermission.

**10:10 INOR 5.** New teaching experiments for inorganic chemistry. **G. Lisensky**

**10:30 INOR 6.** Authoring an inorganic chemistry textbook in the 21st century. **P.J. Fischer**

**10:50 INOR 7.** Teaching inorganic materials chemistry and nanoscience at the undergraduate level. **T.E. Mallouk**

**11:10 INOR 8.** Teaching modern inorganic chemistry: A personal perspective. **G.S. Girolami**

**11:30** Panel Discussion.

#### Section B

San Diego Convention Center  
Room 30C

#### ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Vincent L. Pecoraro

##### Early Years

**B. R. Gibney, A. F. Peacock, Organizers**

**C. M. Zaleski, Organizer, Presiding**

**J. Bodwin, Presiding**

**8:30 INOR 9.** Microbial iron transport: From coordination chemistry to human host competition. **K.N. Raymond**

**9:00 INOR 10.** Inorganic physiology: Distribution and speciation of metal ions in biological systems. **J.E. Penner-Hahn**

**9:30 INOR 11.** Ammonia binding to the manganese of the oxygen evolving complex (revisited). **R.D. Britt**

**10:00 INOR 12.** Bioinspired, alpha-hydroxy acid-containing chelates for tight binding and light-triggered release of metals. **M.J. Baldwin**

**10:30** Intermission.

**10:40 INOR 13.** Withdrawn.

**11:10 INOR 14.** Coordination chemistry of vanadium combined with ligand properties lead to effective phosphatase inhibitors with potential antidiabetic properties. **D.C. Crans, C.C. McClachlan**

**11:40 INOR 15.** Fabricated nano and micro-particles for non-oral delivery. **B. Farrer**

**12:10 INOR 16.** C-H bond cleavage by metalloenzymes and metalloporphyrins. **J.T. Groves**

#### Section C

San Diego Convention Center  
Room 30D

#### ACS Award in Inorganic Chemistry: Symposium in honor of Mercuri G. Kanatzidis

##### Synthesis & Applications of Solid State Materials

**J. A. Aitken, Organizer**

**K. Choi, Organizer, Presiding**

**S. E. Latturmer, Presiding**

**8:30** Introductory Remarks.

**8:35 INOR 17.** Early years/milestones in the career of Mercuri Kanatzidis in the University of Iowa and the University of Michigan. **D.N. Coucouvanis**

**8:50 INOR 18.** Semiquinoid radical-containing molecules and solids with strong magnetic exchange coupling. **D. Harris, I. Jeon, A. Gaudette, J. DeGayer**

**9:15 INOR 19.** Metal-organic frameworks as highly functional catalytic arrays. **S. Moon, Z. Li, S.S. Al-Juaid, P. Li, Y. Liu, A. Howarth, J.B. DeCoste, G.W. Peterson, C.J. Cramer, L. Gagliardi, J.T. Hupp, O.K. Farha**

**9:40 INOR 20.** Emerging biomedical applications of Prussian blue analogue compounds: From oral MRI contrast agents to catalytic anticancer drugs, and to tumorigenic angiogenesis inhibitors. **S. Huang**

**10:05** Intermission.

**10:20 INOR 21.** Design of noncentrosymmetric materials. **K.R. Poeppelmeier**

**10:45 INOR 22.** Quaternary diamond-like semiconductors with infrared nonlinear optical properties. **J.A. Aitken, J. Brant, D. Clarke, J. Jang, J. Zhang, K. Rosmus, S. Wisneski**

**11:10 INOR 23.** Templating of silica mesophases by sustainable oleyl amine surfactants. **T.J. Pinnavaia, C. Canlas**

**11:35 INOR 24.** Surfactants as promising media for the preparation of crystalline inorganic materials. **Q. Zhang**

#### Section D

San Diego Convention Center  
Room 30E

#### ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg

*Cosponsored by WCC*

**N. E. Gruhn, W. D. Jones, Organizers**

**M. S. Sanford, Organizer, Presiding**

**A. J. Miller, Presiding**

**9:00 INOR 25.** New Pd(II) and Ni(II) catalysts for olefin polymerizations. **Z. Chen, D. Bezier, K. Allen, O. Daugulis, M. Brookhart**

**9:20 INOR 26.** Synthesis of allenes via isomerization of internal alkynes. **N. Phadke, M. Findlater**

**9:40 INOR 27.** Tuning olefin isomerization and hydrogenation with cation-responsive catalysts. **A.J. Miller, M.R. Kita, J.B. Smith, S.H. Kerr, J. Grajeda, L.C. Gregor, A.H. Sullivan**

**10:00 INOR 28.** Materials for organic light-emitting diode displays. **N.S. Radu, N. Herron, G. Rossi, F. Gentry, T.N. Hoerter, Y. Wang, A. Fennimore, R. Chesterfield, W. Gao**

**10:20** Intermission.

**10:30 INOR 29.** Organometallic chemistry of nickel(III) and (IV). **M.S. Sanford**

**10:50 INOR 30.** Approaches to the synthesis of Fe(IV) alkylidenes. **P.T. Wolczanski, B.M. Lindley, B.P. Jacobs, R. Agarwal, S.N. MacMillan**

**11:10 INOR 31.** Two decades of lessons in controlling selectivity in Pt (IV) reductive elimination, and new attempts to increase activity in Pt (II) oxidative addition. **N. Williams, M. Van Vleet, A. Liberman-Martin, T. Mortvedt, L.A. Watson, R.J. Cave**

**11:30 INOR 32.** Platinum(IV) and palladium(IV) aryldiazenido complexes. **U.W. Fekl**

**11:50 INOR 33.** Base-free transfer hydrogenation of aldehydes and ketones using Cp\*Ir(pyridinesulfonamide)Cl precatalysts. **A.R. O'Connor**

#### Section E

San Diego Convention Center  
Room 31A

#### Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

**S. A. Koch, Organizer**

**L. E. Cheruzel, Presiding**

**8:30 INOR 34.** Series of N5 ligands as functional mimics of the nickel superoxide dismutase active site. **V.G. Snider, A. Mukherjee**

**8:50 INOR 35.** Bioinspired heterometallic systems for the activation of small molecules. **V. Oswald, A. Borovik**

**9:10 INOR 36.** Reactive copper-oxygen species with mixed benzimidazole/thio- and selenoether platforms relevant to the active site of PHM. **I. Castillo, B. Sanchez-Eguia, M. Orio**

**9:30 INOR 37.** Site-selective characterization of plastocyanin with linear and multidimensional infrared spectroscopy. **A. Le Sueur, M.C. Thielges**

**9:50 INOR 38.** Structural and functional mimic of the NiFe hydrogenase with unprecedented Ni-centered chemistry. **D. Brazzolotto, M. Gennari, N. Queyriaux, F. Meyer, M. Orio, V. Artero, C. Duboc**

**10:10 INOR 39.** Activation of methyl-coenzyme M reductase, the enzyme involved in methane production or consumption in Archaea. **E.C. Duin, D. Prakash, R. Ghebreab, B. Cronin**

**10:30** Intermission.

**10:40 INOR 40.** Targetable, reaction-based small molecule-protein hybrid sensors for detecting mobile zinc. **M.L. Zastrow, Z. Huang, R.J. Radford, S.J. Lippard**

**11:00 INOR 41.** Selective substrate C-H functionalization using light-driven P450 biocatalysts. **L.E. Cheruzel**

**11:20 INOR 42.** Biomimetics of tri-iron arrangements involving cyanide as docking agent in maturases of the H cluster of the diiron hydrogenase. **A.M. Lunsford, C. Beto, S. Ding, N. Wang, M.B. Hall, M.Y. Darensbourg**

**11:40 INOR 43.** Improved method for the spectroscopic determination of inorganic phosphate to quantify nucleotide hydrolysis. **F.E. Katz, F.A. Tezcan**

**12:00 INOR 44.** Development of fatty acid derivatives to inhibit platelet aggregation and investigating their biochemical mechanism. **J. Roy, R. Adili, M. Holinstat, A. Das**

**12:20 INOR 45.** Artificial metalloproteins: Towards a blue copper center. **S.J. Mann, T. Heinisch, T.R. Ward, A. Borovik**

## Section F

San Diego Convention Center  
Room 31B

### Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

A. Ghosh, C. H. Larsen, *Presiding*

**8:00 INOR 46.** Asymmetric ligand approach to design volatile molecular precursors for the Al-Fe intermetallic catalyst. **S. Mishra**, K. Soussi, E. Jeanneau, S. Daniele

**8:20 INOR 47.** Nitrile activation by intramolecular C-C bond coupling to a diimine ligand in group 7 metal tricarbonyl complexes. **V. Yempally**, W.Y. Fan, B. Arndtsen, A. Bengali

**8:40 INOR 48.** Unique highly connected / highly stable RE-MOF for moisture control in confined spaces: Introduction to moisture controlled swing adsorption. **R. Abdul Halim**, M. Eddaoudi, Y. Belmabkhout

**9:00 INOR 49.** Fundamental coordination chemistry for the recycle efforts of scandium. **J. Sears**, T.J. Boyle, L.J. Small, T.M. Alam

**9:20 INOR 50.** Reversible spin state changes in a 4-coordinate iron complex: Valence tautomerism involving redox-active formazanate ligands. **R. Travieso Puente**, E. Otten, M. Chang

**9:40 INOR 51.** Bulky N-heterocyclic thione (NHT) and seleno (NHSe) complexes of mercury(II) and copper(I). **M. Kocherga**, D. Rabinovich

10:00 Intermission.

**10:10 INOR 52.** 5d metallocorrolles: Bis(corrolato)tungsten(VI) sandwich complexes as novel, chiral members in a growing family. **A. Ghosh**, A. Alemayehu, H. Vazquez-Lima, K.J. Gagnon

**10:30 INOR 53.** Bifunctional Cu(II) and Zn(II) ligands for ratiometric metal ion sensing. **M. Abdalrahman**, W.S. Kassel, R. Seitz, **F. Abebe**, S. Burdette, R.P. Planalp

**10:50 INOR 54.** Reactivity of rhodium(I) ( $\beta$ -ketoaminate)(bipyridine) complexes with oxidants. **E. Seraya**, A.F. Heyduk

**11:10 INOR 55.** Toward the synthesis of tetrametallic terminal oxo complexes supported by aminopyrazole ligands. **Z. Han**, K. Horak, T. Agapie

**11:30 INOR 56.** One-step synthesis of substituted 2-(2'-pyridyl)quinoline ligands applied to study the solution and solid phase behavior of gold(III) complexes. **M. Sterling**, E.M. Laguna, P. Olsen, E. Roman, A.L. Rheingold, **C.H. Larsen**

**11:50 INOR 57.** Unraveling trends in metal-metal bonding: A comparison of Ti-M, V-M, and Cr-M heterobimetallics (M = Fe, Co, Ni). **L.J. Clouston**, S. Bernales Candia, L. Gagliardi, C. Lu

**12:10 INOR 58.** Computational study of propene polymerization promoted by postmetallocene octahedral systems: playing with steric and electronic factors. **G. Talarico**, P.H. Budzelaar

## Section G

San Diego Convention Center  
Room 31C

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

N. B. Shustova, *Presiding*

**8:30 INOR 59.** Structure dependent catalytic activity of bimetallic metal organic framework. **A. Pariyar**, A. Choudhury

**8:50 INOR 60.** Electrochemical investigation of MOFs as intercalation materials for batteries. **D.F. Sava Gallis**, H.D. Pratt, T.M. Anderson, J.S. Chavez, K.W. Chapman

**9:10 INOR 61.** Designing electrochromic MOFs. **K. AlKaabi**, M. Li, M. Dinca

**9:30 INOR 62.** Metal-organic frameworks as a versatile platform for renewable energy applications. **N.B. Shustova**, D.E. Williams, E.A. Dolgoplova, A.M. Rice

**9:50 INOR 63.** Development of engineered forms of metal-organic frameworks for chemical defense applications. **J.B. DeCoste**

10:10 Intermission.

**10:25 INOR 64.** Withdrawn.

**10:45 INOR 65.** Layer-by-layer coordinated thin films of metal-organic frameworks (MOFs): New artificial platforms for solar energy capture and directional electronic energy transfer. **M.C. So**, H. Park, D.J. Gosztola, G.P. Wiederrecht, J.D. Emery, A.B. Martinson, S. Er, C. Wilmer, N.A. Vermeulen, J.F. Stoddart, A. Aspuru-Guzik, O.K. Farha, J.T. Hupp

**11:05 INOR 66.** Catalytic hydrocarbon upgrading in metal-organic frameworks. **E. Metzger**, M. Dinca

**11:25 INOR 67.** Dual-ion battery cathode via oxidative insertion of anions in a metal-organic framework. **M.L. Aubrey**, J.R. Long

**11:45 INOR 68.** Electronic conductivity, ferrimagnetic ordering, and reductive insertion in semiquinoid metal-organic frameworks. **L.E. Darago**, M.L. Aubrey, C.J. Yu, M.I. Gonzalez, J.R. Long

## Section H

San Diego Convention Center  
Room 32A

### Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Eric J. Schelter

L. G. Sneddon, P. J. Walsh, *Organizers*

S. C. Bart, N. C. Tomson, *Presiding*

8:30 Introductory Remarks.

**8:40 INOR 69.** Understanding the An=E bonds in  $[K(18\text{-crown-6})][An(E)(NR_2)_2]$  (An = Th, U; E = O, S, Se, Te; R = SiMe<sub>3</sub>). **T.W. Hayton**

**9:00 INOR 70.** Tris(pyrrolide) amine ligands as scaffolds for uranium chemistry. **J.M. Boncella**, M. Winston, B. Scott

**9:20 INOR 71.** Building uranium-nitrogen multiple bonds. **S.C. Bart**, N. Anderson, P.E. Fanwick

**9:40 INOR 72.** Covalency in pentavalent uranium. **S.A. Kozimor**, E.R. Batista, D.L. Clark, J. Cross, M.G. Ferrer, H. La Pierre, S.G. Minasian, A. Olson, B. Scott, D.K. Shuh, B. Stein, C. Stieber, P. Yang

10:00 Intermission.

**10:20 INOR 73.** Playing with plutonium. **D.L. Clark**, S.A. Kozimor, A. Mounce, E.D. Bauer, J.D. Thompson, H. Yasuoaka, G. Koutoulakis

**10:40 INOR 74.** Californium gleaming. **T.E. Albrecht-Schmitt**

**11:00 INOR 75.** Interesting, albeit brief, journey from Yb to Ac: Applications of f-elements. **K. John**

**11:20 INOR 76.** Characterizing temperature-independent paramagnetism in U(VI) bis-imido complexes. **N.C. Tomson**, B. Scott, J.M. Boncella

## Section I

San Diego Convention Center  
Room 32B

### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

P. O. Adelani, T. J. Boyle, *Presiding*

**8:30 INOR 77.** Synthesis and characterization of PtNiCo nanoparticles with controllable size, shape, and composition. **H. Cronk**, S. Kim, Z. Skeete, S. Shan, D.M. Mott, J. Lou, C. Zhong

**8:50 INOR 78.** Loading gold-carbon nanoparticles on nanodiamonds and diamond platforms. **S. Orefuwa**, M. El Naggari, I. Shehadi, **A. Mohamed**

**9:10 INOR 79.** Magnetic isolation of single-domain FePt nanoparticles for controlled optimization. **P.O. Adelani**, J.D. Rinehart, A.N. Duke

**9:30 INOR 80.** Synthetic approaches to iron selenide nanostructures. **S.E. Ingram**, S.L. Stoll

**9:50 INOR 81.** Recent developments and new challenges in the design of EBID precursors. **J. Pedziwiatr**, Y. Wu, J.A. Brannaka, J. Spencer, H. Fairbrother, L. McElwee-White

10:10 Intermission.

**10:25 INOR 82.** Microscopic investigation of chemoselectivity in Ag-Pt-Fe<sub>3</sub>O<sub>4</sub> nanoparticle heterotrimer formation: Mechanistic insights and implications for controlling high-rdred hybrid nanoparticle morphology. **J. Morse**, R. Schaak

**10:45 INOR 83.** On the exploration of a general mechanism of precursor evolution at low temperature to colloidal semiconductor nanocrystals. **K. Yu**

**11:05 INOR 84.** Metal ion exchange in CdS-based molecular clusters. **K.R. Kittilstved**, S. Pittala, M. Mortelliti, F. Kato

**11:25 INOR 85.** Siloxide derivatives of early transition metal alkoxides for production of nanomaterials. **T.J. Boyle**, R.O. Chan, J.M. Sears, P. Lu

**11:45 INOR 86.** Filled tetrahedral semiconductors in the nano-regime: Synthesis and characterization of I-II-V Nowotny-Juza phases. **M.A. White**, M. Thompson, J. Vela-Becerra

**12:05 INOR 87.** DOPED calcium carbonate particles for decolorization of dyes. **H. Ramesh**, K. Radhakrishnan, S. Kumar, A. Raichur

## Section J

San Diego Convention Center  
Room 33A

### Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

C. J. Daley, *Presiding*

**8:00 INOR 88.** Of triangles and squares: Hierarchical self-assembly of interlinked polyoxometalates. **S. Serapian**, G. Izzet, A. Proust, C. Bo

**8:20 INOR 89.** Synthesis and biological testing of cupric phenanthroline complexes: An alternative to cisplatin? **N. Angel**, J.F. Eichler

**8:40 INOR 90.** Structural and efficacy of some mixed antimalarial drugs-metal complexes. **J.A. Obaleye**, N. Simon, M.O. Bamigboye, A.O. Rajee, A.A. Ajibola

**9:00 INOR 91.** Production of carbon disulfide, a potentially relevant biological small molecule, from different vehicles, including photochemically via a cobalt(III) (1,1)-dithiooxalate-based complex. **A.W. DeMartino**, C. Sun, P.C. Ford

**9:20 INOR 92.** Synthetic inorganic chemistry approaches to the development of transition metal complexes as viable qubits. **J. Zadrozny**, J. Niklas, O. Poluektov, D.E. Freedman

**9:40 INOR 93.** Photoswitching in azobenzene-containing metal-organic framework thin films. **Z. Wang**

10:00 Intermission.

**10:10 INOR 94.** Redox-noninnocent and proton-responsive behavior of coordinated bispyrazolyl-pyridine type ligands. **A.V. Polezhaev**, C. Chen, B.J. Cook, K.G. Caulton

**10:30 INOR 95.** Exploring ligand-to-ligand charge-transfer (LL'CT) transitions of Ni(II) coordination complexes. **L.A. Cameron**, A.F. Heyduk

**10:50 INOR 96.** Electrochemical proton reduction using a redox-active W[SNS]<sub>2</sub> cofactor tethered to a Ni center. **K.E. Rosenkoetter**, A.F. Heyduk

**11:10 INOR 97.** Exploring the Mo[SNS]<sub>2</sub> complex as a redox-active cofactor in heterometallic systems. **M. Wojnar**

**11:30 INOR 98.** Cs[H<sub>2</sub>NB<sub>2</sub>(C<sub>6</sub>F<sub>5</sub>)<sub>2</sub>], featuring the first unequivocal 16-coordinate cation. **K. Pörschke**, D. Pollak, R. Goddard

**11:50 INOR 99.** Spectroscopic characterization and application of iron(III) 1,4,7,10-tetra-aza-2,6-pyridinophane derivatives. **S.M. Brewer**, K. Lincoln, K.N. Green

**12:10 INOR 100.** Divergent reactivity of selenoethers with metal reagents: Formation of molecular complexes vs. metal selenide nanoparticles. **S. Mishra**

## Section K

San Diego Convention Center  
Room 33B

### Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

B. J. Holliday, E. J. Werner, *Presiding*

**8:30 INOR 101.** Excited-state metalloradicals: Luminescent cerium(III) complexes for photo-redox chemistry. **H. Yin**, P.J. Carroll, J.M. Anna, E.J. Schelter

**8:50 INOR 102.** Design and evaluation of selective CMPO-based extractants for f-element separations. **E.J. Werner**, S.M. Biros, M.G. Patterson, D.A. Hardy

**9:10 INOR 103.** Use of lanthanide-MOFs for the detection of VOCs derived from tire burning and crude oil emissions. **C.L. Crawford**

9:30 Intermission.

**9:40 INOR 104.** Towards bone-targeting using upconverting nanoparticles decorated with bisphosphonates. **S. Alonso de Castro**, L. Salassa

**10:00 INOR 105.** Excited-state dynamics in heteroleptic ligand environments that are efficient sensitizers of lanthanide ion luminescence. **J. Wilkerson**, A. King, D.J. Strohecker, J. Rack, **B.J. Holliday**

**10:20 INOR 106.** Synthetic routes to multi-metallic f-element complexes with redox-active ligands. **J.H. Farnaby**, J.R. Hickson, N.J. Long

10:40 Intermission.

**10:50 INOR 107.** Visible-emitting lanthanide complexes for multicolor imaging. **E. Borbas**

- 11:10 INOR 108.** Lanthanide complexes as potential luminescent markers and temperature probes. **J. Monteiro**, A. De Bettencourt Dias, F. Sigoli
- 11:30 INOR 109.** Photosensitized down-conversion in rare-earth fluoride nanocrystals. **P. Agbo**, T. Xu, R.J. Abergel

## Section L

San Diego Convention Center  
Room 33C

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

T. Cantat, *Presiding*

- 8:30 INOR 110.** Depolymerization of wood lignin to isolated products using main group and organometallic catalysts. **T. Cantat**, E. Feghali, G. Carrot, C. Genre, P. Thuery
- 8:50 INOR 111.** Synthesis, reactivity, and catalytic applications of iridium pincer complexes. **J.M. Goldberg**, S. Tran, L.M. Guard, S. Bellows, F. Hornig, T.R. Cundari, K.I. Goldberg, D.M. Heinekey
- 9:10 INOR 112.** Directions in pincer chemistry: Progress towards the development of new methodology for catalytic isomerization of internal alkenes to allenenes via C-H bond activation. **N. Phadke**, F. De Jesus Martinez, S. Shafiei-Haghighi, M. Findlater
- 9:30 INOR 113.** Synthesis and reactivity of ruthenium ( $\eta^6$  PCP) complexes with perfluoroethylphosphine substituents. **S. Debnath**, D.M. Roddick
- 9:50 INOR 114.** Synthesis and catalytic activity of air-stable NHC Co(III) pincer complex in C-H borylation. **S.W. Reilly**, M. Zhang, H.U. Valle, C.E. Webster, T.K. Hollis
- 10:10 INOR 115.** Tuning product selectivity in catalytic ethylene tetramerization systems. **A. Lifschitz**, N. Hirscher, J.A. Buss, T. Agapie
- 10:30** Intermission.
- 10:40 INOR 116.** Potential hemi-labile (imino)pyridine palladium(II) complexes as selective ethylene dimerization catalysts: An experimental and theoretical approach. **S. Ojwach**, G. Nyamato, M. Akerman
- 11:00 INOR 117.** Withdrawn.
- 11:00 INOR 1225.** C<sup>+</sup> cyclometalated platinum(II) NHC complexes. **T. Strassner**, A. Tronnier, M. Tenne, J. Soellner
- 11:20 INOR 118.** Ethylene and  $\alpha$ -olefin copolymerization by bimetallic zirconium catalysts. **J. Sampson**, M.N. Akhtar, J. E.A., R. Theravalappil, H.A. Al-Muallem, M. Radlauer, T. Agapie
- 11:40 INOR 119.** Development of chromium compounds supported by chelating multi-aryl ligands for selective ethylene oligomerization. **N. Hirscher**, A. Lifschitz, A.M. Bryan, T. Agapie

### Alpha Olefin Catalysis: Production & Transformations

#### Catalytic Production

Sponsored by I&EC, Cosponsored by CATL and INOR $\ddagger$

### Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Matthew J. Polinski & Thomas E. Albrecht-Schmitt

Sponsored by NUCL, Cosponsored by INOR

## SUNDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 30B

### Undergraduate Research at the Frontiers of Inorganic Chemistry

#### Bioinorganic & Coordination Chemistry

Financially supported by IONIC (Interactive Online Network of Inorganic Chemists)

H. J. Eppley, C. Nataro, *Organizers*

S. K. Goforth, *Presiding*

**1:30** Introductory Remarks.

- 1:35 INOR 120.** Redox-induced ligand switching in mutants of cytochrome c. **K.R. Hoke**, M.R. Chandler, R.J. Quarles
- 1:55 INOR 121.** Sensitive colorimetric assay for light-driven P450 enzymes. **Q. Lam**, M. Kato, L.E. Cheruzel
- 2:15 INOR 122.** Application of molybdate complexes towards the oxidation and hydrolytic chemistry of organophosphate toxins. **L.Y. Kuo**
- 2:35 INOR 123.** Bis- and pendant armed tetraazamacrocyclic transition metal complex dual CXCR4/CCR5 antagonists. **D.J. Davilla**, O. Birdsong, D. Schols, S.J. Archibald, T.J. Hubin
- 2:55** Intermission.
- 3:10 INOR 124.** Multinuclear 51V NMR studies of aqueous vanadium-HEDTA complexes. **D.C. Crans**, X. Wu, B.J. Peters
- 3:30 INOR 125.** Synthetic, spectroscopic, and computational studies of tetraketimide complexes with an emphasis on Group 5. **J.A. Telsler**, P. Damon, C.J. Liss, R.A. Lewis, S. Morochnik, D.E. Szpunar, T.W. Hayton
- 3:50 INOR 126.** Synthesis and reactivity of new N-heterocyclic thione (NHT) and selenone (NHSe) ligands. **M. Styron**, L. Hernandez, M. Kocherga, **D. Rabinovich**
- 4:10 INOR 127.** Synthesis, structure, and catalytic activity of water soluble M-NHC complexes. **R.J. Swails**, S.K. Kariofillis, G.F. Riegel, N.F. Chaudary

### Section B

San Diego Convention Center  
Room 30C

### ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Vincent L. Pecoraro

#### Metallacrowns

A. F. Peacock, C. M. Zaleski, *Organizers*

B. R. Gibney, *Organizer, Presiding*

G. Mezei, *Presiding*

- 1:30 INOR 128.** Controlling the magnetic anisotropy and the single molecule magnet behavior in trigonal bipyramidal mononuclear Co(II) complexes. **M. Talal**, V.E. Campbell, L. Batchelor, F. Shao, G. Zakhia, R. Guillot, R. Ruamps, N. Guihery, A. Barra, W. Wernsdorfer
- 2:00 INOR 129.** Carboxylate ligand modification of heterotrimetallic metallacrown. **C.M. Zaleski**
- 2:30 INOR 130.** Lanthanide/zinc metallacrowns as advanced near-infrared imaging agents for biological applications. **S. Petoud**, S. Eliseeva, I. Martinic, T.N. Nguyen, E.R. Trivedi, V.L. Pecoraro

- 3:00 INOR 131.** Visible and near-infrared luminescence of heterometallic metallacrowns incorporating Ga(III) and Ln(III) ions. **S. Eliseeva**, C. Chow, I. Martinic, V.L. Pecoraro, S. Petoud
- 3:30** Intermission.

- 3:40 INOR 132.** Molecular control of the magnetic exchange between self-assembled metal-complexes and ferromagnetic surfaces for molecular spintronic devices. **V.E. Campbell**

- 4:10 INOR 133.** Fluorescent pyrrolic macrocycles for tumor imaging. **M.A. Kaster**, N. Chaudhary, K.C. Nielsen, B.A. Corbin, J. Hovey, **E.R. Trivedi**

- 4:40 INOR 134.** Origin of ground state instability in new metallo-dichalcogenolenes. **M.L. Kirk**, J. Yang, P. Basu, D. Kersi, B. Mogesa

- 5:10 INOR 135.** Postsynthetic modifications of metal-organic frameworks. **M.S. Lah**

### Section C

San Diego Convention Center  
Room 30D

### ACS Award in Inorganic Chemistry: Symposium in honor of Mercouri G. Kanatzidis

#### Recent Advances in Inorganic Chemistry

J. A. Aitken, K. Choi, *Organizers*

D. Harris, A. L. Odom, *Presiding*

- 1:30 INOR 136.** Pluripotent nanoparticles with programmable and responsive DNA bonds. **C.A. Mirkin**
- 1:55 INOR 137.** Quantum dot-chemosensor conjugates for profiling metabolic states in tumor biology. **C. Lemon**, D.G. Nocera
- 2:20 INOR 138.** Functional molecular materials based on cobalt(II) spin-crossover building units. **X. Zhang**, H. Xie, Z. Wang, **K.R. Dunbar**
- 2:45 INOR 139.** Spin effects on the physical and photophysical properties of molecular systems. **J.K. McCusker**
- 3:10** Intermission.
- 3:25 INOR 140.** Seeing is believing: Coordination chemistry of molecular imaging probes. **T.J. Meade**
- 3:50 INOR 141.** Advances in the inorganic chemistry of biological nitrogen fixation. **B.M. Hoffman**
- 4:15 INOR 142.** Drawing inspiration from nature with a twist. **M.R. Smith**
- 4:40 INOR 143.** Alkanedithiolate  $\neq$  two alkanethiolates for nickel clusters: How and why. **T.B. Rauchfuss**, F. Arrigoni, G.M. Chambers, L. Yulong, G. Zampella
- 5:05 INOR 144.** New tools for high valent catalyst development. **A.L. Odom**, B. Billow, T. McDaniel

### Section D

San Diego Convention Center  
Room 30E

### ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg

Cosponsored by WCC

N. E. Gruhn, M. S. Sanford, *Organizers*

W. D. Jones, *Organizer, Presiding*

B. T. Donovan-Merkert, *Presiding*

- 2:00 INOR 145.** Catalytic, regioselective functionalization of alkyl C-H bonds. **J.F. Hartwig**

- 2:20 INOR 146.** Electrochemically-promoted catalytic asymmetric hydrogenation using C<sub>2</sub>-symmetric rhodium complexes. **B.T. Donovan-Merkert**

- 2:40 INOR 147.** High pressure NMR studies of catalytic alkene hydroformylation and metathesis. **C.R. Landis**, N.J. Beach, S.M. Knapp, A.C. Brezny

- 3:00 INOR 148.** Modeling the controlled burning of organometallics. **T.R. Cundari**

- 3:20 INOR 149.** Iron hydrogenation catalysts relying on ligand-assisted cleavage of dihydrogen. **L. Boisvert**

**3:40** Intermission.

- 3:50 INOR 150.** Homogeneous Ta/Ir tandem catalytic alkane/alkene coupling. **J.E. Bercaw**, J.A. Labinger, D. Leitch, K. Steelman

- 4:10 INOR 151.** New tandem catalytic route for conversion of ethanol to butanol. **S. Chakraborty**, C.E. Hayes, R.T. Baker, **W.D. Jones**

- 4:30 INOR 152.** Investigation of Pd catalysts for the selective methoxycarbonylation of ethylene. **T. Foskey**, L. Huffman, D. Arriola, J. Briggs, K. Frazier

- 4:50 INOR 153.** Catalysts for the decomposition of formic and oxalic acid. **J.M. Boncella**, A. Tondreau, B. Scott

- 5:10 INOR 154.** From fundamentals to catalysis. **D.M. Heinekey**

### Section E

San Diego Convention Center  
Room 31A

### ACS Award in Pure Chemistry: Symposium in honor of Jonathan S. Owen

G. Parkin, *Organizer*

B. Sadtler, *Presiding*

**1:30** Introductory Remarks.

- 1:35 INOR 155.** Size, dimensionality, and strong electron correlation in nanoscience. **L.E. Brus**
- 1:55 INOR 156.** Perovskite fever: Absorbing and emitting light. **H. Zhu**, D. Niesner, X. Zhu
- 2:15 INOR 157.** Electronic doping and redox potential tuning of colloidal semiconductor nanocrystals. **D.R. Gamelin**
- 2:35 INOR 158.** Solid-state chemistry of ternary metal halide nanocrystals. **B. Sadtler**
- 2:55 INOR 159.** Preparation and properties of strongly coupled nanocrystal superlattices: From artificial atoms to mesoscale quantum solids. **C.B. Murray**
- 3:15** Intermission.
- 3:35 INOR 160.** Large exciton-energy shifts by reversible surface exchange in 2D II-VI nanocrystals. **Y. Zhou**, F. Wang, **W.E. Buhro**
- 3:55 INOR 161.** Intrinsic surface energy of graphite. **H. Liu**
- 4:15 INOR 162.** Materials complexity frontier: Nanostructure and heterogeneities. **S. Billinge**
- 4:35 INOR 163.** Role of magic-sized clusters in the growth of InP quantum dots. **B.M. Cossairt**, D. Gary, S. Flowers

## Section F

San Diego Convention Center  
Room 31B

**Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Edward I. Solomon**

**Bioinorganic Models**

K. D. Karlin, *Organizer*

P. Kennepohl, *Presiding*

**1:30 INOR 164.** Protein-like hydrogen exchange in a supramolecular structure. K.N. Raymond, W. Hart-Cooper, C. Sgarlata, C. Perrin, D. Toste, R.G. Bergman

**2:00 INOR 165.** Oxygen reduction reaction of a bio-inspired iron porphyrin with 2nd coordination sphere interaction. T. Ohta, P. Nagaraju, Y. Naruta

**2:30 INOR 166.** Bioinorganic nitrogen oxide chemistry with heme and/or copper complexes. S. Hematian, K.D. Karlin

**3:00 INOR 167.** From non-heme [FeNO]<sup>6</sup> to Fe(II)-HNO complexes: One ligand platform can do it all. N. Lehnert, A. Speelman

**3:30** Intermission.

**3:45 INOR 168.** Non-innocent ligands in bioinorganic chemistry: Detailed electronic structure and reactivity. K. Fujisawa

**4:15 INOR 169.** Tuning the relative stability of metastable Mn- and Fe-dioxygen intermediates. J. Kovacs, J. Rees, M.K. Coggins, A. Johansen, B. Leipzig

**4:45 INOR 170.** Amazing nonheme high-valent iron-oxo reactivity landscape. L. Que, M. Puri, A. Biswas

## Section G

San Diego Convention Center  
Room 31C

**F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Francois P. Gabbaï**

J. D. Hoefelmeyer, T. W. Hudnall, *Organizers*

F. N. Castellano, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 171.** Endeavours in chemistry with Francois Gabbaï. H. Schmidbaur

**2:05 INOR 172.** Low-coordination numbers, unusual bonding, and dispersion force effects. P.P. Power

**2:25 INOR 173.** Reactive intermediates from molecular precursors: Intercepting them in solution and launching them into the gas phase. C.C. Cummins, R. Field, J. Jiang, M. Nava, W. Transue, A. Velian, C. Womack

**2:45 INOR 174.** Room temperature stable phosphinidenes and related species. G. Bertrand

**3:05** Intermission.

**3:15 INOR 175.** Carbene-stabilized main group oxides. G.H. Robinson, Y. Wang, H. Schaefer

**3:35 INOR 176.** Stabilizing low valent arsenic and boron using  $\pi$ -accepting carbene ligands. T.W. Hudnall

**Technical program information known at press time.**

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**3:55 INOR 177.** Stabilization and "transition metal-like" reactivity of low oxidation state/low coordination s- and p-block metal complexes. C. Jones

**4:15 INOR 178.** Syntheses and reactivity studies of boron cations. C. Chiu

**4:35 INOR 179.** Phosphorus-boron and aluminum compounds: Highly reactive boron species & non-innocent ambiphilic ligands. D. Bourissou, B. Chenwa

## Section H

San Diego Convention Center  
Room 32A

**Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Eric J. Schelter**

L. G. Sneddon, P. J. Walsh, *Organizers*

R. K. Thomson, R. J. Trovitch, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 180.** Group 1 and 2 metal alkyl and silyl compounds as precursors for molecular hydrides. J. Okuda

**1:55 INOR 181.** Synthesis of early-transition metals having methylidene and methylidyne ligands. D.J. Mindiola

**2:15 INOR 182.** Redox switchable polymerization processes. P. Diaconescu

**2:35 INOR 183.** Formation of epoxides from olefins via a radical mechanism using atmospheric oxygen in the presence of silver nanoparticles deposited on MCM-41. R.L. Luck, Z. Chen

**2:55 INOR 184.** Application of heterobimetallic catalysts to C-H functionalizations. P.J. Walsh

**3:15** Intermission.

**3:35 INOR 185.** Metalloradical reactivity patterns in even-electron ruthenium complexes: Intermediates and mechanistic insight into bimetallic activation of hydrogen by H-atom transfer. D.H. Berry, M. Noss

**3:55 INOR 186.** Mechanism of bis(imino)pyridine manganese-catalyzed carbonyl hydrosilylation. R.J. Trovitch

**4:15 INOR 187.** Ni(bpy)(cod)-catalyzed hydroboration of ketones, aldehydes, and imines. A.E. King, N. Henson, B. Scott, N.C. Smythe, A.D. Sutton, J.C. Gordon

**4:35 INOR 188.** Single electron transformations to enable cross-couplings via photoredox/Ni dual catalysis. G.A. Molander

## Section I

San Diego Convention Center  
Room 32B

**ExxonMobil Solid State Chemistry Faculty Fellow Award: Symposium in honor of Mircea Dinca**

S. L. Suib, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 189.** Simple interfaces for complex systems: A little oxide goes a long way. J. Schwartz

**2:00 INOR 190.** High-capacity methane storage in flexible metal-organic frameworks with internal thermal management. J.A. Mason, J. Oktawiec, M.K. Taylor, J. Bachman, J.R. Long

**2:25 INOR 191.** Designer interfaces for energy storage and recovery. Y. Surendranath

**2:50 INOR 192.** Lead free inorganic-organic hybrid perovskites: Chemistry and solar cells. M.G. Kanatzidis

**3:15 INOR 193.** High-temperature ion diffusion in colloidal semiconductor nanocrystals: Diffusion doping and cation exchange. D.R. Gamelin, C. Barrows, P. Chakraborty, L.M. Kornowski

**3:40** Intermission.

**3:50 INOR 194.** Energy transfer in metal-organic frameworks. N.B. Shustova

**4:15 INOR 195.** Proton coupled electron transfer mechanism of oxygen evolution and reduction reactions by molecular cobalt complexes. C. Brodsky, G. Passard, A.M. Ullman, D.G. Nocera

**4:40 INOR 196.** Metaphosphate acids. K. Chakarawet, C.C. Cummins, Y. Jiang, I. Knopf, M. Nava, J. Stauber

**5:05 INOR 197.** Conductive metal-organic frameworks: Fundamentals and applications. M. Dinca, K. Al-Kaabi, M. Campbell, E. Miner, S. Park, D. Sheberla, L. Sun, C.R. Wade

## Section J

San Diego Convention Center  
Room 33A

**Inorganic Catalysts**

S. A. Koch, *Organizer*

M. J. Rose, *Presiding*

**1:30 INOR 198.** Visible-light-driven hydrogen photoproduction with Rh(III) catalysts and platinum nanoparticles loaded on graphene oxides. J. Kim, S. Kim, H. Jang, J.H. Lee

**1:50 INOR 199.** Enhancing electrocatalytic hydrogen evolution by nickel molecular catalysts with the aid of Lewis acids in aqueous media. H. Shao, S. Muduli, P.D. Tran, H. Soo

**2:10 INOR 200.** Improving the efficiency of electrocatalysts for the reduction of CO<sub>2</sub> through supramolecular assembly with amino acid-modified ligands. C.W. Machan, S.A. Chabolla, C.P. Kubiak

**2:30 INOR 201.** Stability and reactivity of ligand capped platinum nanoparticles in the semihydrogenation of alkynes to alkenes. P. Wand, J.D. Bartl, U. Heiz, M. Tschurl, M. Cokoja

**2:50 INOR 202.** Ring-opening polymerization of cyclic esters by ferrocene-chelating heteroscorpionate zinc complexes. M. Abubekurov, P. Diaconescu

**3:10 INOR 203.** Heterobimetallic complexes for cooperative CO<sub>2</sub> reduction. A. Reath

**3:30** Intermission.

**3:40 INOR 204.** Cyclic (alkyl) (amino) carbene copper (I) catalyzed dehydrogenative borylation and  $\alpha$ -hydroboration of terminal alkynes. E.A. Romero, R. Jazzar, G. Bertrand

**4:00 INOR 205.** Lithium cobalt oxides as water oxidation catalysts: Correlating structure, electronic properties, and activity. H. Liu, Y. Zhou, R. More, R. Mueller, T. Fox, G.R. Patzke

**4:20 INOR 206.** Thermodynamic and electrochemical studies of [Ni(bis(diphosphine))]2<sup>2+</sup> complex in water and organic solvents. B.M. Ceballos, C. Tsay, J. Yang

**4:40 INOR 207.** Attachment of molecular CO<sub>2</sub> reduction catalysts to gold electrodes. M.L. Clark, C.P. Kubiak

**5:00 INOR 208.** Light-driven homogeneous catalytic oxidation of hydrogen. M. Westwood, M.D. Hopkins

**5:20 INOR 209.** Photo-activation of hydrogen by an [FeFe]-hydrogenase model complex. A.E. Nelson, C.F. Works

## Section K

San Diego Convention Center  
Room 33B

**Nanoscience**

R. M. Richards, *Organizer*

J. L. Colon, N. Shukla, *Presiding*

**1:30 INOR 210.** Man-made microrobots in the mouse's stomach: An *in vivo* study. W. Gao, R. Dong, S. Thamphiwatana, L. Zhang, J. Wang

**1:50 INOR 211.** Renal clearance and degradation of glutathione-coated copper nanoparticles. S. Sun, S. Yang, C. Zhou, G. Hao, X. Sun, J. Zheng

**2:10 INOR 212.** Antibacterial activity and biocompatibility of nitrogen-doped titanium dioxide nanoparticles for use in dental resin formulations. A. Zane, R. Zuo, F.A. Villamena, A. Digeorge Foushee, S. Olsen, P. Dutta, A. Nagy

**2:30 INOR 213.** Enantiomeric separations of chiral pharmaceuticals using chiral tetrahedral Au nanoparticles. N. Shukla, D. Yang, Y. Zhao, A.J. Gellman

**2:50** Intermission.

**3:10 INOR 214.** Functionalized nanoparticles for SERS imaging and detection of biomolecular activities. Z. Skeete, J. Li, C. Salazar, C. Manahan, W. Sun, J. Luo, C. Zhong

**3:30 INOR 215.** Folic-acid functionalized polysilsesquioxane nanoparticles for targeted delivery of protoporphyrin-IX. Z. Lyles, B. Loftin, J.L. Vivero

**3:50 INOR 216.** Self-propelled nanomotors autonomously seek and repair cracks. J. Li, J. Wang

**4:10 INOR 217.** Drug delivery using zirconium phosphate layered structured nanomaterials. J.L. Colon, B. Casanas, A. Diaz

## Section L

San Diego Convention Center  
Room 33C

**Organometallic Chemistry: Synthesis & Characterization—Early Transition Metals**

N. S. Radu, *Organizer*

P. J. Fischer, T. P. Hanusa, *Presiding*

**1:30 INOR 218.** Titanium complexes of 2,6-dimesitylphenylisocyanide. P.J. Fischer, C.E. Moore, A.L. Rheingold, J.S. Figueroa

**1:50 INOR 219.** Reaction of group 4 metallacyclopentenes with isonitriles. T.N. Valadez, J.R. Norton

**2:10 INOR 220.** Exploring the reactivity of terminally bound nitriles of titanium. L. Grant, M. Carroll, G. Wu, P.J. Carroll, D.J. Mindiola

**2:30 INOR 221.** Hydroalkylation of internal alkynes via C(sp<sup>3</sup>)-H bond activation of 2,6-dimethyl-N-heterocycles by cationic alkylhafnium complexes supported by dianionic multidentate ligands. M. Lopez, A. Kondo, K. Yamamoto, H. Tsurugi, K. Mashima

**2:50 INOR 222.** Intermolecular zirconium-catalyzed double hydrophosphination of alkynes. C. Bange, R. Waterman

**3:10 INOR 223.** Routes to early transition metal corrole complexes: Synthesis, characterization, and reactivity. J. Ziegler, R.G. Bergman, J. Arnold

**3:30 INOR 224.** Formation of zwitterionic imido complexes upon activation of coordinated nitriles. D.V. Peryshkov, M. Rahman

**3:50 INOR 225.** Withdrawn.



**4:10 INOR 226.** Nitrene metathesis and catalytic nitrene transfer promoted by niobium bis(imido) complexes. **B.M. Kriegel**, L. Grant, R.G. Bergman, J. Arnold

**4:30 INOR 227.** Synthesis in nonpolar solvents: An unexpected mechanochemical parallel. N.C. Boyde, N.R. Rightmire, T.P. Hanusa

**4:50 INOR 228.** Regioselectivity of addition to the  $\pi$ -bond rich  $\text{Tp}^*\text{W}(\text{CO})(\text{HCCH})$  (NCHMe) molecule. **R. Beattie**, P. White, J.L. Templeton

**5:10 INOR 229.** Molybdenum (I) oxidation state: Preparation, characterization, and reactivity of bis(imino)pyridine Mo complexes. **R. Pal**, M. Flores, T.L. Groy, R.J. Trovitch

## Alpha Olefin Catalysis: Production & Transformations

### Alpha Olefin Transformations

Sponsored by I&EC, Cosponsored by CATL and INOR†

### Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, S&CB and WCC

### Industrial Research at the Interface of Inorganic Chemistry & Polymer Science

Sponsored by POLY, Cosponsored by BMGT and INOR†

## SUNDAY EVENING

### Section A

San Diego Convention Center  
Hall D

### ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Vincent L. Pecoraro

B. R. Gibney, A. F. Peacock, C. M. Zaleski, Organizers

#### 6:00 - 8:00

**INOR 230.** Synthesis and crystal structure of a disodium metallacrown complex with bridging chloroacetate anions. **C. Daly**, M. Zeller, C.M. Zaleski

**INOR 231.** Understanding ligand complexation upon heavy metal binding into different geometries within *de novo* three-stranded coiled coil proteins. **L. Ruckthong**, M.L. Zastrow, J. Stuckey, V.L. Pecoraro

**INOR 232.** Withdrawn.

**INOR 233.** Exploration of single-molecule magnetism of a family of  $[\text{Ln}^{\text{III}}_4\text{Mn}^{\text{II}}_4]$  ( $\text{Ln}^{\text{III}} = \text{Y}^{\text{III}}$ ,  $\text{Dy}^{\text{III}}$ ,  $\text{Ho}^{\text{III}}$ ,  $\text{Er}^{\text{III}}$ ) compound. **T.T. Boron**, A.H. Davis, J.W. Kamp, C.M. Zaleski, V.L. Pecoraro

**INOR 234.** Nitrite-nitro cobalt(III) compound as a carrier prototype for antitumor drugs. **B.M. Pires**, A.J. Bortoluzzi, **R.B. Faria**, M. Scarpellini

**INOR 235.** *De novo* designed metallopeptides: An unexpected binuclear Cu(I) site. **C. Mocny**, F. Yu, J.E. Penner-Hahn, V.L. Pecoraro

**INOR 236.** Fluorinated phthalocyanines as dual-mode fluorescent and MRI contrast agents. **M.A. Kaster**, N. Chaudhary, E.R. Trivedi

**INOR 237.** Combined spectroscopic and DFT investigations of Ni(II) complexes with tridentate ligands containing  $\text{NO}_2$ ,  $\text{N}_2\text{O}$ , and  $\text{N}_3$  donor spheres. **C.S. Mullins**, J.A. Berlanga, C.A. Grapperhaus, L. Bishop

**INOR 238.** Synthesis and crystal structure of a two-dimensional terbium-aluminum metallacrown-like compound. **G. Van Trieste**, M. Zeller, C.M. Zaleski

**INOR 239.** Consequences of methionine oxidation on the structural and functional properties of human calprotectin. **F. Yu**, E.M. Nolan

**INOR 240.** Many faces of designed metalloproteins: From heavy metal sequestration to nitric oxide reduction. **S. Chakraborty**, V.L. Pecoraro, Y. Lu

**INOR 241.** Synthesis and crystal structure of a two-dimensional network of aluminum metallacrowns. **J. Travis**, M. Zeller, C.M. Zaleski

**INOR 242.** Ring metal substitution of 12-metallacrown-4 compounds. **I. Kuhn**, C.M. Zaleski

**INOR 243.** Highly luminescent  $\text{Ga}_2\text{Ln}_2$  metallacrown complexes. **T.N. Nguyen**, S. Eliseeva, C. Chow, J.W. Kamp, S. Petoud, V.L. Pecoraro

**INOR 244.** Metallacrowns as novel near-infrared optical imaging probes for necrotic cells. **I. Martinic**, S. Eliseeva, T.N. Nguyen, V.L. Pecoraro, S. Petoud

**INOR 245.** Glutamate induced asymmetric binding of transition metals in *de novo* designed helical heterotrimers. **A. Tolbert**, C. Mocny, V.L. Pecoraro

**INOR 246.** Exploring metallacrowns: Novel  $\alpha$ -hydroxy hydroxamic acid ligands, platinum, and thermogravimetric analysis. **N.A. Law**, N. Duffy, K. Buxton

**INOR 247.** Designing an antiparallel, asymmetric three-stranded coiled coil. **K. Diffley**, C. Mocny, V.L. Pecoraro

**INOR 248.** Enhanced two-dimensional dispersion of supported group V metal oxides on silica. **J. Grant**, C. Carrero, A. Love, R. Verel, I. Hermans

**INOR 249.** Copper(II) complexes of pyridine and amide donor ligands as precursors to oxidation catalysts. **J. Bodwin**

**INOR 250.** Selective incarceration and extraction of oxoanion contaminants from aqueous media by self-assembled nanojars. **B.M. Ahmed**, B. Szymczyna, S. Jianrattanasawat, G. Mezei

**INOR 251.** Use of non-natural amino acids to bind metals in *de novo* designed 3-stranded coiled coils. **C. White**, K. Koebke, V.L. Pecoraro

**INOR 252.** Telescoping synthesis as an efficient, green method for preparing unsymmetrically derivatized pyrazole ligands. **B.M. Ahmed**, **G. Mezei**

**INOR 253.** Incorporation of electron transfer motifs in synthetic bacterial microcompartment shell proteins. **J.S. Plegaria**, C. Kerfeld

**INOR 254.** Structure and dynamics of the HNOX domain of the human soluble guanylate cyclase. **I.H. Saraiva**, M.C. Almeida, **M. Matzapetakis**

**INOR 255.** Utilization of copper-catalyzed alkyne-azide cycloaddition coupling in luminescent gallium based metallacrowns. **J.C. Lutter**, S. Eliseeva, J.W. Kamp, S. Petoud, V.L. Pecoraro

**INOR 256.** Novel non-chrome thin organic hybrid coatings for coil applications. **T.S. Smith**, B.D. Bammel, J. Comoford, G.T. Donaldson, J.D. McGee, J. Zimmerman

**INOR 257.** Analysis of physical properties of thiodiphenol epoxy resins cured with dicyandiamid. **C. Lim**, D. Kim, S. Kwon, S. Lee, B. Seo

### Section A

San Diego Convention Center  
Hall D

### Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, Organizer

#### 6:00 - 8:00

**INOR 258.** Withdrawn.

**INOR 259.** Assessing density functionals for simulations of structural, redox, and spectroscopic properties of [FeFe]-hydrogenases. **S. Niu**, H. Li, M.B. Hall

**INOR 260.** Novel optical trends in heme enzymes explained by density functional theory. **A. Graves**, M.D. Liptak

**INOR 261.** Biomimetic CFCs degradation: An insight into biotic halogen cycling. **M.A. Crick**, S.K. O'Shea

**INOR 262.** Identification of disulfide bonds by planned digestion and tandem mass spectrometry. **S. Park**, E. Jung, S. Lee

**INOR 263.** Redox non-innocent ligands on first row transition metals: Towards bio-inspired catalysts for C-H bond activation. **J. Bogart**, S.A. Cook, A. Borovik

**INOR 264.** Heme nitric oxide/oxygen binding protein and its role in regulating a bifunctional cyclic-di GMP-processing phosphodiesterase and cyclase in *Agrobacterium vitis*. **D.E. Williams**, N. Nesbitt, S. Muralidharan, L. Nisbett, E.M. Boon

**INOR 265.** NiSOD model complexes that probe the catalytic and electronic implications of a Ni-coordinated Cys-Thiol. **R.A. Steiner**, K.J. Martin, T.C. Harrop

**INOR 266.** Pterin reduction in chemical models of the molybdenum cofactor. **S. Zhu**, B.R. Williams, S.J. Nietzer Burgmayer

**INOR 267.** Comparison of S-H bond vs. S-Au bond beyond the isolobal relationship between proton and gold-phosphine anion. **S. Ding**, D. Crouthers, J. Denny, R.D. Bethel, C. Hsieh, M.B. Hall, M.Y. Darensbourg

**INOR 268.** One Fe(III) model complex for the active site of 2,4'-dihydroxyacetophenone dioxygenase (DAD). **J. Li**, M. Molenda, F.A. Chavez

**INOR 269.** Probing the structural difference between Ca(II) and Pb(II) bound syt1. **C.M. Dashnaw**, J.W. Karr

**INOR 270.** Investigation into the synthesis and characterization of derivatized electrochemical biosensors utilizing a biotin-ferrocene platform. **M. Burnett**, M. Goulet, K.N. Green

**INOR 271.** Using P450 BM3 as a model system to study stability as it relates to the catalytic cycle. **C.A. Denning**, D.K. Heidary, E.C. Glazer

**INOR 272.** Developing a novel dimetallic synthetic model complex for carbon monoxide oxidation. **J.J. O'Connor**, C. Williams, D. Rokhsana

**INOR 273.** Synthetic modeling of the organometallic active site of mono-iron hydrogenase: Fe-acyl complexes derived from CNS (S = thioether, thiophene) and CNP (P = PPh<sub>3</sub>) chelates. **Y. Cho**, M.J. Rose

**INOR 274.** Synthetic modeling of mono-iron hydrogenase: CNS Chelates supporting an iron-hydride species, substitution reactions, and C-H activation of TMAO. **Z. Xie**, M.J. Rose

**INOR 275.** Molybdenum pyranopterin dithiolene complexes: Investigating the steric effects on molybdenum cofactor models. **A. Nagelski**, D.R. Gisewhite, B.R. Williams, S.J. Nietzer Burgmayer

### Section A

San Diego Convention Center  
Hall D

### Chemistry of Materials

C. G. Lugmair, Organizer

#### 6:00 - 8:00

**INOR 276.** Time-resolved observation of reduction kinetics of iron oxides by *in situ* XAFS measurement. **K. Kimijima**, Y. Niwa, R. Muraio, M. Kimura

**INOR 277.** Stable blue phosphorescence Iridium(III) cyclometalated complexes prompted by intramolecular hydrogen bond in ancillary ligand. **S. Kim**, Y. Cho, J. Kim, S. Yi, W. Han, S.O. Kang

**INOR 278.** Synthetic design of cationic porous frameworks for anion immobilization and separation. **X. Bu**, X. Zhao

**INOR 279.** Synthesis and structural characterization of a unique ammonium borate containing a heptaborate anion. **D. Neiner**, Y. Sevryugina, D.M. Schubert

**INOR 280.** Development of lanthanide tagged nanoparticle (T-NP) system for tracking of underground fluid flow. **L.J. Treadwell**, T.J. Boyle, A.C. Cappuccilli, D.T. Yonemoto, P. Lu

**INOR 281.** Adsorption of amyloid beta peptide by metal-organic frameworks. **Z. Mensinger**, B. Cook, E. Wilson

**INOR 282.** Comparative study of *in situ* and pre-synthesized x-pillar ligand in self-assembly of homochiral porous frameworks. **E.T. Nguyen**, X. Zhao, X. Bu

**INOR 283.** CdSe/CdS core-shell nanocrystal sensitizers for molecule-nanocrystal photon upconversion. **Z. Huang**, M.L. Tang

**INOR 284.** Reductive sonochemical synthesis of superparamagnetic nanoparticles (SPMNs). **A.C. Miller**, D.J. Casadonte

**INOR 285.** Fabricating nanowires using site-specific attachment of gold nanoparticles and nanorods to DNA origami templates. **J.K. Jensen**, B. Uprety, K. Lee, J. Harb, R. Davis, A. Woolley

**INOR 286.** Lanthanide separation through size-selective crystallization of homochiral metal-organic frameworks. **X. Zhao**, C. Mao, P. Feng, X. Bu

**INOR 287.** Synthesis of metal-organic frameworks for carbon capture. **M. Cosio**, S.A. Fordham, H. Zhou

**INOR 288.** Postsynthetic cyclodehydrogenation of a large pore zirconium based metal-organic framework. **G. Pour**, F. Uribe-Romo

**INOR 289.** Electrografting organoboron compounds for applications in materials chemistry and catalysis. **S.E. Shaner**, F. Mujid, S. Doden

**INOR 290.** Soft-template synthesis of 3D porous graphene foams with tunable architectures for supercapacitors. **C. Ma**, S. Tong, J. Shen, D. Zhang, Y. Feng, Y. Yu, Y. Liu, Y. Min

**INOR 291.** Investigation of graphene oxide films. **J. Shen**, S. Mo, D. Zhang, Y. Liu, Y. Min

**INOR 292.** Hollow carbon nanospheres: Application and properties. **C. Zhang**

**INOR 293.** Investigating MOF mixed-matrix membranes with cellulosic polymers. **J. Moreton**, M.S. Denny, S. Cohen

**INOR 294.** Metal-organic frameworks constructed from crown ether-based 1,4-benzenedicarboxylic acid derivatives. **T. Chen**, S. Cohen

**INOR 295.** Nanobowls: Creating silica-alumina interfaces to tune metal oxide behavior. **M.A. Ardagh**, Z. Bo, J.M. Notestine

**INOR 296.** Structural optical studies of copper sulphide nanocrystals by solvothermal synthesis from single molecule precursors. **P.A. Ajibade**, N.L. Botha

**INOR 297.** New approaches to the chemical syntheses of azamacrocyclic compounds. **E.J. Parish**, H. Honda, T. Wei, M. Hsiao

**INOR 298.** Highly connected rare-earth molecular building blocks: Assembly of iso-reticular porous metal-organic frameworks having novel topology. **A. PuthanPeedikakkal**, D. Alezi, L. Weselinski, V. Guillem, Y. Belmabkhout, A. Cairns, Z. Chen, L. Wojtas, M. Eddaoudi

**INOR 299.** New approaches to the development of donor-sigma-acceptor materials for organic rectifiers. **Y. Lo**, H. Shyu, **W. Huang**, H. Honda, T. Wei

**INOR 300.** Production of anatase pigment by hydrolysis of low concentration TiOSO<sub>4</sub> solution via short sulfate process. **C. Tian**

**INOR 301.** Flow-driven precipitation in the magnesium and calcium carbonate systems. **B. Bohner**, T. Pivarscik, D. Horvath, A. Toth

**INOR 302.** Achiral routes to the synthesis of chiral inorganic open frameworks and their luminescence properties. **S.L. Wang**

**INOR 303.** Enhancing the visible-light absorption of TiO<sub>2</sub> with the use of key N, Co, and Na dopant concentrations. **Y. Han**, C. Yang

**INOR 304.** Synthesis of highly porous monolithic InNbO<sub>4</sub> aerogels. **R. Lord**, R. Baghi, L. Hope-Weeks

**INOR 305.** 3D DNA origami templated nanoscale device fabrication. **K. Lee**, J.K. Jensen, B. Uprety, R. Davis, J. Harb, A. Woolley

**INOR 306.** Towards the preparation of highly and functionalized porous covalent organic frameworks. **D.A. Vazquez-Molina**, F. Uribe-Romo, M. Lum

**INOR 307.** Preparation of CdTe quantum dots supported on modified silica gel. **K. Silva**, D.V. Freitas, J.M. Dias, M. Navarro

**INOR 308.** Synthesis of polyarylboranes: A new and diverse class of organic/inorganic hybrid materials. **M.W. Lee**

**INOR 309.** Increasing charge transport in metal-organic frameworks via generation of mixed-valency. **R.M. Torres-Gavosto**, L.E. Darago, J.R. Long

## Section A

San Diego Convention Center  
Hall D

### Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

6:00 - 8:00

**INOR 310.** Withdrawn.

**INOR 311.** Squaramide metal-organic frameworks as catalysts. **X. Zhang**, Z. Zhang, J.A. Boissonnault, S. Cohen

**INOR 312.** Spectroelectrochemistry and reactivity of hexacoordinate polypyridylsilicon(IV) complexes. **D.M. Peloquin**, D.R. Dewitt, P. Tran, J. Pope, J. Merkert, B.T. Donovan-Merkert, T.A. Schmedake

**INOR 313.** Rhenium-manganese dinuclear carbonyl complexes as long wavelength absorbing photoCORMs. **Z. Li**, A. Pierri, P.C. Ford

**INOR 314.** Syntheses, spectroscopic characterization, and *in vitro* antibacterial activities of some metal (II) complexes of 2[(E)-(1H-indol-5ylimino)methyl]-6-methoxyphenol. **A.A. Osowole**, **A.O. Abiola**

**INOR 315.** Structure, electrochemistry, and photophysical properties of an Exocyclic di-ruthenium complex and its application as a photosensitizer. **S. Salpage**, B. Som, A. Paul, T. Banerjee, K. Hanson, M.D. Smith, A.K. Vannucci, L.S. Shimizu

**INOR 316.** Combined EPR and *ab initio* multiconfigurational studies of dirhodium(II,III) carboxylates and amidates and computational insight into dirhodium(II,III)-nitrene intermediates. **T. Yang**, K.P. Kornecki, J.F. Berry

**INOR 317.** Synthesis, structure, characterization, and photophysical properties of four copper(I) complexes containing polypyridyl ligands. **A. Báez**, V. Miranda Soto, M.P. Parra Hake, J.D. Campos-Gaxiola, H. Höpfl, A. Cruz-Enriquez

**INOR 318.** Phenylendiamine and phenazine-derived sulfonamides for fluorescent and optical sensing of toxic metals. **I. Lehman-Andino**, N. Bertolotti, G.G. Pena, K. Kavalleratos

**INOR 319.** Coordination chemistry of the rhodizonate anion: Towards understanding the Na-rhodizonate test for Pb. **J.A. Silverman**, E.V. Govor, K. Kavalleratos

**INOR 320.** Mn(II) complex of a new mixed pendant arm cyclen-based ligand: A correlation between chemical structure and relaxivity. **P. Brauchle**, S. Hensiek, T.D. Westmoreland

**INOR 321.** pH and temperature dependent <sup>17</sup>O NMR relaxivities of Mn(II) complexes as a probe of solution speciation and water coordination. **S. Briggs**, A. Lee, T.D. Westmoreland

**INOR 322.** Kinetic and mechanistic investigations on metal-assisted (Zn, Au) thiolate-disulfide exchange. **G.S. Garusinghe**, A.E. Bruce, M.R. Bruce

**INOR 323.** Development of chiral, tridentate, mer-coordinating, nitrogen-based ligands for use in enantioselective catalysis. **K. Zivkovic**, A. Villaseñor, F.F. Faucher, C. Alcocer, C.J. Daley

**INOR 324.** MOF-assisted organic synthesis of drug molecules from natural sources. **J. Garcia**

**INOR 325.** <sup>1</sup>H relaxation rate ratios as a probe of solution speciation for labile manganese (II) complexes. **D.W. Laurenza**, T.D. Westmoreland

**INOR 326.** Water stable metal-organic frameworks for gas separation. **X. Zhang**, **W. Shi**, P. Cheng

## Section A

San Diego Convention Center  
Hall D

### Main Group Chemistry

T. W. Hudnall, *Organizer*

6:00 - 8:00

**INOR 327.** Sodium borohydride amine complexes: A simple way to organic borohydride salts. **S. Schneider**, S.F. Deplazes, **C. Gibson**, Y. Ahmed

**INOR 328.** Bis-bipyridylsilicon(IV) diols as potential dual hydrogen bond donors for chiral catalysis. **C. Waters**, T.A. Schmedake

**INOR 329.** Synthesis of the frustrated Lewis pair dichloro(8-quinolyl)gallium(III) and its reaction with chloroform. **J.J. Fostvedt**, S.R. Tamang, J. Son, J.D. Hoefelmeyer

**INOR 330.** 5-(azido-alkyl)-1H-tetrazoles: Synthesis and characterization. **Y.O. Ahmed**, C. Gibson, S.F. Deplazes, S. Schneider

**INOR 331.** Lithium borohydride complexes of tetrazole derivatives. **S.F. Deplazes**, S. Schneider, Y.O. Ahmed, A.M. Beauchamp, C. Gibson

**INOR 332.** Selective defluorination of polyfluoroaromatics by alkyl-monophosphines. **A.R. Arevalo**, **J.J. Garcia**

**INOR 333.** Rapid synthesis of *hypercloso*-[B<sub>12</sub>(OR)<sub>12</sub>] dodecaalkoxy derivatives. **A.I. Wixtrom**, Y. Shao, S. Kevork, J.C. Axtell, S. Khan, A.M. Spokoyin

**INOR 334.** Synthesis and characterization of carbene-supported boron(II) radicals and radical cations. **A. Ledet**, T.W. Hudnall

**INOR 335.** Ligation of trialkyl antimony to open- and closed-shell first-row transition metals: Copper luminescence and complexes of cobalt and nickel. **M.J. Rose**

**INOR 336.** C-C coupling and sp<sup>2</sup> C-H bond activation catalyzed by transition metal complex (M = Pd<sup>II</sup> and Cu<sup>I</sup>) with the ambiphilic ligand 8-quinolyldimesitylborane. **S.R. Tamang**, J.D. Hoefelmeyer

## Section A

San Diego Convention Center  
Hall D

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

6:00 - 8:00

**INOR 337.** Halogen exchange reactions on *o*-, *m*- & *p*-carborane cages for cancer imaging and therapy. **K. Ishita**, A. Khalil, R. Tiwari, W. Tjarks

**INOR 338.** Computational modeling of Hg-catalyzed methane oxidation in sulfuric acid. **S. Butler**, J.T. Fuller, D. Ess

**INOR 339.** Low-valent Ni catalyzed transfer hydrogenation of benzonitriles with diols as hydrogen source. **J.A. Garduño**, J.J. Garcia

**INOR 340.** From a DFT perspective, Milstein's chemistry can be related to a simple ion-pair formation and slippage metathesis mechanism. **F. Hasanayn**, L. Assi, R. Maousawi

**INOR 341.** Olefin metathesis with Ru-based catalysts containing N-heterocyclic carbenes attached to fullerenes. **A. Poater**, M. Solà, J. Martínez

**INOR 342.** Ruthenium complexes bearing metal-coordinated phosphonates for water oxidation. **J.M. Kamdar**, D.C. Marelius, C.E. Moore, A.L. Rheingold, D.K. Smith, D.B. Grotjahn

**INOR 343.** Stoichiometric reactivity of ruthenium-pincer complexes relevant to polar bond hydrogenation. **L. Le**, A.R. Chianese

**INOR 344.** Bifunctional ruthenium catalysts for the hydrogenation of polar bonds. **T.N. Cervarich**, A.R. Chianese

**INOR 345.** Highly active and (E)-selective bifunctional 16-electron ruthenium monoisomerization catalyst. **E.R. Paulson**, C.E. Moore, A.L. Rheingold, D.B. Grotjahn

**INOR 346.** Withdrawn.

**INOR 347.** Synthesis and water oxidation activity of sterically hindered [Ru(CI)(terpy)pyridyl(naphthyridine) Cl] analogs; an attempt at fluorinated oxidatively resilient ligands. **D.C. Marelius**, R. Shirey, F. Bamare, D.B. Grotjahn

**INOR 348.** Introducing a κ<sup>4</sup>-diazadiene Co(II) hydride catalyst for alkyne hydroboration. **H. Ben-Daaf**, T.L. Groy, R.J. Trovitch

**INOR 349.** Comparative insights into the carbon-hydrogen activation of cycloalkanes by cyclopentadienylcarbonylrhodium and trispyrazolylborate-rhodium complexes. **G. Jia**, M.B. Hall

**INOR 350.** Redox control of an aluminum ring-opening polymerization catalyst. **J. Wei**, P. Diaconescu

**INOR 351.** Gold(I) catalyzed hydroamination of alkenes and alkynes using hemilabile phosphine ligand. **S. Immadi**, C. Hahn

**INOR 352.** Investigation and exploration of transition metal catalysis for site selective C-H bond functionalizations. **D. Kumar**, S. Vemula, R.C. Cook

**INOR 353.** Tuning five-coordinate trisboryl iridium catalyst reactivity through ligand modification. **B. Ghaffari**, B.A. Vanchura, G.A. Chotana, R.E. Maleczka, M.R. Smith

**INOR 354.** Development of new cyclometalated palladium complexes and their catalytic activity in carbon-carbon bond cross coupling reactions. **D. McAteer**, Y. Niyonzima, E. Javed, R. Mroz, **S. Huo**

**INOR 355.** Withdrawn.

**INOR 356.** Synthesis of nickel POCOP-pincer complexes for the catalytic hydrophosphination of unsaturated organic molecules. **A. Roering**, J. Kraai

**INOR 357.** Half-sandwich organometallic complexes incorporating a triazenido ligand functionalized with pyridine. **A.F. Velazquez Ham**, A. Aguilar, J.L. Gomez Lopez, M.P. Parra Hake, V. Miranda Soto

## Section A

San Diego Convention Center  
Hall D

### Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

6:00 - 8:00

**INOR 358.** Ruthenium(II) coordination to pyridylidene remote N-heterocyclic carbenes: A complex story. **T. Cao**, D.C. Marelius, J.M. Kamdar, A.L. Rheingold, C.E. Moore, D.B. Grotjahn

**INOR 359.** Heteroatom polyaromatic hydrocarbon systems with nitrogen ligands. **W. Cross Lopez**, T. Haden, J. Herring, S.M. Kruse, S.K. Hurst

**INOR 360.** Design and synthesis of "para-pyridine-PCP" iridium complexes and their activity as catalysts for alkane dehydrogenation. **N. Lease**, A. Alape Seetharam, S. Martinez, T. Zhou, M. Blessent, A.S. Goldman, K. Krogh-Jespersen

**INOR 361.** Synthesizing redox-active ligand based first row transition metal complexes and studying their catalytic applications. **A. Saini**

**INOR 362.** Yttrium-alkyl complexes supported by a ferrocene-based phosphinimine ligand. **J.L. Brosmer**, P. Diaconescu

**INOR 363.** Synthesis of chiral ligands. **M. Talley**, W. Walker, R. Stokes, D. Michaelis

**INOR 364.** Synthesis and complexation of new multitopic non-chelating N-heterocyclic carbenes. **D. Tapu**, A. Carter, R. Justice

**INOR 365.** Rhodium and Iridium complexes derived from new annulated N-heterocyclic carbenes: Synthesis and catalytic studies. **D. Tapu**, O.J. Buckner, B. Norvell, C. Boudreaux

**INOR 366.** Cooperative reactivity of (PSIP)Rh pincer complexes. **T. Donnell**

INOR **367.** Synthesis and characterization of iron half-sandwich complexes. J. Kephart, E.B. Hulley

INOR **368.** Transition metal complexes of boron-containing heterocycles for multi-electron small molecule activation. L. Essex, W. Harman

## Section A

San Diego Convention Center  
Hall D

### Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **369.** Novel Cr(III)-HMC acetylides complexes: Preparation and emission properties. S. Tyler, E. Judkins, T. Ren

INOR **370.** Novel reactivity in an anionic iron-nitride cluster. M.J. Drance, J.S. Figueroa

INOR **371.** Reaction of  $WN(NR_2)_3$  complexes with alkyl halides. A.J. Touchton, M.M. Nolan, A. Koley, L. McElwee-White

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Bioinorganic Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

INOR **372.** Creation and characterization of rubrerythrin and symerythrin model proteins. J. Pellegrino, K.A. Bell, R. Polinski, S. Cimerol, A.B. Jacobs, E.I. Solomon, A.J. Reig

INOR **373.** Structural and functional characterization of G4DFsc variants containing a 4-His/3-carboxylate active site. K. O'Shea, J. Dorsheimer, K. Biernat, A.B. Jacobs, E.I. Solomon, Y. Wu, W.F. Degrado, A.J. Reig

INOR **374.** Modeling myo-inositol oxygenase (MIOX) using the *de novo* four-helix bundle protein G4DFsc. C. Philip, K. Drost, C.L. Kanya, A.J. Reig

INOR **375.** Structural analysis of a novel group of biomimetic complexes for the active site of nickel acireductone dioxygenase (Ni-ARD). B.Z. Nabona, C.M. Gonzales, D.A. Ivan, S. Sanchez, S.A. Toledo

INOR **376.** Characterization of copper(I) binding to the Sp1 zinc finger domains. A.M. Blumenreich, N.L. Mandel, M.D. Storlie, M.L. Stevens, K.E. Splan

INOR **377.** Investigating the role of riboflavin binding protein in copper transport and storage in oviparous species. H. Masood, S.R. Smith, J.I. Matchynski

INOR **378.** Cloning, expression, and characterization of novel hydroquinone ring-cleaving dioxygenases. E.R. Altman, T.E. Machonkin

INOR **379.** Synthesis and characterization of  $V^O_2(3\text{-methoxysalicylaldehyde semicarbazone})$ . J. Hempfing, V.P. McCaffrey

INOR **380.** Synthesis and characterization of Fe(II) coordination complexes and their reactivity with hydrogen peroxide. R.E. Coleman, K.N. Trotter, N. Arulsamy, E.B. Hulley

INOR **381.** Thermodynamics of Zn(II) and surrogate metal ions binding to the glucocorticoid receptor DNA-binding domain. P. Luong, M.C. Carpenter, D. Wilcox

INOR **382.** New octahedral cobalt(III) complex as a possible anti-cancer prodrug: Synthesis and characterization studies in solid state and solution. N. Joe, A. Morris

INOR **383.** Sensing of biologically relevant anions with a luminescent europium(III) complex. K.H. Felix, K. Johnson, E.J. Werner

INOR **384.** Synthesis and characterization of symmetric and asymmetric water soluble zinc(II) model complexes for liver alcohol dehydrogenase. N.A. Bernier, C.A. Van Akin, J.R. Miecznikowski

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Computational Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

INOR **385.** Redox potentials of ruthenium complexes to understand catalytic ability in water. A.A. Lopez, R.M. Adams, S. Bellows, T.R. Cundari

INOR **386.** Oxidation states "naturally": A natural bond orbital study. F.P. Neil, M. Chelsea, J.S. D'Acchioli, A. Webster

INOR **387.** Theoretical modeling of the asymmetric hydroamination-cyclization of aminoallenes by tantalum amide alkoxide complexes. G.S. Phun, R.J. Cave, A.R. Johnson

INOR **388.** Mechanistic details of hydrogen evolution with  $[Cp^*Rh(phen)(MeCN)]^{2+}$  calculated by DFT. S.L. Corona, S.I. Johnson, L.M. Aguirre Quintana, H.B. Gray, J.R. Winkler, J.D. Blakemore, W.A. Goddard

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Coordination Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

INOR **389.** Evaluating the physical and catalytic properties of complexes containing quinolyl arylsulfonamide ligands. M. Gole, B.C. Chan, A.R. O'Connor

INOR **390.** Electrochemical investigation of tris(triphenylphosphine)rhodium(I) chloride and its analogues utilizing cyclic voltammetry. J. Turner, A. Weinick, B. Ross, A.J. Warhausen

INOR **391.** Synthesis and characterization of TPAP. H.M. Bui, Z. Thammavongsy, J. Yang

INOR **392.** Tripodal CMPO ligands as potential lanthanide extractants: A systematic study of ligand structure and selectivity in acidic aqueous media. M.G. Patterson, D.A. Hardy, S.M. Biros, E.J. Werner

INOR **393.** Structure function relationships of multinuclear copper(II) carboxylate metal-omesogens. B. Musselman, K.A. Wheeler, T.W. Clayton

INOR **394.** Reactivity of nitric oxide with  $[Fe(D(G_2tren)](triflate)_2$ . K. Gomez, A. Speelman, N. Lehnert, R.C. Scarrow

INOR **395.** Reactivity of Rh and Ni silylamides. L. Qiu

INOR **396.** Degrading organophosphate toxins: Fundamental studies of molybdate-mediated phosphonothioate hydrolysis. K.M. Dill, L.Y. Kuo

INOR **397.** Aluminum alkoxide complexes prepared with tridentate  $\gamma$ -aminoalcohols. K.J. Goosherst, D.B. Green, J.M. Fritsch

INOR **398.** Synthesis of early-late heterobimetallic compounds for fluorescence studies. C. Heaney, A. Hill

INOR **399.** Design and characterization of bis(terpyridyl)chromium(III) complexes with enhanced visible absorption and emission. A.J. Kim, A.P. Grorud, B.M. Lovaasen

INOR **400.** Structures of five-coordinate aluminum alkoxide complexes that polymerize  $\epsilon$ -caprolactone and L-lactide. A. Longo, A.L. Rheingold, J.M. Fritsch

INOR **401.** Development of a biomimetic catalyst for dechlorination reactions. I. Lee, K.M. Van Heuvelen

INOR **402.** Hydrosilylation activity of iron complexes supported by conjugated  $\alpha$ -diimine ligands. A. Volkov, G.N. Tran, M. Takemura, K.A. Wheeler, H.M. Hoyt

INOR **403.** Carbon monoxide powered alkaline fuel cell operational at ambient condition. D. Shlian, J. Jiang

INOR **404.** Structure function relationships of cobalt complexes with pendant bases in the secondary coordination sphere. R. Combs, J.F. Khosrowabadi, J. Yang

INOR **405.** Synthesis of gold(III) complexes for chelation-assisted functionalization of strong,  $sp^2$ -hybridized C-H bonds. J.E. Thompson, K.M. Gilmore, R.L. Marley, A.R. McCormick, E.E. Heine, C.P. Owens, N.A. Curry, A. Brown, E. Robbins, M.K. Phillips, A.L. Rheingold, D.R. Weinberg

INOR **406.** Mechanistic investigation of the molybdenum catalyzed oxidation of key phosphines and sulfides. C. Jamieson

INOR **407.** Photochemical reactivity of a binuclear Fe(I)-Fe(I) hydrogenase model compound with cyano ligands. A. Hunt, J. Barrett, M. McCurry, C.F. Works

INOR **408.** Zinc catalysts for the formation of bio-renewable polymers. E.G. Thalacker, J.F. Dunne

INOR **409.** Exploration of the photochemical capabilities of cerium(IV) hexachloride. J. Hertzog, H. Yin, K.C. Mullane, P.J. Carroll, E.J. Schelter

INOR **410.** Ionothermal synthesis and characterization of  $[EMIM]_4[CoS_4(Co(P_2S_6)_2)_2]$ ,  $[EMIM]_2[Cr(P_2S_6)_2]$ , and  $[EMIM]_2[Mn(P_2S_6)_2]$ . C. Juillerat, J.A. Cody

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Environmental Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

INOR **411.** Metallating ligands in catalyst development for carcinogens in groundwater. S. Kim, K.M. Van Heuvelen

INOR **412.** Synthesis and characterization of ruthenium (II) complexes and their reactivity with  $ClO_2^-$ . K.N. Trotter, R.E. Coleman, N. Arulsamy, E.B. Hulley

INOR **413.** Combating organophosphate toxins with molybdenum-peroxo complexes. A. Bennett, L.Y. Kuo

INOR **414.** Developing bio-inspired catalysts for dechlorination. K. Ariola, K.M. Van Heuvelen

INOR **415.** Green metal binding for a brighter future. A. Russell, C. Butler, A.M. Schoffstall, R.M. Henry

INOR **416.** Metal-organic frameworks with embedded basic sites for heavy metal capture from aquatic environments. C. Fast, T.A. Makal

INOR **417.** Degradation of organophosphate pesticides using molybdenum (VI) oxides and ion exchange resin. G. Mehlhaff, L.Y. Kuo

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry General

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

INOR **418.** Expanding the frontiers of inorganic chemistry. H.J. Eppley, C. Nataro, A.K. Bentley, E.R. Jamieson, A.R. Johnson, B.A. Reisner, J.L. Stewart, S.R. Smith, L.A. Watson, N. Williams

INOR **419.** Incorporation of research in the undergraduate inorganic chemistry curriculum: IONIC VIPER workshops. S.K. Goforth, P.J. Fischer, C. Nataro

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Main Group Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

INOR **420.** Aluminum complexes of redox-active ligands: Synthesis, characterization, and preliminary reaction studies. P.M. Wise, T.M. Herb, C. Koelner, A. Poitras, B.E. Cole, J. Bogart, N.A. Piro, P.J. Carroll, W.S. Kassel, E.J. Schelter, C.R. Graves

INOR **421.** Redistribution reactions in organosiloxane complexes of 1-oxo-2-pyridinone. A.E. Ryan, W.W. Brennessel, J.G. Koch, B.M. Kraft

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry Materials & Solid-State Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

INOR **422.** Targeted synthesis of metal-organic frameworks for gas storage and hydrocarbon separations. J.F. Melville, M. Kapelewski, J.R. Long

INOR **423.** Unique crystalline composite displaying three primary zoning events in the solid state and based upon self-assembled, helical coordination polymers. S. Cornell, S.R. Seidel

INOR **424.** Coupling electrochemical and fluorescence investigations of failure modes in aerospace coating systems. K. Hull, E. Blidodeau, E. Sapper, C.E. Immoos

INOR **425.** Synthesis of mixed metal metal-organic frameworks via ion-exchange in solution. S. Shaker, C. Malonzo, A. Stein

**INOR 426.** Synthesis, characterization, and growth kinetics of surface modified zinc oxide quantum dots. **A.D. Mena, B. Colon, D. Francis, P.P. Vaughan, A. Schrock, K. Molek**

**INOR 427.** Synthesis of photoactive gold nanoparticles for biomedical applications. **I. Musri, T. Lafferty, E. Park**

**INOR 428.** Potential nonlinear optical applications for high-temperature solid state and lithium polysulfide flux synthesized diamond-like semiconductors,  $\text{Li}_2\text{-II-IV-S}_4$ . **A. Weiland, J. Brant, J. Zhang, J.A. Aitken**

**INOR 429.** Cation exchange of copper iron sulfide nanoparticles. **A. Kim, R.M. Kozloski, K. Plass**

**INOR 430.** Gold nanoparticle aggregation: The role of capping agent and aqueous environment. **E.R. Carlson, K. Roberts, A.K. Bentley**

**INOR 431.** Energy storage by  $\text{MnO}_2$ -nanoparticle composite supercapacitors. **B.T. Hohman, L.M. Santino, A.K. Bentley**

**INOR 432.** Design and synthesis of cholesteric liquid crystalline porphyrin VOC sensors. **Z.R. Gregg, M.E. Zick, M.E. Langton, E.L. Smith, J.C. Kranick, L.J. Tucker, J.L. O'Donnell**

**INOR 433.** Improved synthetic methodologies for synthesizing polymeric subunits that incorporate extended aromatic acceptors and transition metal chromophores. **J. Callihan, K.A. Walters**

**INOR 434.** Stark absorption studies on supramolecular small molecules and polymers that connect fullerenes and transition metal chromophores. **S. Siemer, K.A. Walters**

**INOR 435.** Supramolecular organometallic sensitized solar cells: Advances in measurement procedures and refinement of cell preparation. **H. Hearn, K.A. Walters**

**INOR 436.** Temperature dependent phase behavior of pluronic F127 triblock copolymers in water. **J. Kim, Y. Han, Z. Zhang, G. Smith, C. Do**

**INOR 437.** Meso-structured styrene / butyl acrylate films containing  $\text{ZnO}$  quantum dots: Stability and fluorescence. **B. Colon, A. Mena, K.S. Molek, A. Schrock**

**INOR 438.** Developing a method to identify potential targets for zeolite encapsulation using computational techniques. **N. Robinson, J. Burkett**

**INOR 439.** Synthesis and characterization of titanium oxide nanopowders. **L. Barnes, H. Hamilton, K.A. Reyes, C.J. Van Leeuwen, K. Molek**

**INOR 440.** Synthesis and physicochemical characterization of quaternary, narrow-bandgap tellurides containing earth-abundant elements. **B. Hogan, J.A. Aitken**

**INOR 441.** Single-step electrodeposition of zinc oxide nanosheets on a compact layer for dye-sensitized solar cell photoanodes. **A. Lim, H. Van Ryswyk**

**INOR 442.** Surface passivation of copper sulfide nanoparticles with tetrathiomolybdate. **M.A. Tomat, Z.N. Georgieva, C. Kim, K. Plass**

**INOR 443.** Solvothermal synthesis of  $\text{Cu}_2(\text{Zn}_{1-x}\text{Co}_x)\text{SnS}_4$  solid solutions and kinetics of methylene blue adsorption. **A. Sharma, A.H. Pinto, R. Penn**

**INOR 444.** Synthesis and characterization of cobalt-zirconium heterobimetallic materials for photocatalysis. **N.G. Celia, M.W. Bedford, I.R. Bogcaz, M.M. Gadzuk-Shea, C.L. Jahncke, A. Hill**

**INOR 445.** Characterization liquid crystalline copper (II) m-toluate dimers. **D. Hong, T.W. Clayton**

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Research at the Frontiers of Inorganic Chemistry

H. J. Eppley, C. Nataro, *Organizers*

6:00 - 8:00

**INOR 446.** Palladium(II) thiocrown and oxathiacrown complexes with cyclometalating ligands. **M.A. Bruening, D.E. Janzen**

**INOR 447.** Synthesis and reactivity of compounds containing 1,1'-bis(phosphino)metallocene ligands. **R.J. Dupuis, E.P. Warnick, C. Nataro**

**INOR 448.** Tetrahedral compounds with bis(phosphino)ferrocene ligands. **S.F. Hartlaub, A.G. Furneaux, C. Nataro**

**INOR 449.** Synthesis and reactivity of compounds with 1,1'-bis(phosphino)ferrocenediyl ligands. **V.A. Decker, B.L. Blass, N.K. Lauricella, C. Nataro**

**INOR 450.** Exploration of the catalytic reactivity of iron-NHC complexes. **L.G. Habgood, C.E. Hedges**

**INOR 451.** Synthesis of group VI pentacarbonyl complexes containing a bidentate phosphine ligand. **H. Drake, B.J. Bellott**

**INOR 452.** Electronic and steric properties of a modified proazaphosphatrane: Tri(pyridylmethyl)azaphosphatrane. **I. Kha, Z. Thammavongsy, J. Yang**

**INOR 453.** Norbornene polymerization initiated by cationic ( $\pi$ -allyl)nickel(II) complexes containing dialkylbiaryl phosphine ligands. **C. Lee, A.R. O'Connor**

**INOR 454.** Synthesis of molybdenum carbon dioxide complexes via oxidation of a carbonyl ligand. **G. Lorzing, J. Vasta, M. Pogash, X. Duan, M.E. Graziani, R. Carden, J. Ohane, P.M. Graham**

**INOR 455.** Mechanistic investigation of Tantalum amide-alkoxide catalyzed asymmetric hydroamination of aminoallenes. **M. Kosich, A.R. Johnson**

**INOR 456.** Synthesis and catalytic activity of water soluble *N*-heterocyclic carbene complexes. **S.K. Kariofillis, R.J. Swails**

**INOR 457.** Synthesis and application of a water soluble Pd-NHC catalyst toward Heck coupling in aqueous solvents. **G.F. Riegel, R.J. Swails**

**INOR 458.** Synthesis and reactivity of nickel silylamides. **M. Schaff, M. Whited**

**INOR 459.** Withdrawn.

## Section A

San Diego Convention Center  
Hall D

### Undergraduate Teaching at the Frontiers of Inorganic Chemistry

*Cosponsored by CHED*

B. A. Reisner, J. L. Stewart, *Organizers*

6:00 - 8:00

**INOR 460.** Writing research proposals across the undergraduate curriculum: Adapting a VIPeR Learning Object for use in multiple courses. **J.L. O'Donnell, J.W. Karr**

**INOR 461.** Exploring scientific communication using infographics. **R.M. Jones**

**INOR 462.** Teaching at the frontiers: Creating an appropriate scaffold the primary literature in a sophomore level inorganic course. **S.R. Smith**

**INOR 463.** Leveraging collegiate consortia to develop literature-based inorganic laboratory experiments. **L.G. Habgood, K.J. Young**

**INOR 464.** Development of synthetic teaching labs for crystallographic analysis. **O. Phillips, L.Y. Kuo**

**INOR 465.** Creating correspondence between teaching and research by "converting" the teaching laboratory to a research laboratory. **R.E. Bachman**

**INOR 466.** Online homework for foundations of inorganic chemistry: A new frontier! **S.G. Sobel**

### My Comments to the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

### My Experience with & Advice for Improving Diversity in Chemistry

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### My Experiences in & Advice for Organic Chemistry Courses

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 20A-C

### ACS Awards in Inorganic Chemistry: Plenary Session

S. A. Koch, N. S. Radu, *Organizers*

C. Turro, *Presiding*

**8:15 INOR 467. Award Address (ACS Award in Inorganic Chemistry sponsored by Aldrich Chemical Company, LLC).** New inorganic solids from synthesis in molten chalcogenide salts: Structural diversity to applications. **M.G. Kanatzidis**

**8:45 INOR 468. Award Address (ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry sponsored by Strem Chemicals, Inc.).** Metallacrowns: From fundamental supramolecular chemistry to SMMs and near IR optical imaging agents. **V.L. Pecoraro**

**9:15 INOR 469. Award Address (Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator sponsored by the Gray Award Endowment).** Advances in coordination chemistry to improve the sustainability of the rare earth elements. **E.J. Schelter**

**9:45 INOR 470. Award Address (Earle B. Barnes Award for Leadership in Chemical Research Management sponsored by the Dow Chemical Company Foundation).** Development of sustainable alternatives for the next generation of chemicals and materials: Leadership in development of renewably-sourced materials. **H.E. Bryndza**

10:15 Intermission.

**10:25 INOR 471. Award Address (ACS Award in Organometallic Chemistry sponsored by the Dow Chemical Company Foundation).** Mechanistic understanding of fundamental organometallic reactions for catalyst development. **K.I. Goldberg**

**10:55 INOR 472. Award Address (F. Albert Cotton Award in Synthetic Inorganic Chemistry sponsored by the F. Albert Cotton Endowment Fund).** Lewis acidic and redox properties of organoantimony compounds: From anion sensing to catalysis. **F.P. Gabbai**

**11:25 INOR 473. Award Address (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation).** Synthesis and coordination chemistry of colloidal quantum dots. **J.S. Owen**

**11:55 INOR 474. Award Address (Alfred Bader Award in Bioinorganic or Bioorganic Chemistry sponsored by the Alfred R. Bader Fund).** Dioxigen binding, activation, and reduction to  $\text{H}_2\text{O}$  by Cu enzymes. **E.I. Solomon**

### Frontiers in Inorganic Chemistry

*Sponsored by SOCED, Cosponsored by INOR*

### Is There a Crisis in Organic Chemistry Education?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## MONDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 30B

### Undergraduate Teaching at the Frontiers of Inorganic Chemistry

#### Innovations in the Classroom

*Cosponsored by CHED*

J. L. Stewart, *Organizer*

B. A. Reisner, *Organizer, Presiding*

**1:30 INOR 475.** New frontier: Foundations of inorganic chemistry to include non-inorganic chemists. **G.P. Wulfsberg**

**1:50 INOR 476.** Chemical philately and education: Teaching inorganic chemistry with postage stamps. **D. Rabinovich**

**2:10 INOR 477.** Apps to aid teaching inorganic chemistry. **C.C. Raymond**

**2:30 INOR 478.** Designing an undergraduate course in organometallic chemistry based on IONiC VIPeR learning objects. **D.A. Laviska**

**2:50 INOR 479.** Using and adapting VIPeR learning objects at Albion College. **V.P. McCaffrey**

### Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**3:10 INOR 480.** Refreshing your local inorganic chemistry course with VIPER learning objects: Adventures in adaptation. K.A. Marek

**3:30 INOR 481.** Teaching molecular orbital theory and computational chemistry at the frontiers of inorganic chemistry. J.L. Stewart

## Section B

San Diego Convention Center  
Room 30C

### ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Vincent L. Pecoraro Metallopeptides

B. R. Gibney, C. M. Zaleski, *Organizers*

A. F. Peacock, *Organizer, Presiding*

M. Matzapetakis, *Presiding*

**1:30 INOR 482.** De novo design of metallo-proteins. W.F. Degrado

**2:00 INOR 483.** Coordination chemistry of designed metalloproteins: Insight into the biological function of natural metalloproteins. B.R. Gibney

**2:30 INOR 484.** Coiled coils as ligands for "non-biological" metal ions: New applications for metalloproteins. A.F. Peacock, M.R. Benwick, L.N. Slope, S.L. Newton, M. Britton

**3:00 INOR 485.** Protein-based radical (Trp<sup>•</sup> and Tyr<sup>•</sup>) intermediates and intramolecular electron transfer in mono- and bi-functional heme peroxidases. T. Kuhl, A. Ivancich

**3:30** Intermission.

**3:40 INOR 486.** Molecular factors that drive mitochondrial Fe-S cluster biosynthesis. T.L. Stemmler

**4:10 INOR 487.** Environmental nitrogen oxide abatement by single-site microporous catalysts. M. Caudle

**4:40 INOR 488.** Designing metalloenzyme inhibitors to be in-VINCE-able. S. Cohen, Y. Chen, C.V. Credille, C. Perez

**5:10 INOR 489.** Bionanotechnology-based enabling technologies. S. Daunert

## Section C

San Diego Convention Center  
Room 30D

### ACS Award in Inorganic Chemistry: Symposium in honor of Mercurio G. Kanatzidis

#### Synthesis & Applications of Solid State Materials

J. A. Aitken, K. Choi, *Organizers*

D. E. Freedman, P. F. Poudeu Poudeu, *Presiding*

**1:30 INOR 490.** How do we design materials for flexible hybrid electronic circuitry? T.J. Marks

**1:55 INOR 491.** Graphene-based supercapacitor. R.B. Kaner, M.F. El-Kady, Y. Shao, J. Hwang, L.J. Wang, K. Marsh, M. Li, H. Wang, M. Kowal, S. Dubin, W. Sun, R. Li, L. Chaney, S. Cho, R. Rizvi

**2:20 INOR 492.** Layered metal oxide nanosheets as model surfaces for understanding nanoparticle-support interactions. M. Strayer, T.P. Sentfle, J.P. Winterstein, N.M. Vargas-Barbosa, R. Sharma, R.M. Rioux, M.J. Janik, T.E. Mallouk

**2:45 INOR 493.** 2D inorganic nanosheets as efficient building blocks for exploring new functional nanohybrids. S. Hwang

**3:10** Intermission.

**3:25 INOR 494.** Multiscale heterostructured materials. G.D. Stucky

**3:50 INOR 495.** Ordered Pd based nanoparticles as low cost, highly efficient, and robust catalysts alternative to Pt in fuel cell applications. S. Peter

**4:15 INOR 496.** Sulfur chemistry in electrochemical energy storage. K.A. See, M.M. Butala, V. Doan-Nguyen, R. Seshadri

**4:40 INOR 497.** Energy and innovation in the chemical industry. S.S. Dhingra

**5:05 INOR 498.** Synthesis, modification, and utilization of BiVO<sub>4</sub> photoanodes. K. Choi

## Section D

San Diego Convention Center  
Room 30E

### ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg

*Cosponsored by WCC*

N. E. Gruhn, W. D. Jones, M. S. Sanford, *Organizers*

A. S. Goldman, J. M. Mayer, *Presiding*

**2:00 INOR 499.** Bonding in organometallic compounds of the actinide elements: Coordination and novel complexes. B.E. Bursten

**2:20 INOR 500.** Chemical surprises at the frontier of the periodic table. J.L. Kiplinger

**2:40 INOR 501.** Toward the development of high oxidation state iridium catalysts for alkane dehydrogenation. Lewis-acid catalyzed olefin insertion/ $\beta$ -hydrogen elimination. Y. Gao, C. Guan, Z.H. Syed, A.M. Wright, K. Allen, D.M. Heinekey, K. Krogh-Jespersen, K.I. Goldberg, A.S. Goldman

**3:00 INOR 502.** Platinum(II) complexes for C-H activation ligated by phosphite ligands. K.A. Grice, J. Kostarut, A.E. Lawando, E.J. Crespo, R. Sommer

**3:20 INOR 503.** New taggants for monitoring underground fluid flows. L.J. Treadwell, J.M. Sears, T.J. Boyle, B.A. Hernandez-Sanchez, R.F. Hess, J.E. Miller, A.C. Cappuccilli, C.D. Cannan, T.M. Roper, M. Spilde, R.A. Kemp

**3:40** Intermission.

**3:50 INOR 504.** Thermal and photochemical reactions mediated by water-soluble host-guest supramolecular systems. R.G. Bergman

**4:10 INOR 505.** Metal and non-metal catalyzed reactions with sulfenate anions. P.J. Walsh

**4:30 INOR 506.** Synthesis and reactivity of mono- and bimetallic complexes of a novel bisimidazole phosphine ligand. B.M. Cossairt, M. Norris, S. Flowers

**4:50 INOR 507.** CpCo(III) fluoride and fluoroalkyl complexes: Selective C-F bond abstraction, C-C bond formation and catalyzed fluorination of acyl chlorides. M. Leclerc, G.M. Lee, J.M. Bayne, S. Gorelsky, D.J. Harrison, M. Vasiliu, D.A. Dixon, R. Baker

**5:10 INOR 508.** Understanding the reactivity of reduced ZnO and TiO<sub>2</sub> nanocrystal. J.M. Mayer, C. Valdez, J. Peper, R. Mitsuhashi, T. Porter

## Section E

San Diego Convention Center  
Room 31A

### ACS Award in Pure Chemistry: Symposium in honor of Jonathan S. Owen

G. Parkin, *Organizer*

J. E. Bercaw, *Presiding*

**1:30 INOR 509.** Catalysis at Dow: Vignettes in olefin production & polymerization. P.N. Nickias

**1:50 INOR 510.** Diazaphospholanes and enantioselective catalysis. C.R. Landis, F. Foarta, B.R. Jones

**2:10 INOR 511.** Pentanuclear and heptanuclear copper hydrides. J.R. Norton, M.S. Eberhart, S. Liu, M.C. Neary

**2:30 INOR 512.** Applications of tetradentate and tridentate tripodal ligands for catalytic and stoichiometric transformations involving zinc and magnesium. S. Ruccolo, M. Rauch, W.I. Sattler, M. Rostami Chajjan, G. Parkin

**2:50** Intermission.

**3:10 INOR 513.** Oligo or poly? A mechanistic interpretation of a switchable catalyst. J.A. Labinger, J.E. Bercaw, E. Despagne-Ayoub

**3:30 INOR 514.** High spin electronic structures in cluster design. T. Betley

**3:50 INOR 515.** Carbon dioxide hydrogenation catalysts encapsulated in the metal organic framework UiO-66. J.A. Byers, C. Tsung, Z. Li, J.V. Morabito, K.F. Beal, L. Chou

**4:10 INOR 516.** Small molecule activation with metal complexes supported by ligands with pendant arene moieties. T. Agapie

## Section F

San Diego Convention Center  
Room 31B

### Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Edward I. Solomon

#### Bioinorganic Enzymology

K. D. Karlin, *Organizer*

T. E. Machonkin, *Presiding*

**1:30 INOR 517.** Electron flow through metalloproteins. H.B. Gray

**2:00 INOR 518.** Genetically encoded sensors to monitor the spatial distribution of zinc in cells. A.E. Palmer

**2:30 INOR 519.** Thermodynamic contributions to the metalloprotein reduction potential. M. Creteau, D. Wilcox

**3:00 INOR 520.** Metal-induced aggregation of human gamma-D crystallin: Insights into the bioinorganic chemistry of cataracts disease. L. Quintanar, J. Dominguez-Calva, E. Serebryany, C. Haasse-Pettingell, J. King

**3:30** Intermission.

**3:45 INOR 521.** Distance, conjugation, and torsional dependence of molecular electronic coupling. M.L. Kirk, D. Shultz, B. Stein, D. Habel-Rodriguez, D.E. Stasiw, C. Tichnell

**4:15 INOR 522.** Cuprous oxidase motifs in multi-copper oxidases: Structural identification and cladistic analysis. D. Kosman, P. Hart, S. Hardies

**4:45 INOR 523.** Oxygenase chemistry of the versatile diiron cluster. J.D. Lipscomb, R. Banerjee, C.J. Knoot, B.S. Rivard, A.J. Komor

## Section G

San Diego Convention Center  
Room 31C

### F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Francois P. Gabbaï

J. D. Hoefelmeyer, T. W. Hudnall, *Organizers*

C. R. Wade, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 524.** My secret life as a main group chemist. J.A. Gladysz

**1:55 INOR 525.** New BN isosteres of polycyclic aromatic hydrocarbons. W.E. Piers, M. Morgan, E. Patrick, D. Spasyuk

**2:15 INOR 526.** Boracycles in Lewis acid chemistry and conjugated materials development. F. Jaekle

**2:35 INOR 527.** Studies of the coupling reactions of carbonyl sulfide (COS) and epoxides. Formation of cyclic- and poly(thiocarbonates). D.J. Darensbourg

**2:55** Intermission.

**3:05 INOR 528.** Experimental and computational approaches to understanding and implementing weak forces involving anions and aromatic  $\pi$ -systems. J.F. Ellenberger, S. Gomez-Coca, I.D. Giles, H.T. Chifitides, K.R. Dunbar

**3:25 INOR 529.** New single-molecule magnets with high blocking temperatures. S. Demir, P.C. Bunting, K.R. Meihaus, J. Zadrozny, J.R. Long

**3:45 INOR 530.** Sustainable manufacturing of functional materials. C.J. Carmalt

**4:05 INOR 531.** Kinetically controlled synthesis of stable metal-organic frameworks. H. Zhou

**4:25 INOR 532.** Energy storing photochemistry with first row transition metal complexes. B.L. Anderson, S. Hwang, A.G. Maher, D.C. Powers, D.G. Nocera

## Section H

San Diego Convention Center  
Room 32A

### Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Eric J. Schelter

L. G. Sneddon, P. J. Walsh, *Organizers*

C. R. Graves, J. R. Walensky, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 533.** Xenon: New applications in materials chemistry and biosensing. Y. Wang, B.W. Roose, B.A. Riggie, I.J. Dmochowski

**1:55 INOR 534.** Competitive heavy atom kinetic isotope effects expose bond forming steps in carbon dioxide reduction catalysis by transition metal complexes. A.M. Angeles Boza

**2:15 INOR 535.** Synthesis and characterization of aluminum complexes of redox-active nitroxide-based ligands. C.R. Graves

**2:35 INOR 536.** Boron formates as surrogates for hydroboranes: Metal free dehydrogenation and disproportionation of formic acid. T. Cantat, C. Chaiver

**2:55 INOR 537.** Group 13 and 15 systems stabilized by electron rich ligands. J.D. Masuda

**3:15** Intermission.

**3:35 INOR 538.** Coordination chemistry and reactivity of polynuclear group 11 amidinate and carboxylate complexes. J.R. Walensky, P. Rungthanaphathophon, A. Lane

- 3:55 INOR 539.** Organosilane reactivity in solvent-borne epoxy coatings. **J.R. Robinson**, N. Caggiano, S.C. Korf, K. Adamsons, B.E. Priore
- 4:15 INOR 540.** Synthesis and coordination chemistry of chelating guanidiniyl ligands. **N.A. Piro**, W.S. Kassel
- 4:35 INOR 541.** New approaches to the synthesis of group 6 metal-element multiple bonds. **R.K. Thomson**

## Section I

San Diego Convention Center  
Room 32B

### Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza

*Cosponsored by ENVR, ORGN and POLY*

M. Harmer, N. S. Radu, *Organizers, Presiding*

#### 1:30 Introductory Remarks.

**1:35 INOR 542.** 20 years of the presidential green chemistry challenge awards: A perspective on chemistry innovation. **D.J. Constable**

**2:05 INOR 543.** Safety by design: Integration of safety / toxicology considerations into the early research process. **J.R. Damewood**

**2:35 INOR 544.** Only the best is good enough: The LEGO group's journey to leave a positive impact. **N. van der Pui**

#### 3:05 Intermission.

**3:15 INOR 545.** Framework to guide selection of chemical alternatives. **T. Fryberger**

**3:45 INOR 546.** Role of the EPA in deploying safer chemicals in both products and manufacturing processes. **J. Jones**

## Section J

San Diego Convention Center  
Room 33A

### Frontiers in Heavy Element Inorganic Chemistry

*Cosponsored by NUCL*

D. K. Shuh, L. Soderholm, *Organizers*

D. L. Clark, *Organizer, Presiding*

#### 1:30 Introductory Remarks.

**1:40 INOR 547.** Early metal chemistry featuring redox non-innocent (RNI) ligands. **P.T. Wolczanski**, S.P. Heins, N. Livezey, S.N. MacMillan, E.B. Lobkovsky

**2:00 INOR 548.** Bis-arene complexes of technetium and rhenium; with and without metal-metal bonds. **R.A. Alberto**, H. Braband, M. Bachmann, G. Meola, P. Schmutz

**2:20 INOR 549.** Metalloporphyrin monolayers as platforms for 3D organization of functional materials. **M.D. Hopkins**, W. Lau, J. Kamm

**2:40 INOR 550.** Mid-valent, early transition metal mononuclear and dinuclear chemistry (as inspired by Al Sattelberger), and novel  $\pi$ -donor ligand clusters as kinetic products. **L. Messerle**

**3:00 INOR 551.** Sustainable acetylde chemistry: 3d metals and tetraazamacrocycles. **T. Ren**, S.F. Tyler, T. Cook, S.N. Natoli, S.D. Banziger

#### 3:20 Intermission.

**3:40 INOR 552.** Adventures with stronger and weaker metal-metal bonds. **A.W. Maverick**, L.G. Butler

**4:00 INOR 553.** Coordination chemistry of 2,2'-biphenylenedithiophosphinate and diphenyldithiophosphinate with U, Np, Pu, and Am. **J. Macor**, S.R. Daly, A. Gaunt, S.A. Kozimor, **G.S. Girolami**

**4:20 INOR 554.** Mechanistic insights into carbon-carbon reductive elimination from tetrabenzyluranium. **S.C. Bart**, S.A. Johnson

**4:40 INOR 555.** Super electron-rich diiron dithiolate analogues of the active site of the [FeFe]-hydrogenases. **T.B. Rauchfuss**, X. Zhou, F. Arrigoni, G. Zampella

## Section K

San Diego Convention Center  
Room 33B

### Organometallic Compounds & Catalysts: Influence on Polymer Science & Synthesis

T. Y. Meyer, *Organizer*

D. E. Bowen, *Organizer, Presiding*

L. Rosenberg, *Presiding*

#### 1:30 Introductory Remarks.

**1:35 INOR 556.** Palladium and nickel catalysts for olefin polymerization and copolymerization with polar monomers. **C. Chen**, S. Dai, M. Chen

**1:55 INOR 557.** Synthesis of polyarylphosphonates and metallopolymers based upon a spirocyclic bisphosphite. **R.A. Stockland**

**2:15 INOR 558.** Phosphine-sulfonate palladium(II) catalysts with rigid, aliphatic backbones for copolymerization of ethylene and polar monomers. **R.E. Black**

**2:35 INOR 559.** Critical role of polymerization catalysis in the production advanced tire elastomers. **S. Rodewald**

**2:55 INOR 560.** Stereocontrol in *rac*-lactide polymerization with copper complexes. **F. Schaper**, P. Daneshmand, S. Fortun

**3:15 INOR 561.** Pd-initiated controlled polymerization of diazoacetates. **E. Ihara**

#### 3:35 Intermission.

**3:50 INOR 562.** Understanding the activity of half-sandwich ruthenium phosphido complexes in P-C bond formation. **R.G. Belli**, J. Yang, D. Pantazis, R. McDonald, **L. Rosenberg**

**4:10 INOR 563.** Reductive functionalization of CO<sub>2</sub>. **S. Bontemps**

**4:30 INOR 564.** Synthesis of biorenewable C5 compounds utilizing D-xylose obtained from agricultural biomass. **C.T. Burns**, M.H. Nantz, J. Satyavolu

**4:50 INOR 565.** From Hyde Park to Ames: An organometallic- and polyolefins-inspired approach to chemical surface modification of colloidal nanocrystal quantum dots. **J. Vela-Becerra**

**5:10 INOR 566.** From group 4 metal mono-dicarbollide complexes to nanocomposites containing boron cage compounds. **D.E. Bowen**, S.M. Wells, E.A. Eastwood, S. Sarkar, J.M. Messman, N. Bowler

**5:30 INOR 567.** Synthesis and applications of styrenic copolymers by metal catalyzed polymerization processes. **A. Grassi**, A. Buonerba, C. Capacchione, S. Milione

## Section L

San Diego Convention Center  
Room 33C

### Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*

A. Beecher, G. Mezei, *Presiding*

**1:30 INOR 568.** Influence of metal vacancy of undoped anatase TiO<sub>2</sub> on p-type conductivity, room-temperature ferromagnetism, and remarkable photocatalytic performance. **S. Wang**, L. Pan, J. Zou, L. Wang, X. Zhang

**1:50 INOR 569.** Withdrawn.

**2:10 INOR 570.** Magnetic study of Fe(III)-loaded synthetic melanin nanoparticles and their implications for MRI contrast agents. **Y. Xie**, Y. Li, N. Zang, Z. Wang, C.M. Andolina, L. Parent, N.C. Gianneschi, J.D. Rinehart

**2:30 INOR 571.** Mechanism of formation, structure, and reactivity of anion-incarcerating nanojars. **G. Mezei**

**2:50 INOR 572.** Assembling oligomers of transition metal clusters with single-atom linkers. **A. Beecher**, J.S. Owen

#### 3:10 Intermission.

**3:25 INOR 573.** Versatile access to polyphosphides by solution- and flow-chemistry activation of red phosphorus. **A. Dragulescu-Andrasi**, L. Miller, D.T. McQuade, M. Shatruk

**3:45 INOR 574.** Formation and reaction mechanisms of molybdenum complex species in acid solutions as precursors of hexagonal molybdenum trioxide. **C. Vargas Consuelos**, M.A. Camacho-Lopez, O. Graeve

**4:05 INOR 575.** Bimetallic molecular precursors for nanocrystalline functional oxides: The relationships between the crystal structure of the precursor and the phase of the metal oxide. **A.M. Moneeb**, A. Alabdulrahman, A. Bagabas, A.W. Appleb

**4:25 INOR 576.** Direct synthesis of polycarbonates from carbon dioxide and diols over a ceria catalyst. **S. Bian**, G. Du

**4:45 INOR 577.** New radical cation hybrid iodoplumbates: Functionalized organics and their impact on structure, stability, and performance. **H. Evans**, A. Lehner, J. Labram

### Diversity-Quantification-Success?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### Undergraduate Research Posters

#### Inorganic Chemistry

*Sponsored by CHED, Cosponsored by INOR and SOCED*

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

S. A. Koch, N. S. Radu, *Organizers*

#### 8:00 - 10:00

329, 334, 373, 385-386, 400-401, 414, 418-420, 442, 446, 450, 454, 456, 458, 461, 463-464. See previous listings.

910, 912, 915, 917, 1090, 1411. See subsequent listings.

## TUESDAY MORNING

### Section A

San Diego Convention Center  
Room 30B

### Undergraduate Research at the Frontiers of Inorganic Chemistry

#### Coordination Chemistry & Materials/Solid-State

*Financially supported by IONIC (Interactive Online Network of Inorganic Chemists)*

H. J. Eppley, C. Nataro, *Organizers*

R. J. Swails, *Presiding*

**8:30 INOR 578.** Structure and properties of coordination polymers containing hydrogen-bonding capable and conformationally flexible dipyrriyl ligands: An introductory undergraduate research program at Lyman Briggs College at Michigan State University. **R.L. Laduca**, C. White, A. Sample

**8:50 INOR 579.** Layer-by-layer assembly of metal-organic coordinated thin films: Fundamentals of formation and sensing. **M.L. Ohnsorg**, M.E. Anderson

**9:10 INOR 580.** Understanding aluminum corrosion at the molecular level: Low-tech and high-tech approaches. **S.G. Sobel**

**9:30 INOR 581.** Surmounting the roadblocks to rechargeable zinc-air batteries by 3D architectural redesign of the air-breathing cathode and Zn anode. **E. Nelson**, J.F. Parker, P. DeSario, J. Long, D.R. Follison, C.N. Chervin

#### 9:50 Intermission.

**10:05 INOR 582.** Aryl-substituted BIAN complexes of iron dibromide: Synthesis, electronic structure, and catalytic hydrosilylation activity. **H.M. Hoyt**, M.J. Supej, A. Volkov, L. Darko, J. Darmon, C. Schultz, K.A. Wheeler

**10:25 INOR 583.** Novel metal alkoxide precursors for the production of high dielectric nanoinks for direct write applications. **D.T. Yonemoto**, T.J. Boyle, A. Cook, N.S. Bell, L.J. Treadwell, J.R. Farrell

**10:45 INOR 584.** Fluxional five-coordinate palladium(II) complexes with sulfur donor macrocycles: Reversible Pd<sup>II</sup> electrochemistry, DFT calculations, and X-ray structure. **D.E. Janzen**

**11:05 INOR 585.** Withdrawn.

### Section B

San Diego Convention Center  
Room 30C

### Transition Metal Chemistry in DNA & RNA Regulation

S. L. Michel, *Organizer*

P. Chen, *Organizer, Presiding*

T. V. O'Halloran, *Presiding*

**8:30 INOR 586.** Exploring protein allostery and dynamics in metalloregulatory proteins. **D.P. Giedroc**, J.J. Braymer, D.A. Capdevila

**9:00 INOR 587.** Loz1, a zinc-responsive transcription factor from fission yeast. **A.J. Bird**

**9:30 INOR 588.** Biliverdin dependent regulation of extracellular heme uptake in *Pseudomonas aeruginosa*. **A. Wilks**

#### 10:00 Intermission.

**10:20 INOR 589.** Siderophore-mediated iron acquisition during nickel stress is controlled by the metalloregulatory protein YqjI in *E. coli*. **F. Outten**

**10:50 INOR 590.** Regulation of zinc homeostasis in *Bacillus subtilis*. P. Chandrangsu, J. Shin, J.D. Helmann

**11:20 INOR 591.** Controlling gene expression through DNA distortion: Structure and mechanism of metalloregulatory proteins. T.V. O'Halloran

## Section C

San Diego Convention Center  
Room 30D

### ACS Award in Inorganic Chemistry: Symposium in honor of Mercurio G. Kanatzidis

#### Synthesis & Applications of Solid State Materials

K. Choi, *Organizer*

J. A. Aitken, *Organizer, Presiding*

P. Trikalitis, *Presiding*

**8:30 INOR 592.** Metal chalcogenides as promising candidate semiconductors for g-ray detection. D. Chung

**8:55 INOR 593.** Synthesis of bismuth sulfide iodides in sulfur/iodine flux mixtures. R. Groom, S.E. Lattner

**9:20 INOR 594.** Magnetic anisotropy arising from main group elements: Bismuth-based molecules and materials. D.E. Freedman, S. Clarke, M. Fataftah

**9:45 INOR 595.**  $\text{FeM}_2\text{Se}_4$ : A fascinating family of high- $T_c$  ferromagnetic semiconductors. P.F. Poudeu Poudeu

**10:10** Intermission.

**10:25 INOR 596.** Enhancement of thermoelectric power factor in type I clathrate  $\text{K}_x\text{Ba}_y\text{Al}_z\text{Si}_{13}$  through charge carrier tuning. F. Sui, S. Kazuichir

**10:50 INOR 597.** Materials modules and systems for thermoelectric based waste heat recovery in passenger vehicles. J.R. Salvador

**11:15 INOR 598.** Thermoelectric properties of polycrystalline Pb-free metal chalcogenide compounds. J. Cha, K. Ahn, I. Chung

**11:40 INOR 599.** Efficient thermoelectric energy conversion in SnTe and GeTe. K. Biswas

## Section D

San Diego Convention Center  
Room 30E

### Memorial Symposium Honoring Karen J. Brewer

*Cosponsored by HIST†  
Financially supported by  
Washington State University*

S. C. Rasmussen, *Organizers*

M. T. Mongelli, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:40 INOR 600.** Karen J. Brewer (1961 - 2014). S.C. Rasmussen

**9:10 INOR 601.** Tribute to 22 years of collaboration and friendship across the chemistry/biology interface. B.S. Winkel

**9:40 INOR 602.** Ru,Rh,Ru supramolecular photocatalysts in Nafion® membranes. E.M. Naughton, K.S. Brewer, R.B. Moore

**10:10** Intermission.

**10:25 INOR 603.** Enhancing coreactant electrogenerated chemiluminescence. M. Richter

**10:55 INOR 604.** Photochemistry of metal organic frameworks: Ruthenium polypyridyl excited state chemistry in a new type of supramolecular material. W. Maza, A.J. Morris

**11:25 INOR 605.** Monitoring the excited state properties of dirhodium(II,II) complexes following visible light photoexcitation with potential applications in solar energy conversion. T.A. White, T.J. Whitemore, R.P. Thummel, K.R. Dunbar, C. Turro

**11:55 INOR 606.** Photo-uncaging and delivery of small molecule bioeffectors. P.C. Ford

## Section E

San Diego Convention Center  
Room 31A

### Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

T. B. Clark, C. J. Daley, *Presiding*

**8:30 INOR 607.** Influencing excited states of iridium(III) cyclometalates by various aryl isocyanides and cyclometalating ligands. A. Maity, T.S. Teets

**8:50 INOR 608.** Mechanistic insights into the reactivity of (Phebox)Ir(H)(OAc) and molecular oxygen. A.M. Wright, D. Pahls, K.I. Goldberg, T.R. Cundari

**9:10 INOR 609.** Withdrawn.

**9:30 INOR 610.** Synthesis and reactivity of methyl-substituted PCP ligands and corresponding iridium complexes. T. Lekich, J.M. Goldberg, G.W. Wong, D.M. Heinekey

**9:50 INOR 611.** Redox-active heterobimetallic complexes with mesoionic carbenes: Electronic structures and catalytic properties. L. Hettmanczyk, S. Manck, C. Hoyer, S. Hohloch, B. Sarkar

**10:10 INOR 612.** Metal complexes with triazoles and triazolylidenes and a ferrocene backbone. S. Manck, T. Bens, M. van der Meer, L. Suntrup, B. Sarkar

**10:30 INOR 613.** Mechanistic studies of carboxylation of isostructural iron methyl complexes with different charge state. K. Lau, R.F. Jordan

**10:50 INOR 614.** Synthesis, structure, and reactivity of hydridosilylene complexes of iron. P. Smith, T. Tilley

**11:10 INOR 615.** Synthesis and characterization of chiral, highly water-soluble pyridyl phosphines derived from 1,3,5-triaza-7-phosphaadamantane (PTA). W.L. Ounkham, W. Lee, B.J. Frost

**11:30 INOR 616.** Effects of ligand modification on accessing various oxidation states in palladium pyridinophane complexes. A. Wessel, L.M. Mirica

## Section F

San Diego Convention Center  
Room 31B

### Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Edward I. Solomon

#### Bioinorganic Methods

K. D. Karlin, *Organizer*

D. R. Gamelin, *Presiding*

**8:30 INOR 617.** Understanding and controlling electrochemistry for fuel cells and electrolyzers. A.A. Gewirth

**9:00 INOR 618.** Nuclear resonance vibrational spectroscopic elucidation of binuclear non-heme iron enzyme intermediates. K. Park, E.I. Solomon

**9:30 INOR 619.** From electronic properties of non-heme iron active sites to biocatalysis. M. Srnc, E.I. Solomon

**10:00 INOR 620.** Vibrational stark effect spectroscopy on the blue light photosensor photoactive yellow protein. M.T. Kieber-Emmons, K.M. Light, V. Cheng

**10:30 INOR 621.** Catalytic cycle of multi-copper oxidases studied by theoretical methods. L. Rulisek, E.I. Solomon, U. Ryde

**11:00 INOR 622.** N2ase & H2ase vibrational spectroscopy with NRVs & FT-IR: The merits of big photons & little ones. S.P. Cramer

**11:30 INOR 623.** Novel mechanisms of transcription regulation in living cells: A lesson from metalloregulators. P. Chen

**12:00 INOR 624.** Synchrotrons and X-ray free electron lasers in structural biology: From "slow" to "ultrafast". B.G. Hedman, K.O. Hodgson

## Section G

San Diego Convention Center  
Room 31C

### F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Francois P. Gabbaï

J. D. Hoefelmeyer, T. W. Hudnall, *Organizers*

W. E. Piers, *Presiding*

**8:30** Introductory Remarks.

**8:35 INOR 625.** Main group strategy for fluorescent dyes. S. Yamaguchi

**8:55 INOR 626.** Organometallic photonics: Pt<sup>II</sup> dimer photochemistry and photophysics. F.N. Castellano

**9:15 INOR 627.** Functionalized triarylborane Lewis acids for anion sensing. M. Lee

**9:35 INOR 628.** Intramolecular frustrated Lewis pair dichloro-8-quinolylgallium(III) activates chloroform. J.D. Hoefelmeyer, S.R. Tamang, J.I. Fostvedt, J. Son

**9:55 INOR 629.** Synthesis of fluoromethyl-substituted organoboranes and their application in frustrated Lewis pair chemistry. H. Wang, Z. Lu, H. Ye, J. Zheng

**10:15** Intermission.

**10:25 INOR 630.** Designing and exploiting reversible small molecule capture by single component frustrated Lewis pairs. S. Aldridge, Z. Mo

**10:45 INOR 631.** Nitrogen fixation with iron complexes. J.C. Peters, T.J. Del Castillo, J. Rittle, N.B. Thompson

**11:05 INOR 632.** (Boryl)iminomethanes: Coordination chemistry and FLP behavior. J.S. Figueroa, B.R. Barnett

**11:25 INOR 633.** Evolving the coordination chemistry of p-block element Lewis acceptors. N. Burford

**11:45 INOR 634.** Electrophilic phosphonium cations in catalysis: New strategies for reactivity. D.W. Stephan

## Section H

San Diego Convention Center  
Room 32A

### Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Eric J. Schelter

L. G. Sneddon, P. J. Walsh, *Organizers*

J. R. Robinson, U. J. Williams, *Presiding*

**8:30** Introductory Remarks.

**8:35 INOR 635.** Designing new energetic chromophores for optical initiation of explosives: Tuning charge transfer in nitrogen-rich Fe(II) tetrazine complexes. J.M. Veauthier, T.W. Myers, D.E. Chavez, J. Ejlorgaard, S. Tretiak, S.K. Hanson, R.J. Scharrf

**8:55 INOR 636.** Dye-sensitized solar cell as a tool to resolve intermolecular interactions. C.P. Berlinguette, G.J. Meyer, F.G. Parlane, S.J. Simon, K. Hu, W.B. Swords

**9:15 INOR 637.** Formal Ce(IV) coordination complexes and the role of configuration interactions: Closed-shell singlet ground states and temperature-independent paramagnetism. C. Booth, R.L. Halbach, G. Nocton, L. Maron, R.A. Andersen

**9:35 INOR 638.** Electronic structures and reactions of metal-oxos. H.B. Gray

**9:55** Intermission.

**10:15 INOR 639.** Spin crossover in mono- and multinuclear Fe(II) complexes with N<sub>4</sub>S<sub>2</sub> coordination environment. A. Dragulescu-Andrasi, A. Arroyave, V. Stubbs, S. Yergeshbayeva, M. Shatruk

**10:35 INOR 640.** New advances in lanthanide magnetism. M. Murugesu

**10:55 INOR 641.** Enhanced processing features in the family of lanthanide double-decker single molecule magnets. J. Galan-Mascaros, N. Gimenez, C. Saenz de Pipaon, P. Ballester, D. Ecija

**11:15 INOR 642.** Recent advances in the chemistry of the rare earth metals in the formal +2 oxidation state. W.J. Evans

**11:35 INOR 643.** Paramagnetic dinuclear complexes with radical diimine ligands. T.J. Woods, M.B. Rivas, K.R. Dunbar

**11:55** Concluding Remarks.

## Section I

San Diego Convention Center  
Room 32B

### Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza

*Cosponsored by ENVR, ORGN and POLY*

M. Harmer, N. S. Radu, *Organizers, Presiding*

**9:00 INOR 644.** Catalysis, mechanistic understanding, and collaboration as tools to sustainable production of chemicals and fuels. K.I. Goldberg

**9:30 INOR 645.** Bridging the gap between homogeneous and heterogeneous catalysis at Argonne National Laboratory. E. Bunel

**10:00** Intermission.

**10:10 INOR 646.** Technology greenhouse: Ideas through commercialization. J.C. Warner

**10:40 INOR 647.** Building a robust biomaterials portfolio: An overview of DuPont's strategy and programs. M.A. Saltzberg

**11:10** Concluding Remarks.

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## Section J

San Diego Convention Center  
Room 33A

**Frontiers in Heavy Element  
Inorganic Chemistry**

Cosponsored by NUCL

D. L. Clark, D. K. Shuh, L. Soderholm,  
Organizers

S. A. Kozimor, *Presiding*

8:30 Introductory Remarks.

8:35 **INOR 648.** Multinuclear metal complexes for challenging chemical transformations. T. Tilley

8:55 **INOR 649.** New ligand platforms for actinide chemistry. J. Arnold, C. Camp, N. Settineri, M. Garner, S. Hohlock

9:15 **INOR 650.** Heavier the better: Something old, something new, nothing radioactive. G.G. Stanley

9:35 **INOR 651.** Exploring redox noninnocence of pincer ligands for delivery to refractory substrates. K.G. Caulton, B.J. Cook, A.V. Polezhaev, N. Maciulis, S. Curtis, N. Labrum, M. Pink, C. Chen

9:55 **INOR 652.** Impact of Al Sattelberger on actinide chemistry at Los Alamos. C. Burns

10:15 **INOR 653.** Recent advances in the chemistry of thorium and uranium in the formal +2 oxidation state. W.J. Evans

10:35 Intermission.

10:55 **INOR 654.** Functional materials by design for energy conversion through integrated theory and experiment. W. Tumas, D.S. Ginley, A. Zakutayev, S. Lany, L. Garten, v. stevanovic, M. Toney

11:15 **INOR 655.** N vs. S: Bifunctional reactivity of Fe complexes bearing svelte thiolato- and amido-SNS ligands. U.K. Das, K. Ghostine, R. Baker

11:35 **INOR 656.** New ligands and metal complexes for efficient outer sphere hydrogenation of ketonic substrates. P.A. Dub, B. Scott, J.C. Gordon

11:55 **INOR 657.** Redox processes of rare-earth metal complexes supported by ferrocene diamide ligands. P. Diaconescu

12:15 **INOR 658.** Proton-coupled electron transfer reactivity of ceria and samarium diiodide. J.M. Mayer, D. Damatov, S. Kolmar, O. Jung, J. Peng

## Section K

San Diego Convention Center  
Room 33B

**Organometallic Compounds &  
Catalysts: Influence on Polymer  
Science & Synthesis**

D. E. Bowen, *Organizer*

T. Y. Meyer, *Organizer, Presiding*

G. M. Diamond, *Presiding*

8:30 Introductory Remarks.

8:35 **INOR 659.** Application of chiral terpenyl groups in imine-type ligand design for olefin polymerization catalysis. F. Zhai, R.F. Jordan

8:55 **INOR 660.** Selectivity-enhanced entropy-driven ring-opening polymerization for the preparation of sequenced copolymers. T.Y. Meyer, R.M. Weiss, A.L. Short, M.A. Washington, D.J. Swiner

9:15 **INOR 661.** Combining N-heterocyclic carbenes with oxophilic and high-oxidation-state metal centers state (group 4, 12 and 13): Fundamental reactivity and use in polymerization and CO<sub>2</sub> functionalization catalysis. C. Fiedel, J. Bruyere, D. Specklin, S. Dagorne

9:35 **INOR 662.** Nature of secondary interactions in molecular and silica-supported organolanthanum complexes from solid-state NMR spectroscopy. M.P. Conley, C. Coperet, R.A. Andersen

9:55 Intermission.

10:15 **INOR 663.** Termination routes in alpha-olefin oligomerization with group IV metallocenes; evidence for beta-alkyl elimination where alkyl is greater than methyl. D.J. Crowther

10:35 **INOR 664.** Synthesis of metal phosphonate cage compounds for tetranuclear Pd polymerization catalysts. Q. Liu, R.F. Jordan

10:55 **INOR 665.** Development of novel D<sub>2h</sub>-symmetric aromatic tetraaza macrocyclic ligands. T. Gardner

11:15 **INOR 666.** Dithiobiuret ligands for the simultaneous leaching and extraction of gold from ore and secondary sources. S.R. Foley

11:35 **INOR 667.** Ethylene oligomerization promoted by chromium complexes bearing imine tridentate ligands. A. Pinheiro, A. Bergamo, A. Casagrande, E. Kirilow, J. Carpentier, O.L. Casagrande

## Section L

San Diego Convention Center  
Room 33C

**Supramolecular Chemistry: A  
Crown & Anchor Approach**

Cosponsored by ORGN

Financially supported by Elsevier,  
*Supramolecular Chemistry, RSC*

A. E. Gorden, *Organizer*

D. W. Johnson, *Presiding*

8:30 Introductory Remarks.

8:40 **INOR 668.** Enzyme-like catalysis in a chiral supramolecular cluster. K.N. Raymond, D. Kaphan, D. Toste, R.G. Bergman

9:10 **INOR 669.** Supramolecular catalyst with cyclic tetrapyrrole compound. Y. Hisaeda

9:30 **INOR 670.** Bioconjugated metallocorroles for medicine and catalysis. Z. Gross

9:50 **INOR 671.** Dynamic covalent self-assembly for determination of enantiomeric excess. P. Anzenbacher

10:10 **INOR 672.** Small pyrrole-based pigments as redox-active ligands. E. Tomat

10:30 Intermission.

10:50 **INOR 673.** Computer-aided molecular design in supramolecular chemistry. B.P. Hay

11:10 **INOR 674.** Exploring reactivity in self-assembled main group coordination clusters: A new route to cyclophanes? D.W. Johnson

11:30 **INOR 675.** Steric and electrostatic effects on the dynamic processes of rotaxane-like complexes. J. Tiburcio

11:50 **INOR 676.** New class of energetic chromophores for optical initiation of explosives: Transition metal complexes of explosive tetrazines. J.M. Vauthier, T.W. Myers, D.E. Chavez, S.K. Hanson, R.J. Scharff

12:10 **INOR 677.** Structured materials from a supramolecular approach. A. Try, M. Hashemi Karouei

## TUESDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 30B

**Undergraduate Research at the  
Frontiers of Inorganic Chemistry**
**Organometallic Chemistry**

Financially supported by IONIC (*Interactive Online Network of Inorganic Chemists*)

H. J. Eppley, C. Nataro, *Organizers*

J. P. Lee, *Presiding*

1:30 **INOR 678.** Catalytic interconversion of primary amines and nitriles by an iridium pincer complex. D.A. Laviska

1:50 **INOR 679.** Alkane dehydrogenation with (supercritical)Phebox)Ir(OAc)(X) complexes. Z.H. Syed, Y. Gao, C. Guan, A.S. Goldman, K.I. Goldberg

2:10 **INOR 680.** Carbon monoxide activation by metal cyano carbonyls. D. Shlian, J. Alboucal, M. Stock, M. Khaloo, J. Jiang

2:30 **INOR 681.** Structural characterization and electrochemical properties of nickel(II) complexes bearing sterically bulky hydrotris(3-phenyl)- and hydrotris(3-tert-butylpyrazol-1-yl)borato ligands. A.K. Frampton, K. Gartland, N.A. Piro, W.S. Kassel, W.G. Dougherty

2:50 Intermission.

3:05 **INOR 682.** Synthesis and characterization of cyclopentadienyl- and pentamethylcyclopentadienyl-Co(II) mixed sandwich compounds containing either tridentate nitrogen or sulfur donor macrocycles. J.P. Lee, P.A. Dean, K.R. Henson, T.P. Latendresse

3:25 **INOR 683.** Structure, bonding, and reactivity of d<sup>9</sup> dioxolene and iminoxolene molybdenum and titanium complexes. T. Marshall-Roth, S.N. Brown

3:45 **INOR 684.** Sudo make me a sandwich complex: Terrifying true tales of organometallic palladium chemistry with undergraduates. S.K. Hurst

4:05 **INOR 685.** Oxidation of a coordinated bis(phosphino)ferrocene ligand. C. Nataro

4:25 **INOR 686.** 4-pyridonate ligands: A pi-basic approach to cleaving C-H bonds with platinum group metals. N. Williams, T. Mortvedt, E. Nesbitt, A. Sullivan, L.A. Watson

4:45 Concluding Remarks.

## Section B

San Diego Convention Center  
Room 30C

**Transition Metal Chemistry in  
DNA & RNA Regulation**

P. Chen, *Organizer*

S. L. Michel, *Organizer, Presiding*

D. Wilcox, *Presiding*

1:30 **INOR 687.** What determines metal specificity and metal affinity of a DNA binding transcriptional de-repressor? N. Robinson

2:00 **INOR 688.** Electron paramagnetic resonance spectroscopy characterizes structural and dynamics features of CueR-DNA-Cu(I) complex. S. Ruthstein

2:30 **INOR 689.** Disruption of zinc finger structure and function upon substitution with copper(I). K.E. Splan, B.T. Buse, A.M. Blumenreich, M.D. Storlie

3:00 Intermission.

3:20 **INOR 690.** Metal coordination and DNA interaction studies of classical and non-classical zinc fingers. S. Lee, S.L. Michel

3:50 **INOR 691.** Thermodynamics of metal ions binding to DNA-binding protein domains. D. Wilcox

4:20 **INOR 692.** Persulfidation of tristetraprolin by hydrogen sulphide. M. Lange, G.D. Shimberg, L. Marko, S.L. Michel, M. Filipovic

## Section C

San Diego Convention Center  
Room 30D

**Metal-Oxygen Oxidants in Synthesis &  
Biology: Beyond Metal-Oxo Species**

M. T. Kieber-Emmons, *Organizer*

T. A. Jackson, *Organizer, Presiding*

1:30 **INOR 693.** Kinetic and spectroscopic interrogation of a promiscuous thiol dioxygenase: 3-mercaptopropionic acid dioxygenase. B. Subedi, J. Crowell, S. Sardar, B.S. Pierce

1:55 **INOR 694.** Intermediates in hydrocarbon oxidations catalyzed by bio-inspired nonheme iron catalysts. L. Que, W. Oloo

2:20 **INOR 695.** Electrochemistry to probe the reactivity of metal-(hydro)peroxy species derived from reductive activation of O<sub>2</sub>. E. Anxolabehere, F. Banse, H. Ching, C. Costentin, H.E. Colmer, P. Dorlet, T.A. Jackson, C. Polcar, M. Robert, N. Segaud, K. Senechal

2:45 **INOR 696.** Tuning the metal-dioxygen, -oxo, -hydroxo, and ligand reactivity landscape in heme-type complexes. D.P. Goldberg, H.M. Neu, G. Baglia, J. Zaragoza

3:10 **INOR 697.** Correlation between the structural, spectroscopic, and kinetic parameters of reactive Mn-peroxy complexes. J. Kovacs, J. Rees, M.K. Coggins, A. Johansen

3:35 Intermission.

3:45 **INOR 698.** Superoxonickel complexes as oxidants. C.G. Riordan, W. Green

4:10 **INOR 699.** Modeling catalytic intermediates of the thiol dioxygenases. A.T. Fiedler, A. Fischer

4:35 **INOR 700.** Involvement of metal-superoxo species in iron and copper C-H activating enzymes. J. Klinman, H. Zhu, S. Peck, F. Bonnot, W. van der Donk

5:00 **INOR 701.** Progress in the generation and characterization of primary copper(I)-dioxygen adducts. K.D. Karlin

Technical program information  
known at press time.

The official technical program  
for the 251st ACS National  
Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)



**5:25 INOR 702.** Differential oxidase and oxygenase reactivities in *de novo* Due Ferri proteins. **A.J. Reig**, R. Snyder, S.C. Butch, W.F. Degrado, E.I. Solomon

## Section D

San Diego Convention Center  
Room 30E

### Memorial Symposium Honoring Karen J. Brewer

*Cosponsored by HIST†  
Financially supported by  
Washington State University*

M. T. Mongelli, *Organizer*

S. C. Rasmussen, *Organizer, Presiding*

**1:30 INOR 703.** Asymmetric bimetallic ruthenium complexes as potential photodynamic therapy agents. **M.T. Mongelli**, K. Thomas, A. Abdulkarim, M. LaCorte, J. Osei-Fosu

**2:00 INOR 704.** Ultrafast photophysics of mixed-metal polyazine supramolecules: Os(II) or Ru(II) with Rh(III). **D.F. Zigler**, Z.A. Morseth, T. Canterbury, J.A. Rodriguez Corrales, K.S. Brewer, J.M. Papanikolas

**2:30 INOR 705.** Ru, Rh, Ru water reduction photocatalysts in ion containing polymers. E.M. Naughton, T. Canterbury, **R.B. Moore**

**3:00 INOR 706.** Emission study of Ir<sup>III</sup>Cp\* compounds and synthesis of Ru<sup>II</sup>-Ir<sup>III</sup>Cp\* bimetallic complex designed for anticancer activity. **S. Molnar**, J.S. Merola, A. Smith

**3:30** Intermission.

**3:45 INOR 707.** Ruthenium and rhodium based anticancer compounds with diimine ligands. **S. Saha**, B. Pena, A. David, C. Turro, **K.R. Dunbar**

**4:15 INOR 708.** Photocatalyst design with consideration for ligand sigma-donating ability and substrate accessibility to catalytically active site. **H.J. Sayre**, K.S. Brewer, C. Turro

**4:45 INOR 709.** Synthesis and characterization of a novel Ru(II)-polypyridyl complex with carboxylate functional groups for supramolecular water reduction photocatalyst-polymer assemblies. **K.M. Felice**, K.S. Brewer, R.B. Moore

**5:15 INOR 710.** Dipyrromethenes bridging ruthenium(II) polypyridyl complexes: Photophysical and electrochemical properties, and DNA photo-induced reactions. **S. Swavey**

## Section E

San Diego Convention Center  
Room 31A

### Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

I. Garcia-Bosch, *Presiding*

**1:30 INOR 711.** Withdrawn.

**1:50 INOR 712.** Synthesis and structural characterization of a  $\beta$ -lactam adduct of a synthetic analogue of a metallo- $\beta$ -lactamase. **S. Rucolo**, G. Parkin

**2:10 INOR 713.** Synthetic modeling of mono-iron hydrogenase (Hmd): Utility of an anthracene scaffold for the facial display of biomimetic donors. **M.J. Rose**, J. Seo, T.A. Manes

**2:30 INOR 714.** Comparison of Mn<sup>IV</sup>(O) and Cr<sup>VI</sup>(O) complexes in HAT and PCET reactivity. **R.A. Baglia**, K. Prokop-Prigge, H.M. Neu, M. Siegler, D.P. Goldberg

**2:50 INOR 715.** Macrocyclic rebellion: TMC Cu(I) conformations lead to dicopper peroxo species with unique spectroscopic, structural, and chemical properties. **I. Garcia-Bosch**, D.E. Diaz, K.D. Karlin

**3:10** Intermission.

**3:20 INOR 716.** Surprise comes twice: Coordinating a thioether-cholesterol ligand to the non-toxic [Ru(tpy)(bpy)(H<sub>2</sub>O)]<sup>2+</sup> complex leads to a highly cytotoxic compound with an unexpected mode-of-action. **B. Siewert**, V.H. van Rixel, E.J. van Rooden, M.J. Moester, S.L. Hopkins, F. Ariese, S. Bonnet

**3:40 INOR 717.** Termolecular proton-coupled electron transfer reactions: Separating proton and electron transfer effects. **W.D. Morris**, J.M. Mayer

**4:00 INOR 718.** Factors influencing acid plus reductant O-O cleavage in low-spin heme-peroxo-copper complexes. **S.M. Adam**, K.D. Karlin

**4:20 INOR 719.** Artificial metalloenzymes with metal-binding motifs made from canonical amino acids. **J. Eppinger**, J. Fischer, M. Groll

**4:40 INOR 720.** Recent advances into mechanistic insights gained from structural and spectroscopic studies of biosynthetic models of nitric oxide reductases. **S. Chakraborty**, J. Reed, M. Ross, H. Matsumura, P. Moenne Loccoz, T. Sage, C. Schultz, Y. Lu

## Section F

San Diego Convention Center  
Room 31B

### Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

L. M. Mirica, D. V. Peryshkov, *Presiding*

**1:30 INOR 721.** Remote multi-proton storage within a pyrrolide-pincer type ligand. **S. Nadif**, M.E. O'Reilly, I. Ghiviriga, K.A. Abboud, A.S. Veige

**1:50 INOR 722.** Metal- and ligand-centered reactivity of *B*-metalated carbonyl pincer complexes of rhodium. **D.V. Peryshkov**, B.J. Eleazer

**2:10 INOR 723.** Variable binding modes of pyridine in molybdenum complexes supported by novel P-pyridine-P ligands. **R. Wan**, K. Horak, J.A. Buss, T. Agapie

**2:30 INOR 724.** Heavy metal for organometallic reactions: Palladium-phosphonium systems and their catalytic potential. **S.M. Kruse**, T. Haden, W. Cross Lopez, J. Herring, S.K. Hurst

**2:50 INOR 725.** Controlling the reactivity of high-valent Pd and Ni complexes with flexible multidentate ligands. **L.M. Mirica**

**3:10 INOR 726.** Extending the  $\pi$ -system: Modulation of arene and phosphine donor lability in polyarene diphosphine-supported molybdenum complexes and its application to small molecule reactivity. **C. Low**, J.A. Buss, T. Agapie

**3:30 INOR 727.** Donor-functionalized cyclic (alkyl)(amino)carbenes (CAACs): Synthesis, coordination, and catalysis. **J. Chu**, D. Munz, M. Melaimi, R. Jazzar, G. Bertrand

**3:50 INOR 728.** 6-membered Cyclic (alkyl)(amino)carbenes as strong donor ligands for transition-metals in catalysis. **C. Weinstein**, G. Junor, M. Melaimi, G. Bertrand

**4:10 INOR 729.** Bimetallic scaffolds for CO<sub>2</sub> reduction. **C.T. Saouma**, L. Mueller

**4:30 INOR 730.** Outer coordination sphere effect on Rh(diphosphine)<sup>+</sup> complexes catalyzed CO<sub>2</sub> hydrogenation. **S. Ni**, **L. Dang**

**4:50 INOR 731.** Role of the chemically non-innocent ligand in the catalytic formation of hydrogen and carbon dioxide from methanol and water with the metal as the spectator: A mechanism study. **H. Li**, M.B. Hall

## Section G

San Diego Convention Center  
Room 31C

### F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Francois P. Gabbai

J. D. Hoefelmeyer, T. W. Hudnall, *Organizers*

H. Wang, *Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 732.** New bond activations, transformations, and catalysis in transition metal-silicon chemistry. **T. Tilley**

**1:55 INOR 733.** Dinuclear gold ylide complexes as catalysts for C—C bond forming reactions. **C.R. Wade**, B. Reiner

**2:15 INOR 734.** Pyrrole-based flexidentate phosphine, polypyrazolyl, and Schiff base ligands for transition and alkali metal complexes. **G. Mani**

**2:35 INOR 735.** N,O-chelates becoming unhinged. New perspectives in metal-ligand cooperativity. **M.W. Drover**, J. Love, **L. Schafer**

**2:55** Intermission.

**3:05 INOR 736.** Magnetization dynamics in heterometallic lanthanide: Transition metal complexes. **M. Nippe**

**3:25 INOR 737.** Sulfur directed acid-base pairs as guiding principle for adjudicating guilt vs. innocence in heterobimetallic complexes derived from metalodithiolate ligands. **M.Y. Darensbourg**, P. Ghosh, N. Wang, S. Ding

**3:45 INOR 738.** Molecular titanium nitrides: Synthesis, characterization, and reactivity studies. **D.J. Mindiola**

**4:05 INOR 739.** New boryl-centered pincer ligands and their complexes. **O. Ozerov**, W. Shih, W. Gu, N. Bhuvanesh, S.D. Timpa, M.C. MacInnis

## Section H

San Diego Convention Center  
Room 32A

### Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

A. Choudhury, *Presiding*

**1:30 INOR 740.** Systematical study of chemical compositions in open framework chalcogenides. **X. Chen**, X. Bu, P. Feng

**1:50 INOR 741.** New insights into the structure, properties, and chemistry of Cu<sub>4</sub>SnS<sub>8</sub>. **A. Choudhury**, S. Mohapatra, H. Yaghoobnejad Asl

**2:20 INOR 742.** Structural variability and thermoelectric properties of transition metal-pnicogen clathrates. **J. Dolyuniuk**, J. Wang, K. Kovnir

**2:40 INOR 743.** Phase formation in mixed divalent hexaborides. **J.T. Cahill**, M. Alberg, S. Misture, D. Edwards, V.R. Vasquez, O. Graeve

**3:00 INOR 744.** Using computer generated decision trees to understand structural adaptivity in [V<sub>2</sub>O<sub>6</sub>(SeO<sub>3</sub>)<sub>3</sub>]<sup>2n-</sup> layered compounds. **P. Adler**, A.J. Norquist, R. Xu

**3:20** Intermission.

**3:35 INOR 745.** Hybrid main-group halide perovskites: Local structure and disorder. **D.H. Fabini**, H. Evans, G. Laurita, C. Stoumpos, M.G. Kanatzidis, R. Seshadri

**3:55 INOR 746.** Exploring degradation of Van Gogh yellow from the inside: A computational study on the PbCr<sub>1-x</sub>S<sub>2</sub>O<sub>6</sub> solid solution. **A.B. Muñoz-García**, A. Massaro, M. Pavone

**4:15 INOR 747.** Structural analysis of the mixed sorosilicate phosphor, Ba<sub>4</sub>Si<sub>6</sub>O<sub>17</sub>·Eu<sup>2+</sup>. **C. Cozzan**, G. Laurita, R. Seshadri

**4:35 INOR 748.** Optical and scintillation properties of metal oxide nanoparticles. **Y. Mao**, M. Pokhrel

**4:55 INOR 749.** Supersaturation of complex ions in crystal growth of ZnO, CaCO<sub>3</sub> and Ca<sub>2</sub>H(PO<sub>3</sub>)<sub>3</sub>. **M.C. Gelabert**, D. Thibault, J. Zinna

## Section I

San Diego Convention Center  
Room 32B

### Environmental & Energy- Related Inorganic Chemistry

S. A. Koch, *Organizer*

S. R. Foley, L. J. Lyons, *Presiding*

**1:30 INOR 750.** Acetic acid process: A viable alternative to cyanide and aqua regia for leaching gold from primary and secondary sources. **S.R. Foley**, H. Salimi, L. Moradi

**1:50 INOR 751.** Homogeneous catalysis of the electrochemical reduction of CO<sub>2</sub> by Re(I) complexes. Role of the pyridine ligands. **J. Nganga**

**2:10 INOR 752.** Withdrawn.

**2:30 INOR 753.** Evidence of a through-bond mechanism for photo-initiated interfacial electron transfer at dye-sensitized titanium dioxide. **G.J. Meyer**, K. Hu, W.B. Swords, E. Piechota, R. Sampaio, C.P. Berlinguette

**2:50 INOR 754.** CO<sub>2</sub> reduction using cobalt aminopyridine complexes. **A. Chapovetsky**, S.C. Marinescu

**3:10 INOR 755.** Design principles for selective CO<sub>2</sub> reduction catalysis. **A. Hall**, A. Wuttig, Y. Yoon, **Y. Surendranath**

**3:30** Intermission.

**3:40 INOR 756.** Promoting interfacial photoinduced iodide oxidation: Halogen bonding at the interface. **W.B. Swords**, S.J. Simon, F.G. Parlani, K. Hu, G.J. Meyer, C.P. Berlinguette

**4:00 INOR 757.** Withdrawn.

**4:20 INOR 758.** Improved ion transport using silyl electrolytes for lithium-ion battery applications. **L.J. Lyons**

**4:40 INOR 759.** DFT study of an unusual proton-relay role for Cp\* in hydrogen evolution catalysis. **S.I. Johnson**, S.L. Corona, J.D. Blakemore, J.R. Winkler, H.B. Gray, W.A. Goddard

**5:00 INOR 760.** Immobilization of molecular electrocatalysts in a coordinating membrane to enhance their activity and selectivity for CO<sub>2</sub> reduction. **W.W. Kramer**, **C.C. McCrory**

**5:20 INOR 761.** High-pressure hydrogen evolution by the decomposition of formic acid in the presence of IR catalyst. **H. Kawanami**, M. Iguchi, Y. Himeda, Y. Manaka, K. Matsuoka

**5:40 INOR 762.** Conversion of cellulosic biomass to fuels and chemicals. **C.L. Marshall**

## Section J

San Diego Convention Center  
Room 33A

Frontiers in Heavy Element  
Inorganic Chemistry

Cosponsored by NUCL

D. L. Clark, D. K. Shuh, L. Soderholm,  
Organizers

J. E. Bercaw, Presiding

**1:30 INOR 763.** Thorium, uranium, f-orbitals, and multiple bonds: These are just a few of Al's favorite things. J.L. Kiplinger

**1:50 INOR 764.** Heavy element molecular magnetism: Exploiting spin-orbit effects and anisotropic coupling. K.R. Dunbar, F.J. Birk, D. Kempe, K. Schulte

**2:10 INOR 765.** Unusual case where plutonium is simpler than cerium. T.E. Albrecht-Schmitt

**2:30 INOR 766.** Mercury-selenium interactions and the protolytic cleavage of Hg-C bonds induced by 1-methyl-1,3-dihydro-2H-benzimidazole-2-selone. J. Palmer, P. Quinlivan, K. Yurkerwicz, G. Parkin

**2:50 INOR 767.** Early transition metal complexes with bicyclic guanidinate ligands: Syntheses, structures, and LMCT spectrofluorimetry. J.R. Olson, C.J. Jensen, D.C. Swenson, L. Messerle

**3:10** Intermission.

**3:30 INOR 768.** Aqueous solution route to actinide thin films. T.M. McCleskey, B. Scott, E. Bauer, S.A. Kozimor, R.L. Martin, A. Burrell, Q. Jia

**3:50 INOR 769.** Uranium imido complexes: A window into uranium bonding and reactivity. J.M. Boncella, N.C. Tomson, A. Tondreau, M. Winston, B. Scott

**4:10 INOR 770.** Spectroscopic studies of metal-metal bonding. W.H. Woodruff

**4:30 INOR 771.** Multiple bonds: Some sojourns in heavy-metal chemistry with Al Sattelberger. B.E. Bursten

**4:50 INOR 772.** Solar-to-fuels conversion by the artificial leaf. D.G. Nocera, M. Huynh, D.K. Bediako, N. Li, C. Liu

## Section K

San Diego Convention Center  
Room 33B

Organometallic Chemistry:  
Applications to Materials  
& Polymer Science

N. S. Radu, Organizer

G. Du, A. M. Spokoyny, Presiding

**1:30 INOR 773.** Metal-free, boron-rich cluster cationic styrene polymerization photocatalysts. A.M. Spokoyny

**1:50 INOR 774.** Synthesis of novel luminescent PAHs featuring a boron ring junction. K.A. Schickedanz, M. Wagner

**2:10 INOR 775.** Zipping up alkynes with zirconocene: Toward a general route to functionalized expanded helicenes and cycloarenes. G.R. Kiel, T. Tilley

**2:30 INOR 776.** Copolymerization of cyclic esters and epoxides via redox-switchable Zr catalyst. S. Quan, P. Diaconescu

**2:50 INOR 777.** Ligand electronic effect in late transition metal catalyzed olefin polymerization and copolymerization. C. Chen, M. Chen, S. Dai

**3:10 INOR 778.** Insight into the mechanism and reactivity of ruthenium ROMP catalysts at the single-molecule and single-particle levels. Q. Easter, V. Trauschke, S.A. Blum

**3:30 INOR 779.** Withdrawn.

**3:50 INOR 780.** Stereoselective synthesis of biodegradable polyesters catalyzed by chiral zinc amido-oxazolinone complexes. G. Du, S. Abbina, V. Chidara, S. Bian

**4:10 INOR 781.** Tuning solid-state emission of push-pull chromophores via embedding into metal-organic materials. L.M. Lifshits, M. Zeller, J.K. Klosterman

**4:30 INOR 782.** Using bulky terphenyl thiolates as capping ligands for gold thiolate nanoclusters. N. Mendelson, J.S. Figueroa

**4:50 INOR 783.** Carboxylic acid functionalized polycarbonates from CO<sub>2</sub>: A versatile platform for the synthesis of functional polycarbonates. Y. Wang, F. Tsai, D.J. Darensbourg

**5:10 INOR 784.** From molecules to materials: The effect of precursor design on functional device synthesis. C.E. Knapp, C.J. Carmalt

## Section L

San Diego Convention Center  
Room 33C

Supramolecular Chemistry: A  
Crown & Anchor Approach

Cosponsored by ORGN

Financially supported by Elsevier,  
Supramolecular Chemistry, RSC

A. E. Gorden, Organizer

P. A. Gale, Presiding

**1:30 INOR 785.** Cation-dependent gold recovery with  $\alpha$ -cyclodextrin facilitated by second-sphere coordination. Z. Liu, J.F. Stoddart

**2:00 INOR 786.** Water-soluble porphyrinoids as G-quadruplex binders and telomerase inhibitors. H. Furuta, Y. Ikawa, S. Katsumata

**2:20 INOR 787.** Imine donor ligands for actinide selective coordination and sensing materials. A.E. Gorden

**2:40 INOR 788.** Metal directed formation of self-assembly supramolecular structures and materials from acyclic ligands. T. Gunlaugsson

**3:00 INOR 789.** Supramolecular behaviors in metal-macrocyclic frameworks. M. Shionoya

**3:20** Intermission.

**3:40 INOR 790.** Mathematical control in the self-assembly of giant M<sub>n</sub>, L<sub>2n</sub> polyhedral complexes. M. Fujita

**4:10 INOR 791.** Synthesis and coordination chemistry of molecular and polymeric Wurster-type receptors: Redox-active hosts for cations and anions. J.W. Sibert

**4:30 INOR 792.** Organizing mechanically interlocked molecules to function inside metal-organic frameworks. K. Zhu, N. Vukotic, S.J. Loeb

**4:50 INOR 793.** Calix[4]pyrroles: From ion pair receptors to molecular switches and self-assembled materials. J.L. Sessler

**5:10** Concluding Remarks.

## TUESDAY EVENING

## Section A

San Diego Convention Center  
Hall D

Bioinorganic Chemistry: DNA,  
RNA & Inorganic Drugs

S. A. Koch, Organizer

**6:00 - 8:00**

**INOR 794.** Synthesis, characterization, and anticancer activity of gold(III) complexes with (1R,2R)-(-)-1,2-diaminocyclohexane. A.A. Isab

**INOR 795.** Antifungal and anti-parasitic transition metal complexes of linked, bridged tetraazamacrocyclic. T.J. Hubin, S.J. Archibald, M. Jacob, B. Tekwani, F. Khan

**INOR 796.** Unsymmetric bis-tetraazamacrocyclic transition metal complexes as CXCR4 antagonists. D.G. Jones, C. Baker, C.D. Garcia, A.N. Walker, D. Schols, P. Symmers, S.J. Archibald, T.J. Hubin

**INOR 797.** Binding events of zinc finger proteins. E. Joung, S. Park, S. Lee

**INOR 798.** Synthesis, characterizations, and DNA-binding and cytotoxicity studies of organorhenium naproxenone complexes. S. Azemati, S. Pramanik, S.K. Mandal, A.J. Winstead

**INOR 799.** Kinetic-mechanistic studies on methemoglobin generation by biologically active thiosemicarbazone iron (III) complexes. M.T. Basha, P.V. Bernhardt

**INOR 800.** Investigation of bimetallic asymmetric ruthenium(II) complexes and their DNA interactions. K. Thomas, M.T. Mongelli

**INOR 801.** Withdrawn.

**INOR 802.** Ruthenium-caged P450 inhibitors for dual antitumor activity. A. Zamora, E. Wachter, D.K. Heidary, C.A. Denning, E.C. Glazer

## Section A

San Diego Convention Center  
Hall D

Coordination Chemistry:  
Synthesis & Characterization

S. A. Koch, Organizer

**6:00 - 8:00**

**INOR 803.** Synthesis, characterization, and CO-releasing properties of rhodium carbonyl complexes containing terpyridine derivatives ligand. B. Zhu, X. Wei, Q. Zhao, J. Xie

**INOR 804.** Bidirectional non-innocence of formazanate in ruthenium complexes. A. Mandal, G.K. Lahiri

**INOR 805.** Synthesis and characterization of new molybdenum(V) complexes with *N*-salicylidene-2-aminothiophenol. N.V. Kolacia

**INOR 806.** Reaction dynamics of simple polyoxometalate ions in water. M.R. Spriet, E.M. Villa

**INOR 807.** Organometallics complexes with triazene ligands functionalized with hindered imidazoles. J. Camarena, V. Miranda Soto, M.P. Parra Hake, D.B. Grotjahn

**INOR 808.** Mixed-valence triruthenium clusters with hydrophobic ligands. M.J. Glover, D.J. SantaLucia, A.L. Eckermann

**INOR 809.** Four new coordination polymers based on p-Terphenyl-3,3',5,5'-tetracarboxylic acid: Syntheses, structures, and photoluminescent properties. C. Zheng

**INOR 810.** Investigating the robustness of disassembly-reassembly methods for the formation of heterometallic MOFs. A. Marton, S. Baudron, M. Hosseini

**INOR 811.** Organometallic complexes of a new electron-rich diketiminato ligand. M.A. Land, K.E. Ylijoki, K. Robertson, P.T. Lee, D. Vidovic, J.A. Clyburne

**INOR 812.** Isomerism and magnetic characteristics of iron heteroscorpionate. K. Demaree, P. Desrochers

**INOR 813.** Synthesis, structural characterization and luminescent behavior of heteroleptic zinc(II) complexes employing novel asymmetric *N,N*-heterocyclic ligands. H. Schoechert, I.M. Klein, S. Kraft, K.L. Cunningham, J.T. Mague, W.F. Wacholtz

**INOR 814.** Computational modeling and analysis of stable 14 electron hemi-chelated Pd-Cr complexes. D. Anstine, J. Djukic

**INOR 815.** Biologically inspired manganese cluster chemistry. D.J. Jovine, M. Zdilla, S. Vaddypally

**INOR 816.** Investigating the electronic and structural properties of trans Co<sup>III</sup>-cyclam acetylides. S.D. Banziger, T. Ren

**INOR 817.** Synthetic strategy for multi-layered Pd(II) complexes via transannular  $\pi$ - $\pi$  interactions. H. Lee, O. Jung

**INOR 818.** Synthesis and crystallographic study of zinc and mercury complexes with a three-N-donor asymmetric pyridine-amine ligand 2,9-di(pyridin-2-yl)-1,3,6-triazabicyclo[4.2.1]nonane. M. Hakimi

**INOR 819.** Novel ligands for organometallic catalysis. B. Wicker, K.M. Gass, M.T. St. Lawrence, Y. Wang, J.H. Davis, R. Sykora

**INOR 820.** Square-planar and octahedral isomers of a Ni(II) complex with a labile sulfur-centered ligand. T. Chivers, J. Konu, S. Haggman, A. Mansikkamaki, I.S. Morgan, H. Tuononen, R. Thirumoorthi, M. Lahtinen

**INOR 821.** Progress towards the synthesis of ligand-free copper(I) carboxylates. H.M. Kidd, S.L. Sandri, A.T. Royappa

**INOR 822.** Synthesis, structural characterization, and magnetic properties of tetranuclear copper(II) and cobalt(II) complexes of Schiff base ligands. Metal catalyzed formation and stabilization of acetal. S.S. Tandon, S.D. Bunge, L.K. Thompson

**INOR 823.** Synthesis and structural characterization of dinuclear 3d-4f complexes, dinuclear (Eu), tetranuclear (Ni), and hexanuclear (Dy) complexes of a Schiff base ligand. S.D. Bunge, S.S. Tandon, V. Hogan, R.R. Boyle

**INOR 824.** Synthesis of 3-functionalized verdazyls. T. Pan, D.J. Brook, A. Herrera

**INOR 825.** Effect of intermolecular forces and linker on metal organic framework secondary structure. M. Johnson, B.A. Doyle, C. Bauer

**INOR 826.** Coordination chemistry of sulfur and selenium oxidized derivatives of tris(2-pyridyl)phosphine with Co(II), Ni(II), Cu(II), Zn(II), and Cd(II) nitrates. A. Bevan, C. Fairfield, A.K. Frampton, D. Pericic, N.A. Piro, W.S. Kassel

**INOR 827.** Solventless and solvent-mediated synthesis and optoelectronic properties of brightly luminescent Ag(I) and Cu(I) azolate/quinoxaline complexes. A.R. Hinkle, K. Reyes, K. Maxwell, S. Hutcheson, M. Wilk, V. Nesterov, M. Omary

**INOR 828.** Synthesis and characterization of Cu(I) and Ag(I) tetrazolate complexes toward active or passive components of electronic devices. R.M. Almotawa, A. Cimino, V. Nesterov, M. Omary, M.A. Omary

**INOR 829.** Synthesis, characterization, and reactivity of small, solvent supported molybdenum clusters. S.C. Haefner

**INOR 830.** Synthesis, single crystal X-ray crystallography and computational studies of Co(II) complex of trimethoprim, [Co(TMP)<sub>2</sub>S<sub>2</sub>]. P.A. Aijbade

**INOR 831.** Synthesis, characterization, and coordination chemistry of poly(2-pyridyl-phosphines) bridged by various linkers. C. Fairfield, N.A. Piro, W.S. Kassel

INOR **832**. Mid-to-late first-row transition-metal complexes of tris(2-pyridyl) phosphine (PPy<sub>3</sub>) and its oxide. **A. Spitzer**, C. Fairfield, A.K. Frampton, N.A. Piro, W.S. Kassel

INOR **833**. Synthesis towards symmetric substituted verdazyl 2 x 2 grid complexes. **B. Ploof**, D.J. Brook, C. Fleming, E. Johnson

INOR **834**. Synthesis of new imine-containing ligand scaffolds for metalloenzyme mimics. **T.M. Dunn**, J.A. Dopke, R.J. Staples

INOR **835**. Bulk synthesis of TCNQ radical anion salts with chemical vapor deposition studying their crystal structure for applications in memory devices. **G.N. Gonzalez**

INOR **836**. Withdrawn.

INOR **837**. Structural studies of manganese carbonyl complexes derived from an anthracene scaffold appended with pyridine, aryl-thioether and aryl-thiolate donors. **T.A. Manes**, M.J. Rose

INOR **838**. Synthesis and electronic description of tetra- and pentametallic, mixed-metal, mixed-valent manganese-cobalt oxido clusters. **A. Nguyen**, D. Suess, L.E. Darago, D.S. Levine, T. Tilley

## Section A

San Diego Convention Center  
Hall D

### Electrochemistry

B. L. Lucht, *Organizer*

6:00 - 8:00

INOR **839**. Consequences of reduction of (T(p-X)PP)Ru(NO)Cl (X= H, Cl, Me, OMe). **J. Zink**, M.J. Shaw, G.B. Richter-Addo

INOR **840**. Analysis of a four H-bond array using cyclic voltammetry: Introducing a new redox center to strengthen dimerization. **B. Tamashiro**, G. Darzi, D.K. Smith

INOR **841**. Proton-coupled electron transfer in an electroactive three hydrogen bond DDA array capable of binding an AAD guest. **R. He**, D.K. Smith

INOR **842**. Novel approaches to the chemical application of electrochemical materials for conducting materials. **E.J. Parish**, M. Hsiao, H. Honda, T. Wei

INOR **843**. Design of a microfluidic electrochemical DNA/RNA hybridization sensor. **J.M. Philippe**, M.C. Buzzeo

INOR **844**. Fluorinated porphyrin as a metal-free electrocatalyst for hydrogen generation. **Y. Wu**, D. Villagran

INOR **845**. Functionalization of Si(111) with sterically spaced molecular wires intercalated within ALD-deposited metal oxides for electron transfer applications. **F. Konopka**, M.J. Rose

## Section A

San Diego Convention Center  
Hall D

### Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **846**. Kinetics of the electrochemical reduction of CO<sub>2</sub> by Re(I) bipyridine complexes: Role of solvents and electrolytes. **J. Nganga**

INOR **847**. Probing structures, spin states, redox properties, and thermodynamics of Co-OEC analogs using broken-symmetry density functional theory. **S. Niu**, E.N. Brothers, M.B. Hall

INOR **848**. Withdrawn.

INOR **849**. Synthesis and study of the photophysics, excited-state properties, and photolabilization pathways of cyclometalated Ir(III)-Pt(II) and Ir(III)-Ir(III) bimetallic complexes bridged by dipyrrolylpyrazine (dpp). **Y. Cho**, S. Kim, D. Cho, H. Son, S.O. Kang

INOR **850**. Oxygen reduction reaction electrocatalysts based on LaFexCo<sub>(1-x)</sub>O<sub>3</sub> thin films prepared by spray-pyrolysis. **D. Dervishogullari**, L.R. Sharpe

INOR **851**. Ionic conductivities of silyl and carbonate blend electrolytes. **L.J. Lyons**, I. Dixon-Anderson, T. Robinson

INOR **852**. Ni-based electrochemical catalysis for water splitting. **Y. Wang**, G. Wang, Y. Huang, X. Duan

INOR **853**. Essential cation-π interaction in a psychrophilic electron transfer protein. **N. Dalchand**, K.S. Montero, G.J. Salerno, M.C. Buzzeo, J.S. Magyar

INOR **854**. Improved electrical energy storage using nanofiller modified flywheels. **T.J. Boyle**, T.N. Lambert, N.S. Bell, W.K. Miller

INOR **855**. Withdrawn.

INOR **856**. Measuring siliceous zeolites for Xe/Kr separations. **A. Sharma**, L. Nemeth, K.V. Lawler, P. Forster

INOR **857**. Development of a photochemical and electrochemical detector of thiocyanate in marine environments. **A.R. McCabe**, C.A. Sweet, C.R. Rockwell, B.S. Sheetz, C. Murphy

INOR **858**. Ecotoxicity study during DEET degradation by ozone. **L. Li**, J. Lee, K. Yeung

INOR **859**. Molecular orbital engineering of a panchromatic cyclometalated Ru<sup>II</sup> dye for p-type dye sensitized solar cells. **M. He**, Z. Ji, Z. Huang, Y. Wu

INOR **860**. Methionine ligand substitution processes provide dynamic stabilization of a psychrophilic metalloprotein. **N.K. Asous**, S.J. Barth, S.K. Lone, K.S. Montero, M.C. Buzzeo, J.S. Magyar

INOR **861**. Metal uptake and regulation in a methanogenic archaeon from the tar pits at Rancho La Brea, Los Angeles. **J. Lee**, P.M. Magyar, J.S. Magyar

INOR **862**. Overexpression, purification, and characterization of a cytochrome P450-type alkane monooxygenase from a psychrophilic marine bacterium. **G.J. Salerno**, J.S. Magyar

INOR **863**. Overexpression and purification of a putative iron uptake protein from the marine diatom *Phaeodactylum tricornutum*. **J. Chou**, K. Farrell, E.M. Shoefelt, B.C. Bostick, J.S. Magyar

INOR **864**. Protein delivery of a Ni catalyst to photosystem I for light-driven hydrogen production. **S.C. Silver**, J. Niklas, O. Poluektov, P. Du, D.M. Tiede, L.M. Utschig-Johnson

INOR **865**. Water splitting through metal oxide photocatalysts: Effect of shape anisotropy, nature of co-catalysts, and surface properties. **K. Latimer**, D. Daniels, K. Senevirathne

INOR **866**. Organosilyl electrolyte conductivities, lithium transference numbers, and solvation shells via PFG-STE NMR diffusion experiments and their application in lithium-ion batteries. **C. Mulligan**, L.J. Lyons

INOR **867**. Optimization and characterization of high-performance CuFeMgW oxide based semiconductors for solar photocatalysis. **C.A. Sharpe**, L.R. Sharpe

INOR **868**. 3-D Interconnected mesoporous tantalum nitride as a novel water splitting photocatalyst. **H. Kang**, S.H. Tolbert

INOR **869**. Bioaccumulation of selenium in the model bryophyte *Physcomitrella patens*. **J. Carsella**, D.C. Crans, S.J. Bonetti, D. Lehmpuhl

INOR **870**. Post-synthetic alkylamine modification on metal-organic frameworks with isostructures for CO<sub>2</sub> capture. **H. Li**, H. Zhou

## Section A

San Diego Convention Center  
Hall D

### Inorganic Catalysts

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **871**. Chlorite dismutation to chlorine dioxide by an [Fe<sup>III</sup>-TAML] complex. **M. Ramachandra**, J. Park, S.D. Hicks, W. Nam, M.M. Abu-Omar

INOR **872**. Increasing ligand denticity: A strategy for a better water oxidation catalyst (WOC). **F. Saeedifard**, J.M. Kamdar, D.C. Mareluis, D.B. Grotjahn

INOR **873**. Improving the efficiency nickel-bisphosphine hydrogen gas production catalysts by lowering overpotential. **A.P. Cardenas**, E.S. Wiedner, M. Helm, A.M. Appel, M.J. O'Hagan

INOR **874**. Synthesis and reactivity of a secondary phosphine ligand with Ni(0) and Ni(II). **N.J. Downes**, T.W. Chapp

INOR **875**. Withdrawn.

INOR **876**. New metals (V, Pd, Ru) and new amide pendant-arms for cross-bridged tetraazamacrocyclic oxidation catalysts. **M. Gorbet**, G. Yin, T.J. Hubin

INOR **877**. Photocatalytic metal-organic frameworks for the aerobic oxidation of arylboronic acids. **X. Yu**, S. Cohen

INOR **878**. Efficient nickel-catalyzed transfer hydrogenation of ketones using ethanol as solvent and hydrogen donor. **N. Castellanos**

INOR **879**. Light-driven dual metal catalysis. **M. Gelwicks**

INOR **880**. Electrocatalytic materials composed of Earth-abundant elements for the hydrogen and oxygen evolution reactions. **J. Mondschein**, J.F. Callejas, C.F. Holder, J.M. McEaney, R.E. Schaak

INOR **881**. Unusual <sup>13</sup>C NMR shift in "tilted" n-heterocyclic carbene complexes explained. **L. Falivene**, L. Cavallo

INOR **882**. Understanding the distinctive electronic structure of Re and Ru tris(thiolate) complexes and its role in chemistry. **H. Tang**, M.B. Hall

INOR **883**. Design and investigations of peptidic platforms on the electrocatalytic reduction of carbon dioxide by a rhenium bipyridine-based complex. **S.A. Chabolla**, C.W. Machan, S. Sahu, E. Dellamaria, J. Yin, M.K. Gilson, F.A. Tezcan, C.P. Kubiak

INOR **884**. Observation and reactivity studies of an unusual RhI intermediate in H<sub>2</sub> evolution catalysis. **L. Aguirre Quintana**, H.B. Gray, J.R. Winkler, J.D. Blakemore

INOR **885**. Aqueous stability and catalytic HER activity of [(DHMP)<sub>2</sub>Ni][BF<sub>4</sub>]<sub>2</sub> under various pH conditions. **S. Ruelas**, C. Tsay, J. Yang

INOR **886**. Hydrodesulfurization of dibenzothiophene using bimetallic and trimetallic: Cobalt, nickel, tungsten sulfide. **D.F. Gonzalez**, J.S. Sollner, J. Parsons

INOR **887**. Aqueous solution palladium catalyzed Suzuki cross coupling reactions: The effect of base and base concentrations. **T. Olson**, J. Parsons

INOR **888**. Metal organic frameworks as catalysts for organic photoredox transformations. **M.W. Logan**, Y. Lau, Y. Zheng, M. Hettinger, R. Marks, M. Hosler, Y. Yuan, F. Uribe-Romo

INOR **889**. Mechanistic investigation of proton reduction by cobaloximes: Insight from H<sub>2</sub> oxidation kinetics. **S.A. Del Ciello**, J.R. Winkler, J.C. Peters, H.B. Gray

INOR **890**. Withdrawn.

INOR **891**. Molecular catalyst incorporation in conductive coordination polymer scaffolds for heterogeneous electrocatalytic carbon dioxide reduction. **G. Merlen**, M.L. Clark, S.A. Chabolla, C.P. Kubiak

## Section A

San Diego Convention Center  
Hall D

### Inorganic Spectroscopy

V. C. Popescu, *Organizer*

6:00 - 8:00

INOR **892**. Mössbauer spectroscopy and electronic structure of bimetallic iron-nitrosyl complexes. **V.C. Popescu**, M. Cohara, P. Ghosh, M.Y. Darenbourg

INOR **893**. Spectroscopic studies of five-coordinate cobalt (II) model complexes: Fluorine substituted hydroxamic acids. **C.D. James**, T. Kuehn, C.N. Worley, D.L. Tierney

INOR **894**. Large and affected by charge: Synthesis and analysis of binaphthoquinone and dibenzoxanthene compounds. **T. Haden**, S.M. Kruse, W. Cross Lopez, J. Herring, S.K. Hurst

INOR **895**. Group 5 (VB) metals speciation in fused chlorides: A spectroelectrochemical study. **I.B. Polovov**, V.A. Volkovich, B.D. Vasin, T.R. Griffiths

INOR **896**. Molybdenum(IV) and tungsten(IV) species in fused chlorides: A spectroscopy study. **V.A. Volkovich**, A.B. Ivanov, B.D. Vasin, I.B. Polovov, T.R. Griffiths

INOR **897**. Measurement of electron delocalization energy in hydrogen-bonded mixed valent Ru<sub>2</sub>O acetate clusters. **T.M. Porter**, G. Canzi, J. Goeltz, C.P. Kubiak

INOR **898**. Excited-state electron transfer from CdSe quantum dots to TiO<sub>2</sub>: Influence of the properties of molecular linkers on electron transfer within mesoporous films. **M.J. Awad**, K.R. Liwosz, D. Watson

INOR **899**. Fiber optic reflectance spectroscopy and multispectral imaging used to assess cadmium sulfide degradation in cadmium yellow paint in paintings by Louise Herreshoff. **M. Stephenson**, B. Becker, E. Timas, **E.S. Uffelman**, P. Hobbs, J. Mass, J. Delaney, K.A. Dooley

INOR **900**. ESR of the heavy-fermion YbRh<sub>2</sub>Si<sub>2</sub>. **C.C. Beedle**, R.D. McDonald, Z. Fisk, N. Harrison, J. Singleton

INOR **901**. Toward ratiometric metal ion sensors based upon thermoresponsive polymers: Polymer collapse and aggregation detected by fluorescence and light scattering. **L. Fulton**, L. Nyranshuti, W. Seitz, R.P. Planalp

INOR **902**. Measurement of NMR relaxation rates in a series of cobalt (II) β-diketonates. **R.R. Baum**, D.L. Tierney

INOR **903**. Stabilization of a combined phenolphthalin/ Cu(II)/EDTA reagent used for the spectrophotometric determination of aqueous cyanide. **S.J. Chalk**, N. Gutierrez

## Section A

San Diego Convention Center  
Hall D

## Interplay of Structure &amp; Transport Properties in Materials for Energy

K. Kovnir, B. C. Melot, *Organizers*

6:00 - 8:00

**INOR 904.** Correlating exciton transport with structural properties in lead sulfide (PbS) nanocrystal films. M.C. Weidman, W.A. Tisdale

**INOR 905.** Inkjet printing of water-processible polyaniline films for clean energy applications. Y. Hu, M.E. Hagerman

**INOR 906.** Effect of polyhedral rotational distortion on the electrochemical properties of polyanionic intercalation electrode materials. S. Zhou, B.C. Melot, R.L. Brutchey, G. Barim

**INOR 907.** Synthesis and characterization of boron phosphide. K. Woo, K. Kovnir

## Section A

San Diego Convention Center  
Hall D

## Lanthanide &amp; Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

6:00 - 8:00

**INOR 908.** Determination of magnetic anisotropy and ligands effect in  $D_{4h}$  molecules with slow magnetic relaxation. D. Paez

**INOR 909.** Separation of 4f- and 5f-elements in a "fused salt - liquid metal" system. V.A. Volkovich, D.S. Maltsev, S.Y. Melchakov, L.F. Yamshchikov, I.B. Polovov

**INOR 910.** Hydrothermal synthesis of lanthanide sulfites and sulfates. J.T. Dvogan, E.M. Villa

**INOR 911.** Aluminum-gadolinium master-alloy for aerospace application: Synthesis and properties. I.B. Polovov, A.V. Krylosov, K.V. Maksimtsev, S.V. Belikov, V.A. Volkovich

**INOR 912.** Synthesis of a library of divalent europium cryptates. L.E. Hopper, M.J. Allen

**INOR 913.** Synthesis of heterometallic rare earth metal precursors to single-molecule magnets with molybdenum and tungsten tetrasulfide bridges. M.D. Boshart, J.W. Ziller, W.J. Evans

**INOR 914.** Computational study of divalent transuranic actinides. G. Chen, F.U. Furche

**INOR 915.** Withdrawn.

**INOR 916.** Organic ligands for actinide extraction in alkaline conditions. E.V. Govor, E. Vasileiadou, S. Kandel, R.G. Raptis, K. Kavallieratos

**INOR 917.** Gemini surfactant-based Ln(III) complexes for bioprobe applications. M. Cendejas, A. McAdams, L. Elmendorf, P.S. Barber

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## Section A

San Diego Convention Center  
Hall D

## Metal-Oxygen Oxidants in Synthesis &amp; Biology: Beyond Metal- Oxo Species

T. A. Jackson, M. T. Kieber-Emmons, *Organizers*

6:00 - 8:00

**INOR 918.** X-ray absorption spectroscopic characterization of the diferric peroxo intermediate of human deoxyhypusine hydroxylase in the presence of its protein substrate. A. Jasniewski, L. Engstrom, V. Vu, L. Que

**INOR 919.** Is ferryl a side-product or an intermediate in catalysis of L-tryptophan dioxygenation by human indoleamine 2,3-dioxygenase (hIDO1)? I.M. Chrisman, L.S. Dameron, V.V. Smirnov

**INOR 920.** Modulating dioxygen activation of manganese corrolazines. H.M. Neu, D.P. Goldberg

**INOR 921.** Characterization and reactivity of a Mn(III)-alkylperoxo species supported by an amide-containing ligand. J. Parham, G. Wijeratne, T.A. Jackson

**INOR 922.** Characterization and oxygen reactivity of a flavonoid-bound manganese complex supported by a scorpionate ligand. M. Denler, T.A. Jackson

**INOR 923.** Electrochemical investigations of peroxomanganese(III) complexes. A.A. Massie, E. Anxolabehere, T.A. Jackson

**INOR 924.** Formation, characterization, and O-O bond activation of a peroxomanganese(III) complex supported by a cross-clamped cyclam ligand. H.E. Colmer, T.A. Jackson

**INOR 925.** Lignin: Utilizing stable metal-oxyl complexes to initiate radical depolymerization. T. Carroll, G. Menard

**INOR 926.** Insights into Mn(III)-OH reactivity: Experimental and theoretical investigations into the role of electronic structure on hydrogen atom abstraction. D. Rice, A. Burr, G. Wijeratne, T.A. Jackson

**INOR 927.** Redox-active ligand mediated oxyl-type O-atom transfer from an exceptionally high valent oxorhenium complex. J.A. Hill, J.D. Soper

## Section A

San Diego Convention Center  
Hall D

## Nanoscience

R. M. Richards, *Organizer*

6:00 - 8:00

**INOR 928.** Colloidal synthesis and transformation of ZnO nanoparticles. J.L. Fenton, J.M. Hodges, R.E. Schaak

**INOR 929.** Cation exchange in quantum dots: Lessons from the Zn/Pb system. W.R. Tilluck, S. Benjamin, C. Mings, A.L. Morris, P.G. Van Patten

**INOR 930.** Controlling the surface modification of magnetic iron oxide nanoparticles: Understanding the binding of benzoic acid and catechol-derived ligands. K.V. Korpany, D. Majewski, C.T. Chiu, S.N. Cross, A.S. Blum

**INOR 931.** One-step ligand exchange for the synthesis of superparamagnetic aqueous-stable iron oxide nanoparticles by mechanochemical milling. K.V. Korpany, C. Mottillo, J. Bachelder, P. Dong, S. Trudel, T. Friscic, A.S. Blum

**INOR 932.** Periodic arrays of gold ellipse dimer nanoantennae with 10-nm gaps as highly active and tunable SERS substrates. A.M. Jubb, Y. Jiao, G. Eres, S. Retterer, B. Gu

**INOR 933.** Influence of ZnO particle size and morphology on photocatalytic degradation of malachite green. J.D. Harris, C.C. Pena, S.C. Bryant, A.J. Christy, A.E. Harris, J.E. Cowen, J.J. Pak

**INOR 934.** Studies towards the formation of novel gold copper alloyed anti-neoplastic agents. B.M. Benin, M. Goomann, S. Huang

**INOR 935.** Dendrimer modified silica nanoparticles as fluorescent chemosensors for the detection of copper and cyanide. A. Luhrs, K. Lyashkevych, C. Feider, L.D. Margerum

**INOR 936.** Multi-step cation exchange of PbS quantum dots. A. Morris, W. Tiluck, S. Benjamin, C. Mings, P. Patten

**INOR 937.** Aqueous phase synthesis of metal nanoparticles and hybrid nanocomposites with controlled geometries. A. Penn, T. Abeywickrama, H.P. Rathnayake

**INOR 938.** Catalytic activity of ultrasmall copper nanoparticles synthesized with a plant-based reducing agent. S.K. St Angelo, G.A. Ferko

**INOR 939.** Controlling the exciton dissociation rates in semiconductor nanocrystal films. N.N. Kholmicheva, M. Zamkov

**INOR 940.** Lowering the valence band of  $Cu_2ZnSnS_4$  through anion substitution: Can it be done? M. Thompson, J. Vela-Becerra

**INOR 941.** Gas-phase synthesis of clusterfullerenes. P.W. Dunk, A.G. Marshall, H.W. Kroto

**INOR 942.** Surface doping of colloidal nanocrystal quantum dots with transition metal complexes. H. Crotty, J. Vela-Becerra

**INOR 943.** Target-specific mesoporous silica nanoparticles for combination therapy of cisplatin and gemcitabine to treat cancer. E.D. Fink, S. Yang, M.P. Alvarez-Berrios, J.L. Vivero

**INOR 944.** Ground state properties and non-adiabatic dynamical studies of  $Pb_{1-x}X_x/Cd_{32}Y_{32}$  ( $X, Y = S, Se, Te$ ) core/shell quantum dots. P.K. Tamukong

**INOR 945.** Withdrawn.

## Section A

San Diego Convention Center  
Hall D

## Organometallic Chemistry: Applications to Materials &amp; Polymer Science

N. S. Radu, *Organizer*

6:00 - 8:00

**INOR 946.** polyMOFs: Exploring polymer structure effects on metal-organic frameworks. S. Ayala, Z. Zhang, H. Nguyen, S.A. Miller, S. Cohen

**INOR 947.** Preparation of metal thiolate complexes for controlled synthesis of nanomaterials. S. Pickle, A.W. Holland

## Section A

San Diego Convention Center  
Hall D

## Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*

6:00 - 8:00

**INOR 948.** C-CN cleavage using palladium supported by a dippe ligand. L. Munjanja, C. Torres-Lopez, W.D. Jones

**INOR 949.** Understanding copper-catalyzed oxidative decarboxylative coupling reactions through the reactivity of copper benzoate and copper aryl complexes. K. Bustin, E. Aguilera, C. Burlas, J.M. Hoover

**INOR 950.** Synthesis and reactivity of aminovinyl carbene complexes. R.M. Padilla, A. Feliciano, J. Tamariz, F. Delgado

**INOR 951.** Sterically-controlled C-H borylation of aryl phosphines. E.E. Albitz, N. Huynh, T.B. Clark

**INOR 952.** Synthesis of alkene-appended dodecaborates. D.T. Buening, J.A. Dopke, R.J. Staples, K.N. Westdorf, A.J. Ramirez

**INOR 953.** Studies toward the mechanism of amine-directed, iridium-catalyzed C-H borylation of *N,N*-dimethylbenzylamines. C.M. Oliver, K.A. McGarry, T.B. Clark

## Section A

San Diego Convention Center  
Hall D

## Organometallic Chemistry: Synthesis &amp; Characterization-Late Transition Metals

N. S. Radu, *Organizer*

6:00 - 8:00

**INOR 954.** Mono- and binuclear Au(I)-complexes of 1,2,3-triazolylidenes: Synthesis, characterization, and trends in catalysis and properties. L. Hettmanczyk, M. van der Meer, S. Hohloch, B. Sarkar

**INOR 955.** Development of new phosphorescent platinum complexes emitting in the deep red to near infrared region. R. Mroz, T. Power, S. Huo

**INOR 956.** C-H and C-P activation by a redox non-innocent ligand supported iron dinitrogen complex. C. Ghosh, T.L. Groy, A.C. Bowman, R.J. Trovitch

**INOR 957.** Perfluoro-olefin, carbene, and carbene complexes of (PNP)Rh. C.J. Pell, Y. Zhu, R. Huacuja, O. Ozerov

**INOR 958.** Tris(3,5-dimethylpyrazol-1-yl)methane and 1,1,1-tris-(3,5-dimethylpyrazol-1-yl)-2-(trimethylsilyloxy)ethane platinum compounds: Synthesis, reactivity and structure. B.P. Quillian, T.B. Gunnoe, A. Lorbecki

**INOR 959.** Reactivity of bi(pyrazol-1-yl)acetic acid ligands with diiodo( $\eta^6$ -*p*-cymene) ruthenium(II). B.P. Quillian, A.E. Fields

**INOR 960.** Synthetic heterocycles and their applications in energy and advanced electronics. N.C. Tice, C. Snyder, D.L. Smith

**INOR 961.** Photophysical properties of platinum group compounds bearing modified pyridine ligands. S.N. Natoli, L.M. Hight, D.R. McMillin

**INOR 962.** Facile aerobic alkylation of rhodium porphyrins with alkyl halides. W. Yang, H. Zuo, Y.W. Lai, S. Feng, S.Y. Pang, E.K. Hung, Y.C. Yu, F.Y. Lau, Y.H. Tsoi, K.S. Chan

**INOR 963.** Synthesis, characterization and reactivity of late transition metal complexes stabilized by bi- and tridentate ligands. S.H. Schreiner, J. Seo

**INOR 964.** Small molecule activation with transition metal-silylene complexes. A.M. Bartrom, W. Harman

**INOR 965.** Synthesis and structural determination of mono- and dinuclear late transition metal ferrocenyl complexes. S.H. Schreiner, P. Koirala

**INOR 966.** Low-valent 3d metals in weak ligand fields for bio-inspired small molecule activation. **P. Pairs, W. Harman**

**INOR 967.** Synthesis and reactivity of high-valent organometallic nickel complexes bearing trifluoromethyl ligands. **J.R. Bour, N. Camasso, M.S. Sanford**

**INOR 968.** Reactivity of bis-protic *N*-heterocyclic carbene (bis-PNHC) complexes of iridium(III). **J.L. Gomez Lopez, V. Miranda Soto, M.P. Parra Hake, D.B. Grotjahn, A.L. Rheingold**

**INOR 969.** Activation of small molecules using transition metal silylene and germylene complexes. **M. Barrientos, W. Harman**

**INOR 970.** Co(CNA<sup>AlMe2</sup>)<sub>2</sub>, an isolobal analogue of Co(CO)<sub>4</sub>, and its reactivity. **C. Chan, J.S. Figueroa**

## Section A

San Diego Convention Center  
Hall D

### Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

#### 6:00 - 8:00

**INOR 971.** Investigation of vanadium-based bronze materials for the detection of peroxide based explosives. **A.A. Allothman, N.F. Materer, Z. Allothman, A.W. Ablett**

**INOR 972.** Geometrical and functional properties of organic ligands on gas sorption properties of metal-organic framework materials. **T.X. Trieu, X. Zhao, X. Bu**

**INOR 973.** Solid state synthesis of copper iron selenostannates. **S.A. Donnelly, B.J. Bellott**

**INOR 974.** Synthesis and characterization of CO<sub>2</sub> chemisorption sites in TMOS/CH<sub>3</sub>OH/H<sub>2</sub>O xerogels. **R. Neuweiler, E.G. Look, H.D. Gafney**

**INOR 975.** Tacticity control of organic polymers inside MOFs via [2+2] photo-polymerization reactions. **I. Park, R. Medishetty, A. Chanthapally, H. Lee, C. Mulljanto, Z. Zhang, H. Quah, S. Lee, M.J. Zaworotko, J.J. Vittal**

**INOR 976.** Comparison of the negative thermal expansion and behavior on compression for CaZrF<sub>6</sub>, CaNbF<sub>6</sub> and MgZrF<sub>6</sub>. **B. Hester**

**INOR 977.** Competing broken inversion symmetry and oxygen octahedral sliding phenomena in *n*=1 Ruddlesden popper derivative HRTIO<sub>4</sub> (R=Nd, Sm, Eu, Gd, and Dy) family. **F. Brown, A. Sen Gupta, H. Akamatsu, M. An Nguyen, T. Mallouk, V. Gopalan**

**INOR 978.** Development of an aqueous synthesis for zinc oxide nanoparticles with biologically benign capping agents. **J. Zinna, M.C. Gelabert**

**INOR 979.** Hydrothermal synthesis of metal homo- and heteropolychalcogenide compounds. **E.G. Yerdon, C.C. Raymond**

**INOR 980.** Synthesis and single crystal structure of (OC)<sub>2</sub>W(Ph<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>PPh<sub>2</sub>)<sub>2</sub>W(CO)<sub>6</sub>. **H. Drake, K.A. Wheeler, B.J. Bellott**

## Section A

San Diego Convention Center  
Hall D

### Supramolecular Chemistry: A Crown & Anchor Approach

A. E. Gorden, *Organizer*

#### 6:00 - 8:00

**INOR 981.** Molecular recognition of uranyl using salen ligand chemosensors. **M. Eddy, E.E. Hardy, A.E. Gorden**

**INOR 982.** Combination of texaphyrin and platinum(IV) prodrugs as a potential new anticancer therapy. **G. Thiabaud, Z.H. Siddik, J.L. Sessler**

**INOR 983.** Dynamic synthesis of diazaborole based oligomers and macrocycles. **S. Lokugama, C. Manankandayalage, D.E. Gross**

**INOR 984.** Allosteric regulation in supramolecular capsules, cages, and polyhedra. **A. d'Aquino, C.A. Mirkin**

**INOR 985.** Design foldamers from fragments: Chloride encapsulation and switchable double helices. **Y. Liu, A. Sengupta, K. Raghavachari, A.H. Flood**

**INOR 986.** Investigation of CB[7] binding effects on organic chromophores. **C.H. Battle, G.H. Aryal, T.A. Grusenmeyer, J. Jayawickramarajah**

**INOR 987.** Evolving small library of nipecotate and isonipecotate cored derivatives for acetylcholine esterase inhibition. **N. Beltrami, D. Calderon, L.P. Dennis, S. Hickmann, E.F. Walsh, H. William, M. Torok, D. Sikazwe, J.M. Davis**

**INOR 988.** Studies of deep-cavity cavitands. **J.H. Jordan, B.C. Gibb**

**INOR 989.** Synthesis and characterization of dipyrinones as supramolecular building blocks. **Z. Nichols, M.T. Huggins, A. Schrock, K. Barnes, T. Jarvis, A. Fisch**

**INOR 990.** Synthesis and characterization of novel fluorescent boron containing molecule. **N.S. Jackson, A.R. Schroeder, S.E. Harrell, M.T. Huggins, A. Schrock, P.P. Vaughan, K. Molek**

**INOR 991.** Exploitation of new five-coordinate vanadyl complexes for comparative uranyl studies and application to metal sequestration. **J. Niklas, A.E. Gorden**

**INOR 992.** Targeting the terminus in peptide recognition by synthetic receptors. **A.R. Urbach**

**INOR 993.** Oxazolidinone-based small molecule libraries for the selective recognition of therapeutically relevant RNA. **B. Morgan, R.N. Culver, B. Blachut, A.E. Hargrove**

**INOR 994.** Expanded porphyrin cyclo[1]furan[1]pyridine[4]pyrrole: A hybrid macrocycle displaying aromatic character upon cation complexation. **J.T. Brewster, I. Ho, Z. Zhan, J.L. Sessler**

**INOR 995.** Molecular recognition of uranyl using a resin supported salen 2-quinoxalino ligand. **C.D. Tutson, A.E. Gorden**

**INOR 996.** Uranyl extractions using a solid supported quinoxalino based salen ligand. **M. West, A.E. Gorden**

**INOR 997.** Analysis of π-π stacking and higher order dimensional crystal packing in recently characterized salphenazine complexes. **E.E. Hardy, A.E. Gorden**

**INOR 998.** Self-assembled pyridine-dipyrrolate cages. **H. Zhang, V. Lynch, J. Lee, E.V. Anslyn, J.L. Sessler**

**INOR 999.** Calix[4]pyrrole-based metal-organic frameworks (MOFs). **J. Lee, V. Lynch, N. Waggoner, S.K. Kim, S.M. Humphrey, J.L. Sessler**

**INOR 1000.** Energetic components of aryl CH•••X<sup>-</sup> hydrogen bonds: Field and resonance effects. **B.W. Tresca, R.J. Hansen, M.M. Haley, D.W. Johnson**

**INOR 1001.** Application of 'Texas-sized' molecular box in molecular device. **Y. Yang, H. Gong**

**INOR 1002.** Redox chemistry of pyrrole-based ligands in transition metal complexes. **K. Lincoln, R. Gautam, E. Tomat**

**INOR 1003.** In-vitro and intracellular metal chelation properties of sirtuin inhibitor sirtinol. **R. Gautam, E. Akam, E. Tomat**

**INOR 1004.** Towards selective ion-pair sensing based on anion and cation complexation and co-extraction: Dual-host combinations of fluorescent sensors for ammonium and nitrate. **T.M. Jonah, C.L. Cortes, R.A. Currie, K. Kavallieratos**

**INOR 1005.** Molecular cluster metalloligand for the synthesis of dual cluster metal-organic frameworks. **C. Bejger, J. Yu, D.W. Paley, M.L. Steigerwald, C.P. Nuckolls**

## Section A

San Diego Convention Center  
Hall D

### Transition Metal Chemistry in DNA & RNA Regulation

P. Chen, S. L. Michel, *Organizers*

#### 6:00 - 8:00

**INOR 1006.** Bioanalytical approaches to measure iron speciation in plasma of patients treated with iron-nanoparticle drug products. **H.M. Neu, A.D. Smith, A. Wilks, J.E. Polli, M.A. Kane, T.Y. Ting, S.L. Michel**

**INOR 1007.** In-cell fluorescence imaging of platinum anticancer compounds detected using click chemistry. **A.D. Moghaddam, J.D. White, M.M. Haley, V. DeRose**

**INOR 1008.** CPSF30, an RNA binding 'zinc-finger' protein with a 2Fe-2S cluster. **G.D. Shimberg, J. Michalek, A. Rodrigues, B.E. Zucconi, S. Ghosh, K. Sureshchandra, G.M. Wilson, T.L. Stemmler, S.L. Michel**

### Industrial Research at the Interface of Inorganic Chemistry & Polymer Science

*Sponsored by POLY, Cosponsored by BMGT and INOR†*

## WEDNESDAY MORNING

### Section A

San Diego Convention Center  
Room 30B

### Interplay of Structure & Transport Properties in Materials for Energy

B. C. Melot, *Organizer*

K. Kovnir, *Organizer, Presiding*

**8:30 INOR 1009.** Influence of lattice flexibility on ionic diffusion in materials for energy storage. **B.C. Melot**

**9:00 INOR 1010.** Electron transport in Ga<sub>2</sub>In<sub>6</sub>Sn<sub>2</sub>O<sub>16</sub>: The role of the 7-coordinate site. **K. Rickert**

**9:20 INOR 1011.** Exploring new electrode materials for Li-ion batteries: Structure and electrochemistry. **G. Rousse**

**9:50** Intermission.

**10:10 INOR 1012.** Thermochemical synthesis of earth-abundant phosphorus-rich metal phosphides and metal thiophosphates for catalytic water splitting applications. **E.G. Gillan**

**10:30 INOR 1013.** Probing function and failure in energy materials with hard X-ray tools. **K.W. Chapman**

**11:00 INOR 1014.** First-principles modeling of Li diffusion in V<sub>2</sub>O<sub>5</sub> as cathode material of Li ion batteries. **S. Suthirakun, A. Genest, N. Roesch**

**11:20 INOR 1015.** Structure-function relationships in electrolytes for reversible magnesium batteries. **B.M. Bartlett, A.J. Crowe**

## Section B

San Diego Convention Center  
Room 30C

### Transition Metal Chemistry in DNA & RNA Regulation

P. Chen, *Organizer*

S. L. Michel, *Organizer, Presiding*

V. DeRose, *Presiding*

**8:30 INOR 1016.** *In vitro* selection and characterization of metal-specific DNAAzymes and their applications in imaging metal ions in living cells. **Y. Lu, K. Hwang, P. Wu, C.E. McGhee, S. Torabi**

**9:00 INOR 1017.** Modulation of DNA/RNA-protein interactions with substitution-inert platinum-metal compounds. **N. Farrell**

**9:30 INOR 1018.** RNA and DNA targets of platinum anticancer compounds detected using click chemistry. **A.D. Moghaddam, K. Plakos, R.M. Cunningham, J.D. White, M.M. Haley, V. DeRose**

**10:00 INOR 1019.** Luminescent zinc fingers: From zinc sensors to sequence-specific RNA sensors. **O. Seneque, L. Raibaut, M. Isaac, C. Cepeda, S.L. Michel, S. Eliseeva, S. Petoud**

**10:30** Intermission.

**10:50 INOR 1020.** *In vivo* inhibition of zinc finger transcription factors by cobalt(III) Schiff base complexes. **T.J. Meade**

**11:20 INOR 1021.** Fe-S cluster biosynthesis provides cofactors to activate proteins that drive gene regulation. **T.L. Stemmler**

**11:50 INOR 1022.** DNA-mediated signaling. **J.K. Barton**

## Section C

San Diego Convention Center  
Room 30D

### Metal-Oxygen Oxidants in Synthesis & Biology: Beyond Metal- Oxo Species

T. A. Jackson, *Organizer*

M. T. Kieber-Emmons, *Organizer, Presiding*

**8:00 INOR 1023.** Role of carboxylic acids in iron-mediated peroxide activation: are peroxycarboxylates involved? **E. Rybak-Akimova, M.C. Piquette, S.G. McKenzie, G. Yang, O. Makhlynets, T. Palluccio**

**8:25 INOR 1024.** Mechanisms and purview of C-H-bond activation by mid-valent metal superoxide complexes. **J.M. Bollinger, C. Krebs**

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**8:50 INOR 1025.** Thermodynamics and mechanistic insights into C-H bond activation by the Cu(III)-OH core. **W.B. Tolman**

**9:15 INOR 1026.** Steric and electronic control of proton-coupled electron-transfer reactions of mononuclear hydroxomanganese(III) complexes. **T.A. Jackson, D.B. Rice, A. Burr, A.W. Howcroft**

**9:40 INOR 1027.** Iron porphyrin electrocatalysts for oxygen reduction. **J.M. Mayer, M. Pegis, B.A. McKeown, S. Raugel, N. Kumar**

**10:05 Intermission.**

**10:15 INOR 1028.** Bio-inspired metal-oxido and metal-hydroxido species. **A. Borovik**

**10:40 INOR 1029.** Dioxxygen activation by a tricopper-dinitrogen complex. **G. Di Francesco, L.J. Murray**

**11:05 INOR 1030.** Superoxo and peroxo intermediates in oxygenase reactions. **J.D. Lipscomb, B. Rivard, M.S. Rogers, C.J. Knoot, E.G. Kovaleva**

**11:30 INOR 1031.** High valent mononuclear iron-oxo species in catalytic O-O cleaving and forming reactions. **M. Costas, O. Cusso, A. Company, Z. Codola, J. Serrano, J. Lloret-Fillol, X. Ribas**

**11:55 INOR 1032.** Mononuclear metal-O<sub>2</sub>(H) adducts in oxidative nucleophilic and electrophilic reactions. **J. Cho**

## Section D

San Diego Convention Center  
Room 30E

### Memorial Symposium Honoring Karen J. Brewer

*Cosponsored by HIST†  
Financially supported by  
Washington State University*

M. T. Mongelli, S. C. Rasmussen, *Organizers*

J. White, *Presiding*

**8:30 INOR 1033.** Excited states of transition metal complexes: Optimizing reactions for solar energy conversion and photochemistry. **C. Turro, K.R. Dunbar**

**9:00 INOR 1034.** Design, synthesis, spectroscopic, electrochemical, and biological studies of strained ruthenium(II) and ruthenium(II)-platinum(II) complexes. **A. Jain, K. Wyland, E. Hoffman, D. Davis, C. Brecht**

**9:30 INOR 1035.** New mechanisms in dye-sensitized solar cells: Catalyzing two-electron-transfer halide redox chemistry at sensitized TiO<sub>2</sub>. **H. Chen, J.M. Cardon, J. Angsono, J. Glancy-Logan, S. Ardo**

**9:50 INOR 1036.** Radically new compounds to combat methicillin resistant *Staph. aureus* (MRSA): Metal complexes as antimicrobials. **J.S. Merola, G. Karpin, D.M. Morris, C.M. DuChane, J.O. Falkingham, M.F. Ehrich**

**10:20 Intermission.**

**10:35 INOR 1037.** Stability of Ru(II), Ru(II),Pt(II) and Ru(II),Rh(II),Ru(II) supramolecular complexes containing enantiomerically pure light absorbing subunits. **A. Wagner, K.S. Brewer**

**11:05 INOR 1038.** Light-activatable Ru-based anticancer complexes in a new light. **S.L. Hopkins, B. Siewert, S.H. Askes, L.N. Lameijer, P. Veldhuizen, R. Zwier, S. Bonnet**

**11:35 INOR 1039.** Redox-active intercalating ligands (RAIL) against cancer: A new approach to using ruthenium polypyridyl complexes as potential anti-cancer drugs. **F.M. MacDonnell, N. Alatrash, C. Griffith, A. Dayoub**

**12:05 INOR 1040.** Supramolecular poly-metallic architectures in the treatment of malignant glioma. **J.A. Rodriguez Corrales, J. Zhu, A. Dominijanni, J.L. Robertson, K.S. Brewer**

## Section E

San Diego Convention Center  
Room 31A

### Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

P. C. Glazer, *Presiding*

**8:30 INOR 1041.** Iron(II) complex as pH-responsive paraCEST MRI contrast agent: Towards imaging of acidosis conditions. **P.B. Tsitovich, J.R. Morrow**

**8:50 INOR 1042.** Ruthenium and platinum antitumor complexes and their activation with 980-nm light. **E. Ruggiero, L. Salassa**

**9:10 INOR 1043.** Targeting specific nucleic acid structures and proteins with ruthenium complexes. **P.C. Glazer**

**9:30 INOR 1044.** Bifunctional compounds as novel theranostic agents for Alzheimer's disease. **L.M. Mirica**

**9:50 Intermission.**

**10:00 INOR 1045.** Role of hydrogen bonding,  $\pi$ - $\pi$  stacking interactions, twist-angle, and solvation on B-DNA. **J. Poater**

**10:20 INOR 1046.** Withdrawn.

**10:40 INOR 1047.** Moving light-based cancer therapy from concept to reality with metalloprotein photosensitizers. **S.A. McFarland, H. Yin, S. Monro, T. Sainuddin, M. Pinto, M. Hetu**

**11:00 INOR 1048.** Insights into the biological activities of clavaniins, potent antimicrobial peptides from tunicate hemocytes. **A.M. Angeles Boza, S. Juliano**

## Section F

San Diego Convention Center  
Room 31B

### Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

J. E. Cloud, V. Doan-Nguyen, *Presiding*

**8:30 INOR 1049.** Reducing the large volume change in alloy anodes through porous nanoscale architecture. **T.C. Lin, J.B. Cook, J.N. Weker, E. Detsi, S.H. Tolbert**

**8:50 INOR 1050.** Porous solid electrolytes for advanced lithium ion batteries. **J.E. Cloud, S. Biswas, S.L. Suib**

**9:10 INOR 1051.** Effect of rotational polyhedra distortions on guest ion intercalation in anti-NASICON Fe<sub>3</sub>(MoO<sub>4</sub>)<sub>3</sub>. **G. Barim, S. Zhou, B.C. Melot, R.L. Brutchey**

**9:30 INOR 1052.** Unraveling the mechanism of transition metal sulfide conversion electrodes with local structure methods. **V. Doan-Nguyen, M.M. Butala, M. Lumley, R. Seshadri**

**9:50 Intermission.**

**10:05 INOR 1053.** Graphite-conjugated catalysis. **S. Chu, T. Fukushima, M. Jackson, S. Oh, M. O'Reilly, Y. Surendranath**

**10:25 INOR 1054.** Electro-catalytic oxidation of glycerol on free-standing monolithic nanoporous silver. **Y. Liang, E. Detsi, S.H. Tolbert**

**10:45 INOR 1055.** Modular method for non-covalent attachment of homogeneous electrocatalysts to electrode surfaces. **B.R. Lydon, A. Germann, J. Yang**

**11:05 INOR 1056.** Single and multi-doped transition metal (Mn, Fe, Ni and Co) ZnO and its electrocatalytic activities for oxygen reduction reaction. **M.R. Shakil, A. El-Sawy, H. Tassim, S.L. Suib**

## Section G

San Diego Convention Center  
Room 31C

### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

S. H. Pang, C. T. Saouma, *Presiding*

**8:30 INOR 1057.** Flexible Ti- and Zr-MOFs based on 1,4-*trans*-cyclohexanedicarboxylate linkers. **B. Bueken, F. Vermoortele, H. Reinsch, M. Cliffe, M. Wharmby, C. Tsou, D.E. Vanpoucke, R. Ameloot, V. Van Speybroeck, A. Goodwin, F. Taulelle, J.M. Mayer, D. De Vos**

**8:50 INOR 1058.** Protein-based metal-organic frameworks. **J. Bailey, F.A. Tezcan**

**9:10 INOR 1059.** Computational study of the dehydration process of the NU-1000 MOF. **A. Mavrandonakis, A.E. Platero Prats, L.C. Gallington, Y. Liu, J.T. Hupp, O.K. Farha, K.W. Chapman, C.J. Cramer**

**9:30 INOR 1060.** Withdrawn.

**9:50 Intermission.**

**10:05 INOR 1061.** Rendering water unstable Cu<sub>2</sub>(NH<sub>2</sub>btc)<sub>2</sub> moisture-resistant via post synthetic modification. **H. Rubin, M.M. Reynolds**

**10:25 INOR 1062.** Thermodynamic considerations for CO<sub>2</sub> reduction at Zr-based MOFs. **C.T. Saouma, T. Elkin, M. Bhattacharya**

**10:45 INOR 1063.** Understanding the formation of defects on metal-functionalized metal-organic frameworks. **G. González Miera, A.E. Platero Prats, P.J. Chupas, K.W. Chapman, B. Martin-Matute**

**11:05 INOR 1064.** Effect of acid gas exposure on the external surfaces of ZIF-8. **S.H. Pang, C.W. Jones, R.P. Lively**

## Section H

San Diego Convention Center  
Room 32A

### Inorganic Catalysts

S. A. Koch, *Organizer*

R. N. Austin, *Presiding*

**8:00 INOR 1065.** O-O bond formation in woc by iridium complexes. **A. Poater, L. Cavallo**

**8:20 INOR 1066.** Cobalt complexes supported by a ferrocene-based ligand as redox switches for hydroelectrolysis reactions. **S. Shepard, P. Diaconescu**

**8:40 INOR 1067.** Mechanistic studies of oxygen atom transfer in [ONO]Re complexes. **J.M. Hoffman, S.N. Brown**

**9:00 INOR 1068.** Cobalt cubane water oxidation catalysts: On the way to photosystem II. **F. Evangelisti, R. More, F. Hodel, S. Lubner, G.R. Patzke**

**9:20 INOR 1069.** New ideas for hydrogen-efficient direct deoxygenation catalysts. **R.N. Austin, L. Grabow, B. Frederick, R. Nelson, B. Baek, P. Ruiz, M. Wheeler**

**9:40 INOR 1070.** Water oxidation pathways using a cobalt oxide dimer catalyst. **P. Petrovic, S. Zanic, E. Brothers, P.T. Anastas**

**10:00 INOR 1071.** Withdrawn.

**10:20 Intermission.**

**10:30 INOR 1072.** Electrocatalytic H<sub>2</sub> production is favored over formate production by including a proton shuttle on [Fe<sub>2</sub>N(CO)<sub>2</sub>]. **N.D. Loewen, E.J. Thompson, M. Kagan, C. Bañales, T.W. Myers, J. Fettingler, L.A. Berben**

**10:50 INOR 1073.** Mechanistic details and thermodynamic insights for electrocatalytic reduction of CO<sub>2</sub> or H<sup>+</sup> by metal carbonyl clusters. **A. Taheri, L.A. Berben**

**11:10 INOR 1074.** Modification of electrode surfaces with Ni(II) cyclam, CO<sub>2</sub> reduction catalyst. **A. Zhanaidarova**

**11:30 INOR 1075.** Covalent attachment of molecular electrocatalysts to high surface area carbon materials. **B. Johnson, Z.R. Jones, S.L. Scott, L.A. Berben**

**11:50 INOR 1076.** Overlooked reaction involving a catalyst, [Co(dmgBF<sub>2</sub>)(OH<sub>2</sub>)<sub>2</sub>], and a sacrificial electron donor, triethylamine during the production of hydrogen in acidified acetonitrile: A mechanistic study that must not be ignored! **M.J. Celestine, M.A. Lawrence, J. Combs, C.E. Galbraith, L.S. Joseph, A. Holder**

## Section I

San Diego Convention Center  
Room 32B

### Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

S. T. Liddle, D. A. Penchoff, *Presiding*

**8:30 INOR 1077.** Uranyl hybrid materials: Synthesis and characterization. **M. Payne**

**8:50 INOR 1078.** Phosphorus-stabilized rare earth(III) and (IV) methanediides: Structure, bonding, and magnetism. **S.T. Liddle, M. Gregson, E. Lu, F. Tuna, E. McInnes, W. Lewis, A. Blake**

**9:10 INOR 1079.** Synthesis and characterization of thorium-chalcogen multiple bonds. **D.E. Smiles, G. Wu, T.W. Hayton**

**9:30 Intermission.**

**9:40 INOR 1080.** Supramolecular assembly of actinide bearing hybrid materials: structural systematics and properties. **R. Surbella, K.L. Pellegrini, B. McNamara, D.E. Meier, J. Schwantes, C.L. Cahill**

**10:00 INOR 1081.** Organometallic actinide complexes with nitrogen-rich ligands. **K.A. Maerzke, K. Browne, P. Yang, N. Henson, J.L. Kiplinger, J.M. Veauthier**

**10:20 INOR 1082.** Towards low limit SERS detection of uranyl ions with tailor made bifunctional ligands. **J.F. DeJesus, M.J. Trujillo, D.A. Penchoff, J.A. Bradshaw, J.P. Camden, D.M. Jenkins**

**10:40 Intermission.**

**10:50 INOR 1083.** Investigation of organo-actinide metal complexes with soft-donor ligands through reactivity studies. **A. Behrle, J.R. Walsensky**

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**11:10 INOR 1084.** Nitrogen-rich, organometallic complexes of thorium and uranium with 5-methyl-1H-tetrazole. **K. Browne**, K.A. Maerzke, N.E. Travia, N. Henson, D.E. Morris, B. Scott, P. Yang, J.L. Kiplinger, J.M. Veauthier

**11:30 INOR 1085.** Synthesis of  $(C_2H_5SiMe_3)_4U$  reveals that a  $(C_2H_5SiMe_3)_3UCl/(C_2H_5SiMe_3)_3UMe$  mixture is more crystalline than the pure compounds. **C.J. Windorff**, M.R. MacDonald, J.W. Ziller, W.J. Evans

## Section J

San Diego Convention Center  
Room 33A

### Main Group Chemistry

T. W. Hudnall, *Organizer*

S. Aldridge, *Presiding*

**8:30 INOR 1086.** Oxidation of carbene-stabilized main group diatomic molecules. **Y. Wang**, P. Wei, G.H. Robinson

**8:50 INOR 1087.** Bottleable (amino)(carboxy) radicals derived from cyclic (alkyl)(amino) carbenes. **J. Mahoney**, D. Martin, C.E. Moore, A.L. Rheingold, G. Bertrand

**9:10 INOR 1088.** Application of a donor-acceptor strategy to generate molecular main group element precursors to nanodimensional materials. **A.K. Swarnakar**, T.K. Purkait, J.G. Veinot, E. Rivard

**9:30 INOR 1089.** Molecular precursor to phosphathyne: Synthesis, characterization, and further reactivity. **W.J. Transue**, A. Velian, M. Nava, C. Womack, J. Jiang, G. Hou, X. Wang, R. Field, C.C. Cummins

**9:50 INOR 1090.** Encapsulated peroxide dianion in solution and the solid state: Fundamental properties and reactivity with CO and CO<sub>2</sub>. **M. Nava**, S. Zhang, N. Lopez, C.C. Cummins

**10:10** Intermission.

**10:20 INOR 1091.** Metal-free dehydrogenation of amine-boranes by tunable *N*-heterocyclic iminoboranes. **M. Lui**, N. Paisley, R. McDonald, M. Ferguson, E. Rivard

**10:40 INOR 1092.** Bond activation by highly reactive low valent germanium complexes. **S. Aldridge**, A. Rit

**11:00 INOR 1093.** Development of frustrated Lewis pairs featuring antimony(V) acids. **D. Tofan**, F.P. Gabbaï

**11:20 INOR 1094.** Boron, silicon, and phosphorus catalysts for the reduction of CO<sub>2</sub>. **T. Cantat**, N. von Wolff, E. Blondiaux, G. Lefevre, J. Berthet, P. Thuery

**11:40 INOR 1095.** Synthesis and properties of bidentate Lewis acids with large binding pockets. **C. Chen**, F.P. Gabbaï

**12:00 INOR 1096.** Distiboranes based on *ortho*-phenylene backbones: Synthesis and anion binding. **D. You**, M. Hirai, F.P. Gabbaï

## Section K

San Diego Convention Center  
Room 33B

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

J. Okuda, O. Serrano, *Presiding*

**8:30 INOR 1097.** Carbon dioxide hydrogenation by late transition metal phosphine and *N*-heterocyclic carbene complexes. **M. Reineke**, A. Lilio, C.P. Kubiak

**8:50 INOR 1098.** Lewis acid enhancement in catalytic CO<sub>2</sub> reduction at low cost metals. **Y. Zhang**, **W.H. Bernskoetter**, N. Hazari

**9:10 INOR 1099.** Hydrosilylation of carbon dioxide catalyzed by triphenylborane. **J. Okuda**

**9:30 INOR 1100.** Carbon dioxide reduction to formate by a multi-functional, redox-active borane. **J. Taylor**

**9:50 INOR 1101.** Cascade conversion of carbon dioxide to methanol: New catalytic, kinetic, and mechanistic insights. **D.C. Samblanet**, M.S. Sanford

**10:10** Intermission.

**10:20 INOR 1102.** Photochemical reduction of carbon dioxide using a CN-modified *fac*-Mn(bpy)(CO)<sub>3</sub> catalyst. **P. Cheung**, C.W. Machari, A. Malkhasian, J. Agarwal, C.P. Kubiak

**10:40 INOR 1103.** Small molecule activation by mid-valent group 6 metal complexes supported by a sterically-reduced monocyclopentadienyl, amidinate ligand environment. **L.M. Duman**, L.R. Sita

**11:00 INOR 1104.** Synthesis of stereoregular and cyclic poly(lactic acid) using an iron-based catalyst. **J.A. Byers**, A. Kaur, C.M. Manna, L. Yablon, B. Li, F. Haefner

**11:20 INOR 1105.** Fully aliphatic aziridination employing a macrocyclic *N*-heterocyclic tetracarbenes iron(II) catalyst. **P.P. Chandrachud**, H.M. Bass, D.M. Jenkins

**11:40 INOR 1106.** Ester hydrogenation by an octahedral iron-amino hydride catalyst: DFT comparisons of bifunctional and ion-pair slippage mechanisms. **F. Hasanayn**, A. Abotaka

**12:00 INOR 1107.** Substitution of labile solvent ligands of an iron(II) NHC complex by isocyanides. **A. Lindhorst**, S. Haslinger, J. Kueck, M. Cokoja, A. Pothig, F.E. Kuehn

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Materials Genome & Materials Informatics

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

#### Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger

*Sponsored by NUCL, Cosponsored by INOR†*

#### Supramolecular Chemistry

*Sponsored by ORGN, Cosponsored by INOR*

## WEDNESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 30B

#### Interplay of Structure & Transport Properties in Materials for Energy

K. Kovnir, *Organizer*

B. C. Melot, *Organizer, Presiding*

**1:30 INOR 1108.** Crystal chemistry and transport properties of novel layered Li pnictides. **K. Lee**, **K. Kovnir**

**2:00 INOR 1109.** Silicon clathrates for electrochemical energy storage applications. **C.K. Chan**

**2:20 INOR 1110.** Characterization of multi-valent electrochemical reactions in spinel oxide hosts. **J. Cabana**

**2:50 INOR 1111.** Rational design of heterometallic molecular precursors for the synthesis of energy-related materials. **E. Dikarev**, Z. Wei, H. Han, C.M. Lieberman

**3:20** Intermission.

**3:40 INOR 1112.** Structure and transport of lithium ions in lithium garnet oxides as solid electrolytes for lithium-ion batteries. **W. Lai**

**4:10 INOR 1113.** Germanium nanoparticle synthesis involving other group IV elements. **K.A. Newton**, A.L. Holmes, W. Blacklock, S. Kauzlarich

**4:30 INOR 1114.** Rational nanostructure design for high performance Mg rechargeable batteries. **Y. Yao**

### Section B

San Diego Convention Center  
Room 30C

#### Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

V. V. Smirnov, *Presiding*

**1:30 INOR 1115.** Examining outer-sphere effects on coordination chemistry using disulfide bond networks in engineered metalloprotein scaffolds. **L. Churchfield**, F.A. Tezcan

**1:50 INOR 1116.** Aryl-amine oxygenation mechanism for a diiron enzyme involved in antibiotic biosynthesis. **A. Komor**, B. Rivard, L. Que, J.D. Lipscomb

**2:10 INOR 1117.** Effect of Lewis acids on transition metal complexes. **M. Swart**, M. Gruden, K. Ray, F. Meyer

**2:30 INOR 1118.** Binding of a potent pyridine inhibitor in an iron-sulfur enzyme IspH and NO in the non-heme center of a biosynthetic nitric oxide reductase model. **Y. Zhang**

**2:50 INOR 1119.** Design of protein-based hybrid catalysts for renewable fuel production. **D. Sommer**, A. Roy, M. Vaughn, G. Ghirlanda

**3:10 INOR 1120.** Nitrosyl hydride (nitroxyl) complexes of iron porphyrins. **E.G. Abucayon**, R.L. Khade, Y. Zhang, G.B. Richter-Addo

**3:30** Intermission.

**3:40 INOR 1121.** Synthesis and reductive coupling reactivity of tripodal iron isocyanide complexes. **J.M. Hoover**, A. Gowda, J.L. Petersen

**4:00 INOR 1122.** Effects of ionic liquids on stability, structure, and reactivity on biological macromolecules. **H.U. Valle**, T.A. Rogers, T. Al-Mohanna, J.P. Emerson

**4:20 INOR 1123.** Optimizing immobilization of ferrocene peptide bioconjugates for biosensor development. **M. Goulet**

**4:40 INOR 1124.** Electrochemical characterization of isolated nitrogenase cofactors. **J. Yang**, B.R. Lydon, N. Sickerman, C. Lee, Y. Hu, M. Ribbe

**5:00 INOR 1125.** Tryptophan radical in azurin: Effects of deuteration and metal substitution on quantum yields of fluorescence and radical formation. **J. Liang**, J. Rivera, J.E. Kim

**5:20 INOR 1126.** Why heme enzymes that decyclize free tryptophan react as dioxygenases: Mechanistic study on O<sub>2</sub> activation and timing of the O-O bond cleavage in indoleamine 2,3-dioxygenase (hIDO1). **I.M. Chrisman**, L.S. Dameron, **V.V. Smirnov**

### Section C

San Diego Convention Center  
Room 30D

#### Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

B. M. Leonard, S. Marinescu, *Presiding*

**1:30 INOR 1127.** Imobilized one dimensional cobalt dithiolene metal organic surface (MOS) for efficient electrochemical and photoelectrochemical H<sub>2</sub> evolution from water. **C.A. Downes**, S.C. Marinescu

**1:50 INOR 1128.** Two-dimensional cobalt dithiolene metal-organic surfaces (MOS) as immobilized catalysts for the conversion of acidic water to H<sub>2</sub>. **A.J. Clough**, J.W. Yoo, M.H. Mecklenburg, S. Marinescu

**2:10 INOR 1129.** Ligand removal from CdS quantum dots for enhanced photocatalytic H<sub>2</sub> generation in pH neutral water. **C. Chang**, K.L. Orchard, B.C. Martindale, E. Reiser

**2:30 INOR 1130.** Synthesis and water splitting electrocatalysis of metal carbide compounds. **B.M. Leonard**

**2:50** Intermission.

**3:05 INOR 1131.** One- and two-dimensional cobalt dithiolene metal-organic surfaces (MOS) for efficient electrochemical and photoelectrochemical H<sub>2</sub> evolution from water. **S. Marinescu**, A.J. Clough, C.A. Downes, J.W. Yoo

**3:25 INOR 1132.** Effect of interlayer anions on [NiFe]-LDH nanosheet water oxidation activity. **B.M. Hunter**, J.R. Winkler, H.B. Gray, **A.M. Mueller**

**3:45 INOR 1133.** Nanoparticulate RuO<sub>2</sub> deposited on practical electrode substrates: Efficient water oxidation from vanishingly small loadings of an expensive platinum-group metal. **C.N. Chervin**, P. DeSario, E. Nelson, M.B. Sassin, J. Long, D.R. Rolison

**4:05 INOR 1134.** In situ spectroscopies of mixed-metal nanosheet water oxidation catalysts made by pulsed laser ablation in liquids. **B.M. Hunter**, J.R. Winkler, H.B. Gray, A.M. Mueller

**4:25 INOR 1135.** Designing nickel based ceramics as catalysts for the hydrogen evolution reaction combining theoretical and experimental observations. **M. Ledendecker**, H. Schlott, B. Meyer, M. Antonietti, M. Shalom

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## Section D

San Diego Convention Center  
Room 30E

### Memorial Symposium Honoring Karen J. Brewer

*Cosponsored by HIST†  
Financially supported by  
Washington State University*

M. T. Mongelli, S. C. Rasmussen, *Organizers*  
M. Richter, *Presiding*

**1:30 INOR 1136.** Catalytic water oxidation: From Ru(II) to Fe(III). L. Wickramasinghe, L. Tong, R. Zong, R. Zhou, R.P. Thummel

**2:00 INOR 1137.** Ru(II)-anthraquinone complexes: redox and spectroscopic properties and light-activated interactions with DNA. J.K. White, T.A. White, C. Turro

**2:30 INOR 1138.** Tyrosine-histidine mimic with stepwise oxidation and concerted reduction by proton coupled electron transfer. G. Manbeck, E. Fujita, J.J. Concepcion

**3:00 INOR 1139.** What I learned from Karen Brewer about teaching undergraduates. P.A. Deck

**3:30** Intermission.

**3:45 INOR 1140.**  $\pi$ -Extended metal thiophenedithiolenes: Synthetic approaches to tuning electronic and optical properties. K. Konkol, E. Uzelac, C.M. Amb, S.C. Rasmussen

**4:15 INOR 1141.** Light that pleases the world in science: The Karen Brewer's effect on my academic career. A. Holder

**4:45 INOR 1142.** New hydrophilic supramolecular complex for the photocatalytic production of hydrogen from aqueous solutions. T. Canterbury, S.M. Arachchige, R.B. Moore

**5:15 INOR 1143.** Photoredox reactions of Pt(II)  $\sigma$ -metalated bis-pyridylbenzene complexes: Photoreduction and H<sub>2</sub> generation in chromophore-sacrificial donor systems. A.D. Kulkarni, A.C. Neuberger, R.H. Schmehl

## Section E

San Diego Convention Center  
Room 31A

### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*  
R. Beaulac, M. W. Lee, *Presiding*

**1:30 INOR 1144.** Formation and interlayer decoupling of colloidal MoSe<sub>2</sub> nano-flowers. D. Sun, S. Feng, M. Terrones, R.E. Schaak

**1:50 INOR 1145.** Multiscale simulations of formation and dissolution of nanomaterials in liquid cells. S. Sen, P. Kral

**2:10 INOR 1146.** Facile synthetic approach to MoS<sub>2</sub> monolayer-PbSe QDs hetero-structures. Q. Ding, S. Jin

**2:30 INOR 1147.** Solution-liquid-solid (SLS) approach to colloidal nitride semiconductor nanomaterials. R. Beaulac, N. Karan, Y. Chen, Z. Liu

**2:50 INOR 1148.** Cubic Sn<sub>3</sub>Ge<sub>1-x</sub> nanoalloys: Beyond bulk composition limit. K. Ramasamy, J.M. Pietryga, S. Ivanov

**3:10** Intermission.

**3:25 INOR 1149.** Amine-copper (II) formates for the generation high conductivity copper films at low temperatures: Towards printing copper on PET. C. Paquet, T. Lacelle, B. Deore, A. Kell, I. Korobkov, S. Lafreniere, P.R. Malenfant

**3:45 INOR 1150.** Radical functionalization of boron nitride nanotubes. T. Sainsbury

**4:05 INOR 1151.** Polyarylboranes: A new and diverse class of small, metal-free quantum dots exhibiting high fluorescence quantum yields. M.W. Lee

**4:25 INOR 1152.** Fabrication of aluminum nanoparticles in constricted environments. C.O. Nyapete, P.A. Jelliss, S.W. Buckner

**4:45 INOR 1153.** Oxide-free functionalized silicon nanowires for versatile applications. J. Veerbeek, J. Huskens

## Section F

San Diego Convention Center  
Room 31B

### Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*  
M. P. Campos, B. Fokwa, *Presiding*

**1:30 INOR 1154.** Experimental and theoretical studies of the hard borides A<sub>3</sub>MB<sub>2</sub> (A = Nb, Ta; M = Fe, Ru, Os). R. Touzani, M. Mbariki, B. Fokwa

**1:50 INOR 1155.** Nanostructuring of superhard materials. M. Yeung, G. Akopov, R. Mohammadi, R.B. Kaner

**2:10 INOR 1156.** Characterization and surface organization of ligand substituted Mn<sub>2</sub> single molecule magnets. N.M. Khatiri, M. Pablico-Lansigan, K.D. Pires, S.E. Lofland, J.A. Borchers, P. Butler, M. Pileni, K. Plass, D. Keavney, S.L. Stoll

**2:30 INOR 1157.** Lanthanides-TTF complexes displaying single molecule magnet behaviour and luminescence. L. Ouahab, F. Pointillart

**2:50 INOR 1158.** New mixed-valence Mn<sub>3</sub> and Mn<sub>2</sub> clusters: Single-molecule magnetism and base-catalyzed transformation of alcohol into hemiacetals. O.A. Adebayo, K.A. Abboud, G. Christou

**3:10** Intermission.

**3:25 INOR 1159.** Tunable library of substituted thiourea and selenourea precursors to metal chalcogenide nanocrystals. M.P. Campos, J.S. Owen, M.P. Hendricks, I. Jen-La Plante, G.T. Cleveland, R.A. Swain, A.W. Graham

**3:45 INOR 1160.** One-step synthesis of core/shell nanocrystals with a graded interface. L. Hamachi, I. Jen-La Plante, J.S. Owen

**4:05 INOR 1161.** Solution-phase conversion of bulk oxides to metal chalcogenides. C. McCarthy, R.L. Brutchey

**4:25 INOR 1162.** Magneto-optical properties of europium sulfide-europium selenide solid solutions in the bulk and nanoscale. N. Rosa, H.A. Dalafa, A. Kawashima, S. Omagari, T. Nakanishi, Y. Hasegawa, S.L. Stoll

**4:45 INOR 1163.** Alkylation of CdSe nanocrystals with organometallic reagents. P. Chen, N.C. Anderson, Z. Norman, J.S. Owen

## Section G

San Diego Convention Center  
Room 31C

### Electrochemistry

B. L. Lucht, *Organizer*  
M. J. Rose, *Presiding*

**1:30 INOR 1164.** Chemically and electrochemically triggered assembly of viologen radicals: From the control of the  $\pi$ -dimerization to molecular switches. A. Milet, E. Saint-Aman, C. Kahlfuss, G. Bucher

**1:50 INOR 1165.** Bonding and function of nickel-phosphine H<sub>2</sub> catalysts to silicon(111) photoelectrodes: C-C covalent attachment and metal-oxide-phosphonate adsorption. M.J. Rose, J. Seo, H. Kim

**2:10 INOR 1166.** Composite  $n$ -Si(111) | R | metal-oxide photoelectrodes: Effect of interfacial organic linkers on charge transfer and ALD-based growth of TiO<sub>2</sub> ultra-thin films. R. Pekarek, M.J. Rose

**2:30 INOR 1167.** Investigating the mechanism of O<sub>2</sub> reduction with iron porphyrin electrocatalysts in the context of structure: Activity relationships. M. Pegis, N. Kumar, F.S. Menges, S. Raugel, M.A. Johnson, J.M. Mayer

**2:50 INOR 1168.** Dynamics of deposition, stripping, and passivation for Mg batteries. D.J. Wetzel, A.A. Gewirth, R.G. Nuzzo

**3:10 INOR 1169.** Fully-integrated wearable sensor array for multiplexed perspiration analysis. W. Gao, S. Emaminejad, H. Nyein, S. Challa, R.W. Davis, A. Javey

## Section H

San Diego Convention Center  
Room 32A

### Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*  
S. K. Hurst, *Presiding*

**1:30 INOR 1170.** Towards the stabilization of late transition oxo and imido complexes by cyclic (alkyl)(amino)carbenes (CAACs). D. Munz, J. Chu, M. Melaimi, R. Jazzar, G. Bertrand

**1:50 INOR 1171.** Oxidation chemistry facilitated by cryptand encapsulated M-O-M complexes. J. Stauber, E.D. Bloch, K.D. Vogiatzis, L. Gagliardi, D.G. Nocera, C.C. Cummins

**2:10 INOR 1172.** Selective two-electron reduction of carbon monoxide mediated by molybdenum complexes supported on an asymmetric phenol phosphine ligand. S. Riduan, J.A. Buss, T. Agapie

**2:30 INOR 1173.** Heterolytic activation of C-H bonds via bifunctional transition metal platforms. E.B. Hulley, W. Christman, T. Morrow

**2:50 INOR 1174.** Curved carbon-rich polyaromatic ligands: Convex and concave binding of multiple metal ions. S.N. Spisak, Z. Zhou, N.J. O'Neil, Z. Wei, M.A. Petrukhina

**3:10 INOR 1175.** Withdrawn.

**3:30 INOR 1176.** Photophysically innocent boron cluster ligand scaffolds for organic light emitting diode materials. K. Kirlikovali, J.C. Axtell, A. Gonzalez, A.C. Phung, S. Khan, A.M. Spokoyiny

**3:50 INOR 1177.** Activation of a gold catalyst by oxidation of a redox-noninnocent chlorostibine Z-ligand. H. Yang, F.P. Gabbai

**4:10 INOR 1178.** Exploring the promises of open cage fullerene coordination. A. Aghabali, M.M. Olmstead, A.L. Balch

**4:30 INOR 1179.** Synthesis of a series of aryl-14H-dibenzo[a,j]xanthene derivatives. S.K. Hurst

## Section I

San Diego Convention Center  
Room 32B

### Inorganic Spectroscopy

S. A. Koch, *Organizer*  
V. C. Popescu, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 INOR 1180.** Computational prediction on nuclear resonance vibrational anisotropy applied to Iron porphyrates. Q. Peng, R.W. Scheidt

**1:55 INOR 1181.** Probing valence orbitals using Co K $\beta$  X-ray emission. F. Li, E. Farquhar

**2:15 INOR 1182.** Homogenous approaches to solar hydrogen production from water. K. El Roz, R.S. Khnazyer, F.N. Castellano

**2:35 INOR 1183.** Cobalt and zinc complexes of hexamine cage ligands with multiple conformations in solution. L. Alcock, G. Cavigliasso, R. Stranger, A. Willis, J. Hook, D. Lawes, S. Ralph

**2:55 INOR 1184.** Withdrawn.

**3:15** Intermission.

**3:25 INOR 1185.** Unexpected photoluminescence enhancement from cyclometalated Ir(III) complexes in water. M. McGooty, R.S. Khnazyer, A. Singh, Y.G. Yingling, F.N. Castellano

**3:45 INOR 1186.** Effect of transition metal ions on the thermal transition of poly-N-isopropylacrylamide. L. Fulton, W. Seitz, R.P. Planalp

**4:05 INOR 1187.** Photo-induced electron and energy transfer in Heisenberg spin-coupled donor-acceptor complexes. D.M. Arias-Rotondo, J.K. McCusker

**4:25 INOR 1188.** Instrumentation for cyclotron resonance and electron spin resonance in high fields/frequencies. C.C. Beedle, R.D. McDonald, N. Harrison, J. Singleton

**4:45 INOR 1189.** Access to a second-order excited-state quenching mechanism. W.B. Swords, G.J. Meyer

**5:05 INOR 1190.** Tracking the excited state equilibrium in an Ir(III) bichromophore system: A combined time resolved spectroscopy and computational study. J. Yarnell, F.N. Castellano

## Section J

San Diego Convention Center  
Room 33A

### Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*  
K. Szabo, *Presiding*

**1:30 INOR 1191.** Probing early transition metals with macrocyclic tetracarbene ligands for catalytic aziridination. L.C. Keller, G.R. Elpittia, P.P. Chandrachud, D.M. Jenkins

**1:50 INOR 1192.** Ring expansion reactions of the anti-aromatic borole to prepare conjugated heterocycles. C. Martin

Technical program information  
known at press time.

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**2:10 INOR 1193.** Rhodium catalyzed C-H activation and hydroamination in a highly selective redox [4+2] imine/alkyne annulation. **R.S. Manan, P. Zhao**

**2:30 INOR 1194.** Application of rhodium-bis(diazaphospholane) catalyzed asymmetric hydroformylation in the enantioselective synthesis of quaternary aldehydes and sequence specific oligoesters. **F. Foarta, C.R. Landis**

**2:50 INOR 1195.** Asymmetric transformations using 1,1-disubstituted olefins as challenging substrates. **O. Pamies, M. Dieguez**

**3:10 INOR 1196.** Organometallic chemistry of adamantane: Toward novel functionalization of diamondoid hydrocarbons. **D. Armstrong, F. Taullaj, U.W. Fekl**

**3:30 INOR 1197.** General and green protocol for the allylation of tautomeric amidic nucleophilic centers through palladium catalysis. **S. Vemula, D. Kumar, G.R. Cook**

**3:50 INOR 1198.** Withdrawn.

**4:10 INOR 1199.** Alkyl carbon-nitrogen bond formation from Ir<sup>III</sup>. **T.E. Stevens, T.R. Cundari, K.I. Goldberg**

**4:30 INOR 1200.** Catalysis at metal-metal bonds. **C. Uyeda, T. Steiman, S. Pal, Y. Zhou**

**4:50 INOR 1201.** Metal mediated fluorination with fluoro-benziodoxole reagents. **K. Szabo**

## Section K

San Diego Convention Center  
Room 33B

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

J. S. Figueroa, *Presiding*

**1:30 INOR 1202.** Effect of ligand exchange processes in asymmetric catalysis and redox chemistry of rare earth alkali metal BINOLate heterobimetallic complexes. **J.R. Robinson, J. Gu, P.J. Carroll, P.J. Walsh, E.J. Schelter**

**1:50 INOR 1203.** Mesoionic carbenes in copper(I) catalyzed reactions. **S. Hohloch, L. Suntrup, F. Duecker, B. Sarkar**

**2:10 INOR 1204.** Pd-Cy\*Phine catalyzed copper-free sonogashira cross-coupling: Mechanism and insights from electronic structure calculations. **A.M. Mak, Y. Lim, H. Jong, E.G. Robins, C. Johannes, M.B. Sullivan**

**2:30 INOR 1205.** Ligand-free copper catalyzed hydrazination of terminal alkynes. **J. Peltier, R. Jazzar, M. Melaimi, G. Bertrand**

**2:50** Intermission.

**3:00 INOR 1206.** Theoretically-guided optimization of new ligand libraries for asymmetric reduction and C-C bond coupling reactions. **M. Diéguez, O. Pamies**

**3:20 INOR 1207.** Well-defined molybdenum isocyanide catalysts for regioselective hydrostannation. **K. Mandla, J.S. Figueroa**

**3:40 INOR 1208.** Withdrawn.

**4:00 INOR 1209.** Development of a rhodium(I) catalyst for single-step styrene production. **B.A. Vaughan, M. Webster-Gardiner, S. Karbalaeei Khani, T.R. Cundari, T.B. Gunnoe**

**4:20 INOR 1210.** New developments in the catalytic dehydrogenative borylation of terminal alkynes and the applications of alkynylboronates. **C.J. Pell, C. Lee, O. Zherov**

**4:40 INOR 1211.** Analysis on olefin hydrosilylation catalyzed by a cationic nickel allyl complex. **Y. Choe, J. Mathew, Y. Nakajima, S. Shimada, k. sato**

**5:00 INOR 1212.** Influence of Lewis acids on organometallic species. **J. Becica, D. Chen, L.V. Dinh, G. Dobreiner**

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Powering the Future: Novel Materials for Solar Cell Technologies

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#### Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger

*Sponsored by NUCL, Cosponsored by INOR‡*

#### Supramolecular Chemistry

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## THURSDAY MORNING

### Section A

San Diego Convention Center  
Room 30B

#### Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

K. N. Green, C. T. Saouma, *Presiding*

**8:30 INOR 1213.** Cobalt (III) complexes as pro drugs for cancer therapy. **C. Zhang, M. Sutherland, L. Chiang, R. Clarke, J. Thompson, C. Walsby, T.J. Storr**

**8:50 INOR 1214.** Pyridol derived N-heterocyclic amines and applications in catalysis and medicine. **K.N. Green, S.M. Brewer, H.M. Johnston, M. Burnett**

**9:10 INOR 1215.** Titanium(IV) serum transferrin structure: New insight into the use of chemical transferrin mimetics for Ti(IV) anticancer drug development. **A.D. Tinoco, S.A. Loza-Rosas, A.M. Vázquez, K.I. Rivero, L.M. Negrón, M. Saxena, S. Sharma, N. Zambrana, T.B. Parks**

**9:30 INOR 1216.** Evaluating the potential of deferasirox, a commercial chemical transferrin mimetic, in Ti(IV) anticancer drug design. **S.A. Loza-Rosas, A.M. Vázquez, K.I. Rivero, L.M. Negrón, T.B. Parks, A.D. Tinoco**

**9:50** Intermission.

**10:00 INOR 1217.** Structural features that influence photochemical reactivity and phototherapeutic activity of Ru(II) polypyridyl complexes. **E. Wachter, A. Zamora, Y. Sun, D.K. Heidary, E.C. Glazer**

**10:20 INOR 1218.** Redox-activated MRI contrast agents to detect oxidative stress. **C.T. Saouma, C. Mathis**

**10:40 INOR 1219.** Disulfide-masked thiosemicarbazone prochelators targeting the iron metabolism of cancer. **E. Akam, E. Tomat**

### Section B

San Diego Convention Center  
Room 30C

#### Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

S. Gage, R. Sardar, *Presiding*

**8:30 INOR 1220.** Improving the efficiency and stability of photochemical CO<sub>2</sub> reduction mediated by dye-sensitized ternary system (dye/TiO<sub>2</sub>/Re(I)). **H. Son, C. Pac, S.O. Kang, W. Dong-II, J. Lee**

**8:50 INOR 1221.** Withdrawn.

**9:10 INOR 1222.** Synthesis and photocatalytic properties of ternary metal halide nanocrystals. **B. Yin, B. Sadtler**

**9:30 INOR 1223.** Spectroscopic investigations of surface-immobilized molecular photocatalysts for CO<sub>2</sub> reduction. **M.E. Louis, T. Fenton, G. Li**

**9:50 INOR 1224.** Anisotropically shaped perovskite nanostructures synthesis and photovoltaic applications. **R. Sardar, M. Teunis**

**10:10** Intermission.

**10:25 INOR 1226.** Perovskite mysteries revealed: Amorphous and dopant phases studied by annealing, <sup>207</sup>Pb ssNMR, and XRD. **B. Rosales, L. Men, S. Cady, J. Vela-Becerra**

**10:45 INOR 1227.** Tiny TiN: Solution ammolysis reactions towards nanoparticulate titanium nitride and titanium-niobium nitride alloys. **J. Brancho, B.M. Bartlett**

**11:05 INOR 1228.** Size-controlled synthesis of later transition metal nitrides by templating using mesoporous silica. **S. Gage, M.R. Davidson, C.A. Cadigan, S. Pylypenko, B.G. Trewyn, R.M. Richards**

**11:25 INOR 1229.** Bendable zeolite membranes for pervaporation separation. **B. Wang, P. Dutta**

### Section C

San Diego Convention Center  
Room 30D

#### Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

M. E. Anderson, O. Miljanic, *Presiding*

**8:30 INOR 1230.** Metal-organic frameworks as scaffolds for probing HSAB properties. **T.A. Makal**

**8:50 INOR 1231.** 2D metal-organic frameworks as supramolecular building blocks for constructing ordered arrays of aromatic panels. **L.M. Lifshits, M. Zeller, J.K. Klosterman**

**9:10 INOR 1232.** Developing design rules for MOF thin film integration. **M.E. Anderson**

**9:30 INOR 1233.** Chemical vapour deposition of zeolitic imidazolate framework thin films. **I. Stassen, M. Styles, G. Greci, H. Van Gorp, W. Vanderlinden, S. De Feyter, P. Falcaro, D. De Vos, P. Vereecken, R. Ameloot**

**9:50 INOR 1234.** Synthesis and property of porous coordination polymer nano/micro-materials. **W. Sun**

**10:10** Intermission.

**10:25 INOR 1235.** Investigation of the surface properties and potential application areas of novel copper based metal organic framework synthesized by solvothermal and microwave assisted method with different heating and drying temperatures and durations, washing and filtration procedure. **A. Yurdusen, Y. Yurum**

**10:45 INOR 1236.** Withdrawn.

**11:05 INOR 1237.** Structure transitions of the Zr<sub>6</sub>(O)<sub>4</sub> clusters in NU-1000 and related MOFs. **A.E. Platero Prats, L.C. Gallington, A. Mavrandonakis, Y. Liu, J.T. Hupp, H.K. Farha, C.J. Cramer, K.W. Chapman**

**11:25 INOR 1238.** Nitrogen-rich porphyrinic metal-organic frameworks synthesized by postsynthetic metathesis method: From inert material to active catalyst. **X. Wang, H. Zhou**

**11:45 INOR 1239.** Withdrawn.

### Section D

San Diego Convention Center  
Room 30E

#### Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

C. W. Li, J. D. Rinehart, *Presiding*

**8:30 INOR 1240.** Solution-processed semiconductor materials for electronic and thermoelectric devices. **Z. Lin, A. Yin, Y. Huang, X. Duan**

**8:50 INOR 1241.** Multidimensional functional graphene materials and their applications. **T. Fan, S. Tong, S. Mo, Y. Yu, Y. Liu, Y. Min**

**9:10 INOR 1242.** Optimizing permanent magnetic materials through post-synthetic modification on the single-domain level. **J.D. Rinehart, P. Adelman**

**9:30 INOR 1243.** End-bonded contacts for carbon nanotube transistors with low, size-independent resistance. **Q. Cao**

**9:50 INOR 1244.** Optical characterization of oxides and sillenites of bismuth doped with Li<sup>+</sup>, Eu<sup>3+</sup> and Mn<sup>4+</sup>. **J. Ortiz Q, I. Zumeta Lubé, D. Diaz**

**10:10** Intermission.

**10:25 INOR 1245.** Surface reactivity of lead sulfide nanocrystals. **I. Preza, J.S. Owen**

**10:45 INOR 1246.** Band-edge potentials of colloidal semiconductor nanocrystals. **C. Brozek, G.M. Carroll, D.R. Gamelin**

**11:05 INOR 1247.** Intercolloidal charge transfer between ZnO nanocrystals and amorphous TiO<sub>2</sub> nanoparticles. **J. Lora, R. Mitsuhashi, J.M. Mayer**

**11:25 INOR 1248.** Distinctive, selective ligand binding sites on CdS nanocrystals affecting energy and charge transfer. **X. Li, L. Slyker, V. Nichols, G. Pau, C.J. Bardeen, M. Tang**

**11:45 INOR 1249.** Tailoring the surface of colloidal ZnO quantum dots for efficient photocatalytic charge transfer. **C.W. Li, P. Alivisatos**

**12:05 INOR 1250.** Proton coupled electron transfer at nanocrystals: Effects of protons on ZnO redox chemistry. **C. Valdez, J.M. Mayer**

### Section E

San Diego Convention Center  
Room 31A

#### Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

D. J. Brook, *Presiding*

**8:00 INOR 1251.** Using a Ru(II) building block and a rapid screening approach to identify nucleic acid selective "light switch" compounds. **E. Wachter, D. Moyá, E.C. Glazer**

**8:20 INOR 1252.** Rhodamine based turn-on fluorescent sensor for the detection of chromium ions. **R. Madawala, E. Sinn**

**8:40 INOR 1253.** New class of heterobimetallics with potential for CO<sub>2</sub> activation. **A.M. Lunsford, K. Goldstein, M. Cohan, M.Y. Darensbourg**

**9:00 INOR 1254.** Effect of redox-inactive metals toward reactivity of biomimetic Fe complexes. **T. Chantarojsiri, J. Yang**

**9:20 INOR 1255.** Four-electron reductive coupling of carbon monoxide: Evidence for dicarbyne and terminal carbide reaction intermediates. **J.A. Buss, T. Agapie**

**9:40 INOR 1256.** Metal-assisted (Zn, Au) thiolate-disulfide exchange: Explorations of the mechanism using 2D NMR. **G.S. Garusinghe, A.E. Bruce, M.R. Bruce**

10:00 Intermission.

10:10 INOR 1257. Evidence for valence tautomerism in the iron and cobalt complexes of verdazyls. D.J. Brook, C. Fleming, B. Ploof

10:30 INOR 1258. Synthesis and characterization of novel gold (III) thiolate complexes. M. Johnson

10:50 INOR 1259. Synthesis, characterization, crystallography, and antimicrobial activity of novel gold(II) complexes with phosphine ligands (L<sub>2</sub>) tris(4-methoxy-3,5-dimethylphenyl)phosphine and (L<sub>2</sub>) Bis(2-methoxyphenyl) chlorophosphine. K.J. Brown

11:10 INOR 1260. Why MLCT excited-states make poor photoacids, and how to overcome it. C.P. Ramirez, S. Ardo

11:30 INOR 1261. Chemical and spectroscopic characterization of a monomeric Ni(II)-OH complex derived from water. N. Lau, A. Borovik

11:50 INOR 1262. Dinitrogen activation by a zerovalent cobalt complex: Exploiting its reducing power. I. Reim, B.J. Cook, M. Pink, S. Bidwell, R.L. Lord, K.G. Caulton

12:10 INOR 1263. Generation of coordinatively unsaturated, Lewis acidic manganese(I) complexes via controlled *cis*-labilization of CO. D.W. Agnew, J.S. Figueroa

## Section F

San Diego Convention Center  
Room 31B

### Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

Z. Assefa, P. Desrochers, *Presiding*

8:00 INOR 1264. Withdrawn.

8:20 INOR 1265. Ruthenium polypyridyl complexes with antimony-substituted cyclometalating ligands. A.M. Christianson, F.P. Gabbaï

8:40 INOR 1266. Effects of the  $\mu_4$ -bridging atom in a tetranuclear iron cluster on the activation of nitric oxide. C. Reed, T. Agapie

9:00 INOR 1267. Thermally mediated decoherence in high-spin, nuclear spin-free transition metal complexes. J. Zadrozny, D.E. Freedman

9:20 INOR 1268. Investigating computational, structural, physicochemical and biological properties of a family of pyridoxine-lanthanide metal complexes. A. Saha, C.E. Stouder, K. Warren, C.W. Padgett, A.L. Stewart, K.S. Aiken, S.M. Landge, A. Amonette

9:40 INOR 1269. Structure and photoluminescent properties of dinuclear and tetranuclear Au(I) and Ag(I)-complexes with 1-methylbenzimidazole diphenylphosphine (MBDP) ligand. Z. Assefa, D.E. Jenkins

10:00 INOR 1270. Iron and cobalt chemistry of ferrocenyl substituted hydrotris(pyrazolyl)borate ligands. D.C. Cummins, K.H. Theopold, G.P. Yap

10:20 Intermission.

10:30 INOR 1271. Synthesis of a masked terminal nickel(II) sulfide via reductive deprotection. N.J. Hartmann, G. Wu, T.W. Hayton

10:50 INOR 1272. Curious stability of binuclear alkyl hydrides of chromium and their reaction with hydrocarbons. Y. Hung, K.H. Theopold, G.P. Yap

11:10 INOR 1273. Highly-reduced complexes of platinum and palladium supported by *m*-terphenyl isocyanides. B.R. Barnett, J.S. Figueroa

11:30 INOR 1274. Bimetallic indium complexes for the polymerization of cyclic esters. P. Kelley, P. Mehrhodavandi

11:50 INOR 1275. Chromium complexes of the redox-active [ONO] ligand and oxygen-atom transfer reactivity. A. Hollas, A.F. Heyduk

12:10 INOR 1276. Rapid synthesis of a functional resin-supported scorpionate and its copper(I, II), rhodium(I), and chromium(III) complexes. P. Desrochers, A. Pearce, T.R. Rogers

## Section G

San Diego Convention Center  
Room 31C

### Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

J. D. Blakemore, J. Yang, *Presiding*

8:00 INOR 1277. Withdrawn.

8:20 INOR 1278. Development of bis(arylimino)acenaphthene (BIAN) copper complexes as visible light harvesters for photovoltaic and artificial photosynthetic applications. J. Kee, Y. Lu, R. Ganguly, H. Soo

8:40 INOR 1279. Solvation effects on transition metal hydricity and electrocatalytic aqueous hydrogen production. J. Yang, C. Tsay, B. Livesay, S. Ruelas

9:00 INOR 1280. Proton-hydride tautomerism in hydrogen evolution catalysis. J.D. Blakemore, L.M. Aguirre Quintana, S.I. Johnson, J.R. Winkler, H.B. Gray

9:20 INOR 1281. Reusable materials in chemical sensing utilizing supramolecular  $pK_a$  shifts. N. Saleh

9:40 INOR 1282. Manifold of excited states and density of acceptors: Disentangling excited state electron injection into nanoporous titania. D.F. Ziegler, Z.A. Morseth, L. Wang, D.L. Ashford, M.K. Brennaman, E. Grumstrup, E.C. Brigham, M.K. Gish, R. Dillon, L. Alibabaei, G.J. Meyer, T.J. Meyer, J.M. Papanikolas

10:00 INOR 1283. Cation-dependent charge recombination to solution phase electron acceptors in dye-sensitized solar cells. B.N. DiMarco, R.M. O'Donnell, G.J. Meyer

10:20 Intermission.

10:30 INOR 1284. Nanoporous black silicon as a platform for photoelectrochemical hydrogen production: Exciting catalysts and nailing down the flatband potential. N.C. Anderson, N.R. Neale

10:50 INOR 1285. Hydrogenation of CO<sub>2</sub> and dehydrogenation of formic acid using Cp\*Ir complexes with imidazoline ligands. Y. Himeida, N. Onishi, M.Z. Ertem, A. Tsuruzaki, Y. Manaka, J.T. Muckerman, E. Fujita

11:10 INOR 1286. Hybrid molecule-nanocrystal photon upconversion across the visible and near-infrared. Z. Huang, X. Li, M. Mahboub, B. Yip, J. Rubalcava, K.M. Hanson, V. Nichols, H. Le, C.J. Bardeen, M.L. Tang

11:30 INOR 1287. Ternary Zn/Al/Ir layered hydroxide as efficient water oxidation catalyst. L. Fagiolarì, A. Scafuri, F. Costantino, R. Vivani, A. Macchioni

11:50 INOR 1288. Synthesis and surface chemistry of cadmium carboxylate passivated CdTe nanocrystals from cadmium bis(phenyltelluroate). M.P. Campos, J.S. Owen

12:10 INOR 1289. Distance-dependent energy transfer pathway between CdSe nanoparticles and anthracene during hybrid inorganic-organic upconversion. X. Li, R. Zavala, M. Tang

## Section H

San Diego Convention Center  
Room 32A

### Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

E. Borbas, J. Monteiro, *Presiding*

8:30 INOR 1290. Structural trends and solution behavior of actinide and lanthanide thiocyanate complexes. R. Wilson, T.J. Carter, S. Skanthakumar, L. Soderholm

8:50 INOR 1291. Chemical and electrochemical approaches to recycling rare-earth metals. J.A. Vigil, L.J. Small, T.N. Lambert, R.F. Hess, T.J. Boyle, M. Kelly

9:10 INOR 1292. Integrated toolkit of synchrotron X-ray and atomistic simulations for rare earth element refinery. B. Qiao, G. Ferru, M. Olvera De La Cruz, R.J. Ellis

9:30 Intermission.

9:40 INOR 1293. Reactivity of [K(18-crown-6)]([C<sub>5</sub>H<sub>3</sub>(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub>Th), the first complex containing thorium in the formal +2 oxidation state. R. Langeslay, M. Fieser, J.W. Ziller, F.U. Furcher, W.J. Evans

10:00 INOR 1294. Sequestering uranium from seawater: Accurate predictions of thermochemistry and structural properties. D.A. Penchoff, C. Peterson, J.P. Camden, D.M. Jenkins, A.K. Wilson

10:20 INOR 1295. Open frameworks assembling from selected *f*-elements and various di-carboxylic acids. R.A. Zehnder, M. Zeller

10:40 Intermission.

10:50 INOR 1296. Recycling rare earth elements using ionic liquids: An electrochemical approach. R.F. Hess, T.J. Boyle, J. Sears, L.J. Small, T.N. Lambert, D.R. Kammiller

11:10 INOR 1297. Biologically (RE)levant metals: Model studies of a new rare-earth dependent methanol dehydrogenase. W.L. Dornier, P.J. Carroll, E.J. Schelter

11:30 INOR 1298. X-ray absorption spectroscopy of actinium and americium. M. Ferrier, E.R. Batista, J.M. Berg, E. Birnbaum, J. Cross, J. Engle, K. John, S.A. Kozimor, V. Radchenko, B. Stein

## Section I

San Diego Convention Center  
Room 32B

### Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

D. Ess, *Presiding*

8:30 INOR 1299. Computation and experiment reveal unique reactivity and mechanisms of heterobimetallic and homobimetallic catalysts. D. Ess

8:50 INOR 1300. Ligand substituent effects on enantio- and regioselectivity in carbophilic catalysis with metal-acyclic diaminocarbene complexes. A. Ruch, X. Zhang, F. Kong, L.M. Slaughter

9:10 INOR 1301. Metal-carbon bond functionalization in the context of methane oxidation. R.J. Nielsen, M. Cheng, W.A. Goddard

9:30 INOR 1302. Exploiting electrophilic interactions to go beyond traditional pathways in hydrogenations with Wilkinson's catalyst. J.E. Perea-Buceta, I. Fernández, S. Heikkinen, K. Axenov, A. King, T. Niemi, M. Nieger, M. Leskela, T. Repo

9:50 INOR 1303. On the mechanism of the dual metal catalysis. A. Poater, S. Vummaleti, L. Falivene

10:10 INOR 1304. Highly enantioselective allylic alkylations in water. J. Eppinger, D. Sawant

10:30 INOR 1305. Base-free and acceptorless ruthenium-catalyzed dehydrogenative coupling of alcohols to esters. D. Nguyen, R. Gauvin, G. Raffia, L. Zhang, L.C. Demailly, P. Fongarland, S. Dasset, P. Sebastien, F. Dumeignil

10:50 Intermission.

11:00 INOR 1306. Redox non-innocent ligand supported manganese complexes for solar-light generation. T.K. Mukhopadhyay, T.L. Groy, R.J. Trovitch

11:20 INOR 1307. Transition-metal-catalyzed decarbonylation of biomass-derived carboxylic acids: A DFT study. M.A. Ortuno, B. Dereli, C.J. Cramer

11:40 INOR 1308. Light activated H<sub>2</sub> release from amine borane by [FeFe]ase mimics. J. Blank, A. Lunsford, S. Moncho Escrivá, S. Haas, M. Sohail, E.N. Brothers, M.Y. Darensbourg, A. Bengali

## Section J

San Diego Convention Center  
Room 33A

### Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

J. M. O Connor, *Presiding*

8:30 INOR 1309. Reactivity of Cp\*Co(IPr) with E-H Bonds: Experimental and computational studies of oxidative addition to a 16 electron Co(I) fragment. J. Andjaba, C.A. Bradley

8:50 INOR 1310. Withdrawn.

9:10 INOR 1311. Conversions of a metallocyclobutene to conjugated dienes. P. Qin, B. Cenzano-Fong, K.K. Baldrige, R.L. Holland, J.M. O Connor

9:30 INOR 1312. Structure and reactivity of a Ru(0) N-heterocyclic carbene pincer complex. A. Sasayama, C.P. Kubiak

9:50 INOR 1313. Reactions of pincer-type Pd<sup>II</sup>-Me complexes with molecular oxygen. K. Smoll, W. Kaminsky, K.I. Goldberg

10:10 INOR 1314. Withdrawn

10:30 INOR 1315. Synthesis and reactivity of (C<sub>2</sub>F<sub>5</sub>-PONOP) pincer complexes of iridium. P. Miller, J. Addams, T. Parson, D.M. Roddick

10:50 INOR 1316. DFT Calculations of spectra and binding mechanisms of bimetallic complexes. A.L. Cooksy, H. Amouri

11:10 INOR 1317. Stimuli induced, "on-off" ligation in a simple [Cu<sub>2</sub>(dppm)<sub>2</sub>(solvent)<sub>2</sub>]<sup>2+</sup> system. T.M. Brown, V.J. Catalano

11:30 INOR 1318. New paramagnetic rhodium(II) dimers without Rh-Rh bonds. D. Zhu, A. Sharma, C. Wiebe, P.H. Budzelaar

## Section K

San Diego Convention Center  
Room 33B

## Solid-State Inorganic Chemistry

C. G. Lugmair, V. Politavets, *Organizers*

J. Chan, *Presiding*

**8:30 INOR 1319.** Piezoelectrics: Putting the "squeeze" on new materials. A. Manjon-Sanz, T. Surta, R. McQuade, M. Dolgos

**8:50 INOR 1320.** Local order parameters: Descriptors for databases, synthesizability, interstitial relaxation, and diffusion paths. N.E. Zimmermann, M. Haranczyk

**9:10 INOR 1321.** Influence of Sn<sup>2+</sup>-substitution on the local structure of the Pb-free ferroelectric perovskites (Sr,Sn)TiO<sub>3</sub> and (Ba,Ca,Sn)TiO<sub>3</sub>. G. Laurita, K. Page, S. Suzuki, R. Seshadri

**9:30 INOR 1322.** Local structure influence on the insulator-metal transition in complex palladium oxides. L. Lamontagne, G. Laurita, M. Knight, H. Yusuf, R. Seshadri

**9:50 INOR 1323.** M&M process for ferrite synthesis. A.W. Apblett, A. Vecoven

**10:10** Intermission.

**10:25 INOR 1324.** Withdrawn.

**10:55 INOR 1325.** Withdrawn.

**11:15 INOR 1326.** Withdrawn.

**11:35 INOR 1327.** Synthesis, crystal growth, structural and magnetic characterization of NH<sub>4</sub>MCl<sub>2</sub>(HCOO), M = (Fe, Co, Ni). J.T. Greenfield, K. Kovnir

**11:55 INOR 1328.** Structural properties of ammonia borane/polymer composites. O. Gunaydin-Sen, R. Gangineni, S. Pati, R. Suwari

## Computational Materials &amp; Nanoscience: Theory Meets Experiment

## Forum: The Future of Spectroscopies: Quantum &amp; Classical Fields; Theoretical Perspectives

Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY

## Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger

Sponsored by NUCL, Cosponsored by INOR†

## THURSDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 30B

## Chemistry of Materials: Materials for Energy &amp; Catalytic Applications

C. G. Lugmair, *Organizer*

L. A. Fredin, M. Yadav, *Presiding*

**1:30 INOR 1329.** Potential of imogolite nanotubes as (co-)photocatalyst: A linear-scaling density functional theory study. E. Poli, J.D. Elliott, G. Teobaldi

**1:50 INOR 1330.** High energy hot electron generated from Mn-doped quantum dots: A new way to enhance photocatalysis. Y. Dong, J. Choi, H. Jeong, D. Son

**2:10 INOR 1331.** Understanding the photochemistry of earth abundant iron light harvesters for sensitization. L.A. Fredin

**2:30 INOR 1332.** One-pot synthesis of photocatalytically active metal chalcogenide aerogels. D.A. Ramirez, B. Pacheco, L. Luberski, L. Hope-Weeks

**2:50 INOR 1333.** New family of earth-abundant materials for solar energy conversion applications. K. Ramasamy, H. Sims, S. Ivanov, A. Gupta

**3:10** Intermission.

**3:25 INOR 1334.** Withdrawn.

**3:45 INOR 1335.** Organic-inorganic hybrid catalyst for alkane oxidation. M. Yadav, A.J. Karkamkar

**4:05 INOR 1336.** Sol-gel synthesis of composite Cu/ZnO/Y<sub>2</sub>O<sub>3</sub> nanomaterials as potential heterogeneous catalysts. R. Baghi, R.W. Lord, L. Hope-Weeks

**4:25 INOR 1337.** Immobilization of transition metal complexes on composite surfaces: Metal sensing and catalysis. E. Rosenberg, G. Abbott, J. Ross, R. McVay

**4:45 INOR 1338.** Palladium intercalated in the walls of mesoporous silica for robust, high temperature catalytic applications. R.M. Richards, S. Gage, M. Davidson, M. Menart, Y. Ji, J. Leong, S. Pylypenko, B.G. Trewyn, C. Ngo, S. Kodambaka

## Section B

San Diego Convention Center  
Room 30C

## Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

K. V. Lawler, A. Mavrandonakis, *Presiding*

**1:30 INOR 1339.** Light gas separations and storage with MOFs via DFT modeling, synthesis, and pressurized induced structural changes. T.M. Nenoff, D.F. Sava Gallis, M.V. Parkes, J. Greathouse, M. Rodriguez, K. Chapman

**1:50 INOR 1340.** MOF crystal chemistry paving the way to gas storage needs: Aluminum-based soc-MOF for CH<sub>4</sub>, O<sub>2</sub>, and CO<sub>2</sub> storage. D. Alezi, Y. Belmabkhout, M. Suyetin, M. Eddaoudi

**2:10 INOR 1341.** Separation of xylene isomers in the metal-organic frameworks CO<sub>2</sub>(dobdc) and CO<sub>2</sub>(m-dobdc): Adsorption differences and unexpected framework flexibility. M. Kapelewski, E.D. Bloch, M.I. Gonzalez, M.R. Hudson, D. Reed, G. Barin, C.M. Brown, J.R. Long

**2:30 INOR 1342.** polyMOFs as a strategy to obtain water tolerant materials for selective carbon dioxide separations. Z. Zhang, S. Cohen

**2:50 INOR 1343.** Multi-functional rare-earth porphyrinic shp-MOF platform meets the needs for gas storage, catalysis, and electron sensitizer. Z. Chen, K. Adil, Y. Belmabkhout, M. Eddaoudi

**3:10 INOR 1344.** Dramatic tuning on carbon dioxide uptake through pore space partition. X. Zhao, Q. Zhai, X. Bu, P. Feng

**3:30** Intermission.

**3:45 INOR 1345.** Computational investigation of C1-C2 hydrocarbons interacting with the open-metal sites of the MIL-127 framework. A. Mavrandonakis, V. Bernalles, L. Gagliardi, C.J. Cramer

**4:05 INOR 1346.** Importance of a precise crystal structure for simulating gas adsorption in nanoporous materials. K.V. Lawler, Z. Hulvey, P. Forster

**4:25 INOR 1347.** Reversible, low-concentration carbon monoxide binding in a metal-organic framework utilizing a unique spin state change mechanism. D. Reed, J.R. Long

**4:45 INOR 1348.** Carbon dioxide chemical fixation on metal-organic framework (MOF) platforms. W. Gao, S. Ma

**5:05 INOR 1349.** Evaluating Ni<sub>2</sub>(m-dobdc) and other metal-organic frameworks for high-pressure hydrogen storage. M. Kapelewski, T. Runcevski, H. Jiang, K. Hurst, T. Gennett, S. Fitzgerald, J.R. Long

**5:25 INOR 1350.** Extraordinary versatility of the metal-organic framework UiO-66-NH<sub>2</sub> for toxic chemical removal. G.W. Peterson, J.B. DeCoste

## Section C

San Diego Convention Center  
Room 30D

## Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

J. Florek, I. Jen-La Plante, *Presiding*

**1:30 INOR 1351.** Compact voltage sensitive nanocrystals for the imaging of neuron activity. I. Jen-La Plante, L. Hamachi, J.S. Owen

**1:50 INOR 1352.** Mesoporous silica nanoparticles: Selective surface functionalization and particle size control for optimal theranostic performances. M. Bouchoucha, R. C.-Gaudreault, M. Fortin, F. Kleitz

**2:10 INOR 1353.** Exploring disulfide and metal-mediated bonding as design principles for protein self-assembly. R. Subramanian, F.A. Tezcan

**2:30 INOR 1354.** Enzymatically responsive nanoparticle superlattices. S.N. Barnaby, R.V. Thamer, M.B. Ross, K. Brown, G.C. Schatz, C.A. Mirkin

**2:50 INOR 1355.** Synthesis of nanoinks using novel precursors for advanced Direct Write applications. L.J. Treadwell, T.J. Boyle, A. Cook, N.S. Bell

**3:10** Intermission.

**3:25 INOR 1356.** Molecular magnets gone dimensional. S.A. Corrales, T. Jenkins, D. Pistey, N. Mhesn, B. Voss, A.M. Mowson, G. Christou, A. Ozarowski, C. Lampropoulos

**3:45 INOR 1357.** Withdrawn.

**4:05 INOR 1358.** Nanoporous organo-functionalized materials as selective and regenerable sorbents for rare earth extraction. J. Florek, A. Mushtaq, E. Juère, F.G. Fontaine, D. Larivière, F. Kleitz

**4:25 INOR 1359.** Supercapacitors based on CuSbS<sub>2</sub> nanoplates. K. Ramasamy, R. Gupta, H. Sims, S. Ivanov, A. Gupta

**4:45 INOR 1360.** Observing different electronic sites in reduced titanium dioxide nanoparticles. J. Peper, J.M. Mayer

## Section E

San Diego Convention Center  
Room 31A

## Coordination Chemistry: Synthesis &amp; Characterization

S. A. Koch, *Organizer*

P. Chandrasekaran, *Presiding*

**1:30 INOR 1361.** Coordination chemistry of N-heterocyclic thione (NHT) and selone (NHSE) derivatives of caffeine. M. Styrón, D. Rabinovich

**1:50 INOR 1362.** Synthesis and characterization of bimetallic coordination complexes of tris(2-pyridyl)phosphine and its derivatives. A.K. Frampton, C. Fairfield, N.A. Piro, W.S. Kassel

**2:10 INOR 1363.** Magnetism of two-coordinate transition metal complexes. P. Bunting, J.R. Long

**2:30 INOR 1364.** Radical stabilization and ligand-based redox chemistry on oligopyrrolic fragments. R. Gautam, E. Tomat

**2:50 INOR 1365.** Towards terminal high-valent metal-oxo motifs on multimetallic scaffolds. G. de Ruiter, N.B. Thompson, T. Agapie

**3:10 INOR 1366.** Effects of methyl viologen on aminoethylglycine-functionalized [Ru(bpy)<sub>3</sub>]<sup>2+</sup> with pendant phenothiazines. B. Biber, M. Williams

**3:30 INOR 1367.** Structural properties of silver(I) and mercury(II) coordination polymers based on benzene-1,2,4,5-tetrathioether. P. Chandrasekaran, S. Kakumanu, T. Selby-Karani

**3:50** Intermission.

**4:00 INOR 1368.** Tetranuclear complexes as precursors for the rational design of pentanuclear oxido clusters reminiscent of the oxygen evolving complex in photosystem II. H. Lee, E. Tsui, T. Agapie

**4:20 INOR 1369.** Extremes of π-backdonation: The isolation of a m-terphenyl isocyanide stabilized Co-carbyne. C.C. Mokhtarzadeh, J.S. Figueroa

**4:40 INOR 1370.** Withdrawn.

**5:00 INOR 1371.** Modular approach to tuning the equatorial ligand field strength around a series of Co<sup>II</sup>-OH complexes with hydrogen bonding cavities in trigonal symmetry. J. Jones, A. Borovik

**5:20 INOR 1372.** Withdrawn.

**5:40 INOR 1373.** Intramolecular arene C-H and C-F activation by multimetallic tetramanganese clusters relevant to the oxygen-evolving complex of photosystem II. K.M. Carsch, G. de Ruiter, T. Agapie

## Section F

San Diego Convention Center  
Room 31B

## Nanoscience

R. M. Richards, *Organizer, Presiding*

**1:30 INOR 1374.** Photoinduced electron donor/acceptor processes between colloidal CdSe quantum dots and nitroxide free radicals. P. Dutta, R. Beaulac

**1:50 INOR 1375.** Hydrothermal synthesis of substitutionally-doped transition metal ions in SrTiO<sub>3-δ</sub> colloidal nanocrystals. W. Harrigan, S.E. Michaud, K.A. Lehuta, K.R. Kittilstved

**2:10 INOR 1376.** Electronic transport in self-assembled gold nanoparticle-molecular networks. P. Zhang, C. Papadopoulos

**2:30 INOR 1377.** Plasmonic metallurgy enabled by DNA. M.B. Ross, J.C. Ku, B. Lee, C.A. Mirkin, G.C. Schatz

**2:50 INOR 1378.** N-heterocyclic carbene precursors for Ag, Ag<sub>2</sub>S and Ag<sub>2</sub>Se nanocrystals syntheses. H. Lu, R.L. Brutchey

**3:10** Intermission.

**3:30 INOR 1379.** Tuning the magic size of atomically precise gold nanoclusters via isomeric methylbenzenethiols: Small change makes big difference. Y. Chen, R. Jin

**3:50 INOR 1380.** Computationally guided synthetic approaches to nanoscale metal carbide/nitride materials. S. Gage, C.A. Cadigan, C. Ciobanu, S. Pylypenko, B.G. Trewyn, R.M. Richards

**4:10 INOR 1381.** Mixed halide organolead perovskites: Dimensionality control and role of excess precursor on photoluminescence stability. L. Men, D. Freppon, U. Bhattacharjee, F. Zhu, B. Rosales, J.W. Petrich, E.A. Smith, J. Vela-Becerra

**4:30 INOR 1382.** Exploring the surface chemistry of semiconductor nanocrystals: From CdS to CsPbI<sub>3</sub>. H. Andaraarachchi, J. Vela-Becerra

## Section G

San Diego Convention Center  
Room 31C

## Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

S. N. Brown, M. Findlater, *Presiding*

**1:30 INOR 1383.** Transition metal oxos as frustrated Lewis pairs. E.A. Ison, N.S. Lambic

**1:50 INOR 1384.** Ligand-centered dehydrogenation reactions of metal bis- and tris-iminoxolones. S.N. Brown

**2:10 INOR 1385.** Pt(II) complexes supported on mesoporous silica nanoparticles: New catalyst for olefin hydroarylation. T.S. Gray, P. Kunal, M.M. Otting, N. Hirscher, J.R. Andreatta, L.G. Habgood, B.G. Trewyn, T.B. Gunnoe

**2:30 INOR 1386.** Withdrawn.

**2:50 INOR 1387.**  $sp^2$  C-H activation and C-C coupling catalyzed by Cu(I) complex with the ambiphilic ligand 8-quinolylidimesitylborane. S.R. Tamang, J.D. Hoefelmeyer

**3:10** Intermission.

**3:20 INOR 1388.** C-H activation by a titanium neopentylidene complex. D. Ninkovic, E. Brothers, S. Zaric, M.B. Hall

**3:40 INOR 1389.** Ir(III)-arene complexes as active catalysts for the oxidation of  $sp^3$  C-H bonds. S. Hohloch, S. Kaisser, F. Duecker, A. Bolje, R. Maity, J. Kosmirj, B. Sarkar

**4:00 INOR 1390.** Alkane dehydrogenation co-catalyzed by an iridium(III) complex and Lewis acids. Catalyst design and mechanistic study. Y. Gao, C. Guan, Z. Syed, T.J. Emge, A.S. Goldman

**4:20 INOR 1391.** Palladium complexes with electron-poor biscarbenes. P. Piernaria

## Section H

San Diego Convention Center  
Room 32A

## Organometallic Chemistry: Synthesis &amp; Characterization-Late Transition Metals

N. S. Radu, *Organizer*

D. B. Grotjahn, *Presiding*

**1:30 INOR 1392.** Ligands possessing C- and N-donors for ruthenium catalyzed water oxidation: Synthesis, characterization, and electrochemistry. A.G. Nash, D.B. Grotjahn

**1:50 INOR 1393.** High-valent Pd and Ni complexes supported by 1,4,7-trimethyl-1,4,7-triazacyclononane. M. Watson, L.M. Mirica

**2:10 INOR 1394.** Synthesis, characterization, and reactivity of mononuclear palladium complexes bearing nitrogen and carbon-donor ligands. N. Ruhs, N.P. Rath, L.M. Mirica

**2:30 INOR 1395.** Late transition metal complexes of protic bifunctional ligands: Activation of molecular oxygen. W.D. Bailey, R.A. Kemp, K.J. Goldberg

**2:50 INOR 1396.** First late transition metal cyclopentadienyl chelate complexes with silylphosphane or secondary phosphane tethers. I. Werner, S. Heinisch, H. Butenschoen

**3:10 INOR 1397.** Withdrawn.

**3:30 INOR 1398.** Synthesis and reactivity of copper hydride nanoclusters. T.D. Nguyen, G. Wu, T.W. Hayton

**3:50 INOR 1399.** Development and investigations into a bispyrazolyl mono-triazolyl heteroscorpionate platinum system. K. Lavoie, B. Frauhiger, P. White, J.L. Templeton

**4:10 INOR 1400.** Synthesis and characterization of  $(\text{N}4)\text{M}(\text{COD})$  ( $\text{R} = \text{Me}$  or  $\text{tBu}$ ,  $\text{M} = \text{Rh}$  or  $\text{Ir}$ ) complexes. K. Fuchigami, L.M. Mirica

**4:30 INOR 1401.** Incorporating a proaza-phosphatrane donor into a tripodal ligand. Z. Thammavongsy, I. Kha, J. Yang

**4:50 INOR 1402.** Towards transition metal complexes having 1,3-benzoxaphosphole ligands. A. Grimm, J. Protasiewicz

## Section I

San Diego Convention Center  
Room 32B

## Main Group Chemistry

T. W. Hudnall, *Organizer*

A. M. Spokoiny, *Presiding*

**1:30 INOR 1403.** Tin catalyzed hydrophosphination of secondary phosphines. J.P. Stelmach, R. Waterman

**1:50 INOR 1404.** Cationic gallium and indium complexes as Lewis acids for molecular catalysis: Structure-stability-activity relationships. V. Gandon

**2:10 INOR 1405.** Computational evidence for bond activation by main-group metals. D. Ess

**2:30 INOR 1406.** Mechanistic insight into ligand-based proton transfer reactions with a molecular aluminum complex. T. Sherbow, L.A. Berben

**2:50 INOR 1407.** Synthesis and characterization of low-valent aluminum clusters. L. Stevens, Y. Peng, D. Mayo, S.M. DeCarlo, P. Zavalij, K.H. Bowen, B.W. Eichhorn

**3:10** Intermission.

**3:20 INOR 1408.** Selective vertex cross-coupling of bromo-carboranes using electron-rich phosphine ligands. R.M. dziedzic, L.M. Saleh, S.L. Stevens, A.M. Spokoiny

**3:40 INOR 1409.** Hydrogen peroxide and dihydroperoxy alkane adducts of phosphine oxides as solid, stoichiometric, and soluble oxidizing agents. S. Ahn, J. Bluemel

**4:00 INOR 1410.** S-block grind: Mechanochemical synthesis of bulky allyl complexes of the s-block metals. N.R. Rightmire, T.P. Hanusa

**4:20 INOR 1411.** Lewis acidic properties of tryarylstibines. M. Yang, F.P. Gabbai

**4:40 INOR 1412.**  $\text{B}(\text{C}_6\text{F}_5)_3$  - A unique  $\pi$ -Lewis acid: Rearrangement and carboboration reactions. M.M. Hansmann

**5:00 INOR 1413.** Forming new bonds: Ditopic organoboranes in reduction reactions. T. Kaese, M. Wagner

## Computational Materials &amp; Nanoscience: Theory Meets Experiment

## Forum: Exciting Aspects of Excitation Dynamics &amp; Dissociation at the Nanoscale

Sponsored by MPPG, Cosponsored by COMF, ENFL, INOR, ORGN and POLY

## MEDI

## Division of Medicinal Chemistry

W. Young, *Program Chair*

## BUSINESS MEETINGS:

**MEDI Executive Committee Business Meeting,** 8:30 AM: Sun

**MEDI Division Business Meeting,** 4:30 PM: Sun

**Long Range Planning Committee,** 6:00 PM: Mon

## SUNDAY MORNING

## Section A

San Diego Convention Center  
Room 6F

## Bromodomain Inhibition: BETs &amp; Beyond

A. S. Duerfeldt, W. D. Schmitz, *Organizers, Presiding*

**9:00** Introductory Remarks.

**9:05 MEDI 1.** Bromodomain inhibitors: from chemical probe to clinic candidate. J. Qi

**9:35 MEDI 2.** New benzazepine and pyridopyrazinone BET-inhibitors for cancer treatment. N. Schmees

**10:05 MEDI 3.** BET proteins: Biology beyond cancer. G.V. Denis, J.T. Deeney, A.C. Belkina, O.O. Shirihai, B.E. Corkey

**10:35 MEDI 4.** From epigenetic mechanism to targeted therapy. M. Zhou

**11:05 MEDI 5.** Discovery and development of a potent dual TRIM24/BRPF1 bromodomain inhibitor, IACS-9571, using structure-based drug design. W.S. Palmer, G. Poncet-Montagne, G. Liu, A. Petrocchi, N. Reyna, G. Subramanian, J. Theroff, M. Kost-Alimova, J. Bardenhagen, E. Leo, H. Sheppard, T. Tieu, S. Xi, Y. Zhan, S. Zhao, M. Barton, G. Draetta, C. Toniatti, P. Jones, M. Geck Do, J. Andersen

**11:35 MEDI 6.** Hijacking ubiquitin E3 ligases using PROTAC technology to effectively degrade BRD4 and achieve anti-tumor efficacy. Y. Qian, J. Lu, K. Raina, M. Altieri, D. Gordon, A. Rossi, J. Wang, H. Dong, X. Chen, K. Siu, J. Winkler, C.M. Crews, K. Coleman, A. Crew

## Section B

San Diego Convention Center  
Room 6E

## General Orals

W. B. Young, *Organizer*

J. B. Schwarz, *Presiding*

**8:30 MEDI 7.** Scaffold hopping and optimization of maleimide based porcupine inhibitors. A. Poulsen, S.Y. Ho, W. Wang, J. Alam, A.J. Duraiswamy, G.R. Lin, S.H. Ang, E.S. Tan, M.A. Lee, Z. Ke, B. Madan, D. Virshup, L. Ding, V. Manoharan, C.Y. Shan, L.C. Bing, V. Pendharkar, K. Sangthongpitag, T.H. Keller

**8:50 MEDI 8.** Solubility sorted: Solid form disruption to improve solubility. C. Groom, E. Davis, J. Cole

**9:10 MEDI 9.** Targeting the transcriptional activation of human oncogenes with small molecules. D. Sun

**9:30 MEDI 10.** Alternative core development around HCV NS5A inhibitor MK-8742 scaffold. L. Tong, J.A. Kozlowski, W. Yu, C.A. Coburn, P.T. Meinke, A.G. Nair, M.P. Dwyer, O. Selyutin, S.B. Rosenblum, Y. Jiang, R. Liu, E. Asante-Appiah, S. Agrawal, E. Xia, S. Curry, P. Ingravallo

**9:50 MEDI 11.** Identification of a novel series of indole core protein modulators of the hepatitis B virus. S.D. Kuduk, A.M. Lam, C. Esperitu, R. Vogel, K. Klumpp, L. Flores, G.D. Hartman

**10:10 MEDI 12.** Evolution of synthetic cannabinoid designer drugs. S. Banister, M. Longworth, J. Stuart, R. Kevin, M. Glass, R. Gerona, M. Connor, I. McGregor, M. Kassiou

**10:30 MEDI 13.** Development of novel and selective factor IXa inhibitors. T. Zhang

**10:50 MEDI 14.** Selective deubiquitylase inhibitors for cancer immunotherapy. J. Wu, S. Kumar, G. Fegley, F. Wang, M. Kodrasov, S. Agarwal, M. Mattern, J. Weinstock

**11:10 MEDI 15.** Novel indole-2-carboxamides are highly potent against drug-sensitive and drug-resistant strains of *Mycobacterium tuberculosis*. J. Stec, O.K. Onajole, S. Lun, W.R. Bishai, A.P. Kozikowski

**11:30 MEDI 16.** Identification of a potent and selective covalent inhibitor of lysophospholipase-like 1 (LYPLAL1). J. Chen, K. Ahn, D. Anderson, M. Boehm, M.F. Brown, Y. Che, K.F. Fennell, K.F. Geoghegan, A.M. Gilbert, J. Gutierrez, J.J. Calloway, A.S. Kalgutkar, A. Lanba, C. Limberakis, T.V. Magee, I. O'Doherty, R. Oliver, B. Pabst, J. Pandit, K. Parris, R. Patel, J.A. Pfefferkorn, T. Rolph, B.P. Schuff, J. Starr, A. Varghese, N.B. Vera, C. Vernochet, J. Yan

**11:50 MEDI 17.** Discovery of CCT251921: A potent, selective and orally bioavailable small molecule modulator of the mediator complex-associated kinases CDK8 and CDK19. A. Mallinger, K. Schiemann, C. Rink, F. Stieber, M. Calderini, M. Stubbs, O. Poeschke, M. Busch, P. Czodrowski, D. Musil, D. Schwarz, M. Ortiz-Ruiz, R. Schneider, M. Valenti, A. de Haven Brandon, P. Workman, T. Dale, D. Wienneke, P. Clarke, C. Esdar, F. Raynaud, s. Eccles, F. Rohdich, J. Blagg

## From Synthesis to Design: Modeling Tools for Medicinal Chemists

Sponsored by COMF, Cosponsored by CINF and MEDI

## SUNDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 6F

## General Orals

W. B. Young, *Organizer, Presiding*

**1:30 MEDI 18.** Discovery of an iminopyridine derivative, TAK-259, as a novel, selective, and orally active  $\alpha_{1D}$  adrenoceptor antagonist with anti-urinary frequency effects. N. Sakauchi, Y. Kohara, A. Sato, T. Suzuki, Y. Imai, Y. Okabe, S. Imai, R. Saikawa, H. Nagabukuro, H. Kuno, H. Fujita, I. Kamo, M. Yoshida

**1:55 MEDI 19.** Minimizing CYP2C9 inhibition of exposed-pyridine inhibitors of NAMPT (nicotinamide phosphoribosyltransferase). M. Zak, N.J. Skelton, T. O'Brien, B.M. Liederer, D. Sampath, J. Oeh, W. Wang, X. Zheng, Y. Ho, P. Yuen, P.S. Dragovich

**2:20** **MEDI 20.** Creative medicinal chemistry solutions to complex metabolic and tissue distribution issues for the hepatitis C virus polymerase nucleoside inhibitor MK-0608. **Q. Dang,** Z. Zhang, T. Chen, H. Wang, J. Yin, S. He, G. Njoroge, L. Miesel, H. Huang, P.T. Meinke, D. Olsen

**2:45** **MEDI 21.** Discovery of MK-2548: A P2X3 receptor antagonist for the treatment of chronic pain. **D. Paone**

**3:10** **MEDI 22.** Targeted covalent and non-covalent ITK Inhibitors as useful tool compounds to evaluate ITK as an anti-asthma target. **Z. Pei**

**3:35** **MEDI 23.** Lead optimization of a series of selective TrkA inhibitors for the treatment of pain. **W.D. Shipe,** S. Mercer, M.E. Fraley, B. Wood, K. Babaoglu, N. Bhandari, C.W. Boyce, Y. Chen, A. Cooke, K. Feng, D. Henze, A. Kim, Y. Kuo, J. Lee, P. Liu, L. Xiaoyi, B. Ma, P. Manley, J. McCauley, M. McWherter, D. Meng, H. Mitchell, W. Morris, X. Niu, D.L. Parker, E. Price, K. Schirripa, A. Struyk, C. Stump, H. Su, J. Wu

**4:00** **MEDI 24.** Identification of selective JAK1 inhibitors for treatment of autoimmune diseases. **N. Kaila,** M.L. Vazquez, R.J. Unwalla, J.W. Strohbach, J. Trzupuk, S. Han, R.P. Robinson, M.D. Parikh, E. Arnold, C. Choi, S. Drozda, M. Dowty, J. Tellez, M. Hegen, P. Symonowicz, J. Jussif, Z. Radi

**4:25** **MEDI 25.** Strategies toward optimizing the metabolism of a novel series of 5HT4 partial agonists. **M.A. Brodney,** A. Sawant, R. Obach, E.A. LaChapelle, M. Vanase-Frawley

**4:50** **MEDI 26.** Recent advances in the design and synthesis of oncology drug candidates. **S. Bailey**

## Section B

San Diego Convention Center  
Room 6E

### Medicinal Chemists' Toolbox: Recent Strategies & Tactics for Resolving Off-Target Liabilities

N. A. Meanwell, P. M. Scola, K. Yeung, *Organizers, Presiding*

**2:00** Introductory Remarks.

**2:05** **MEDI 27.** Incorporation of transporter data for driving decision making in drug discovery. **M. Soars**

**2:45** **MEDI 28.** Intramolecular H-bonding and other recent approaches to circumvent P-gp efflux. **M.J. Blanco-Pillado**

**3:25** **MEDI 29.** Predicting, identifying, and managing aldehyde oxidase metabolism in drug discovery. **A.C. Burns**

**4:05** **MEDI 30.** Dealing with reactive drug metabolites in drug discovery: Can we predict toxicities of drug candidates that form reactive metabolites? **D.K. Dalvie**

**4:45** **MEDI 31.** Considerations of plasma protein and tissue binding in drug design. **X. Liu**

### Discussions with the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

### Global Initiatives in Research Data Management & Discovery

#### Global Landscape

*Sponsored by CINF, Cosponsored by ANYL, COMP, MEDI and PHYS*

## SUNDAY EVENING

### Section A

San Diego Convention Center  
Hall F

#### General Posters

W. B. Young, *Organizer*

**7:00 - 9:00**

**MEDI 32.** Impact of injection solvent choice on peak shape and resolution in reversed-phase flash chromatography. **J.R. Bickler**

**MEDI 33.** Options available for green flash chromatography. **J.R. Bickler**

**MEDI 34.** Quantitative analysis of proteins by selected reaction monitoring mass spectrometry and application to clinical samples. **S. Kurono, S. Niwayama**

**MEDI 35.** Drug-herb interaction: A crossover study of the effect of a polyherbal herbal formulation, Katoka<sup>®</sup>, on metronidazole pharmacokinetic profile drug-herb interaction: a crossover study of the effect of a polyherbal herbal formulation, Katoka<sup>®</sup>, on metronidazole pharmacokinetic profile. **G.E. Ukpo**

**MEDI 36.** Pyrroloacridiniums as chemiluminescent reagents for immunoassay diagnostics. **B. Bax,** R. Himmelsbach, J.P. Skinner

**MEDI 37.** Stability of total prostate specific antigen in serum kept under unique storage conditions. **A. Elezzi,** W.R. Zaidan, K. Weitze, M. EL-Saidi

**MEDI 38.** Extraction and purification of some chloroplast pigments from the leaves of *Telfaria Occidentalis* and study of solvent effects on their absorption spectra 1. **F.U. Akhigbe**

**MEDI 39.** Discovery of functionalized *N,N*-biarylamines as potent and selective exchange proteins directly activated by cAMP isoform 2 (EPAC2) inhibitors. **C. Wild,** Y. Zhu, N. Ye, M. Fang, M.A. Ynalvez, H. Chen, X. Cheng, J. Zhou

**MEDI 40.** Withdrawn.

**MEDI 41.** Novel pH-dependent H<sub>2</sub>S donors and their biological applications. **J. Kang,** C. Park, Z. Li, C. Organ, C. Yang, A. Pacheco, D.J. Lefler, M. Xian

**MEDI 42.** Synthesis of amphiphilic cyclic and linear peptide-fatty acid conjugates and studying their interactions with siRNA. **H. Do,** R. Tiwari, **K. Parang,** H. Montazeri Alabadi

**MEDI 43.** Synthesis and evaluation of fatty acyl derivatives of (HR)<sub>n</sub> peptides as cell-penetrating peptides. **N. Aboud,** T. Miyake, A. Shirazi, **A. Suzuki,** A.I. Shiroishi, K. Parang, R.K. Tiwari

**MEDI 44.** Withdrawn.

**MEDI 45.** Cooperativity and hydrophobic collapse can be potential factors for micro-molar to pico-molar change in binding affinity: A case study using thrombin inhibitors. **A.M. Said,** D.G. Hangauer

**MEDI 46.** Discovery of potent and selective factor 11a arylpyrrolidine benzothioephene inhibitor. **A.K. Ogawa,** E. VandeBunte, C. Lesburg, Z. Guo, Y. Gao, R. Mal, R. Moningka, A. Romero, R. Anand, V.J. Colandrea, W. Geissler, R. Patel, X. Song, R. Tschirret-Guth, B. Hawes, B. Wood, S. Edmondson

**MEDI 47.** Synthesis and *in vitro* activity of ectonucleotide pyrophosphatase / phosphodiesterase 1 inhibitors. **E. Forcellini,** E. Shayhidin, M. Boulanger, A. Mahmut, C. Lefevre, S. Boutin, X. Barbeau, P. Lague, P. Mathieu, J. Paquin

**MEDI 48.** Small molecule KLF5 inhibitors: New agents for treating colorectal cancers. **C. Wang,** A. Eguizabal, Y. He, T.D. Bannister, M. Garcia-Barros, A. Bialkowska, V. Yang

**MEDI 49.** Synthesis and biological evaluation of naphthoquinones as HER2 kinase inhibitors. **R. Schroeder,** M. Stoudouris, P. Tram, T. Stone, K. Nguyen, F. Jones, J. Sridhar

**MEDI 50.** Design, synthesis and biological evaluation of diarylheptanoids. **W. Yin,** Y. Jahng, Y. Kwon, **A.M. Rahman**

**MEDI 51.** Homology model guided design and synthesis of MCT1 and four inhibitors. **S. Wood,** J. Choi, J. Doherty, C. Yang, T.D. Bannister, J. Cleveland, W.R. Roush

**MEDI 52.** Thio-disaccharides induces an oxidative stress that kills cervix epitheloid carcinoma cells. **Z.J. Witczak,** J. Sarnik, A. Czubatka, A. Maciejka, T. Poplawski

**MEDI 53.** Vitamin D3 analogues as selective hedgehog pathway inhibitors. **C. Maschinot,** M.K. Hadden

**MEDI 54.** Repurposing itraconazole as an anticancer chemotherapeutic. **J.R. Pace,** M.K. Hadden

**MEDI 55.** *In vitro* cell viability and mice tumor xenograft effect of doxorubicin analogs on soft tissue sarcomas. **P. Moon,** D.L. Warner, K. Cornell, R. Carfi

**MEDI 56.** Synthesis of indazole derivatives and evaluation of their antiproliferative activity. **J. Zhao,** H. Chen, G. Yu, G. Li, C. Sun, W. Li

**MEDI 57.** Plinabulin: A marine drug candidate for anti-tumor. **W. Li,** T. Sun

**MEDI 58.** Deuteration in drug discovery. **F. Li,** W. Jiang, A.W. Czarnik, W. Li

**MEDI 59.** Discovery of a potent broad spectrum antiproliferative benzothiazole derivative with nanomolar multikinase activity. **A.K. El-Damasy**

**MEDI 60.** Chromenone MCT inhibitors: Targeting unique metabolic properties of tumor cells. **C. Wang,** H. Wang, C. Yang, J. Cleveland, T.D. Bannister

**MEDI 61.** Synthesis and biological evaluation of 4,6-diaryl-2-aminopyrimidine analogues as anticancer agents. **A. Khurana,** R. Bansal, K. Dhar

**MEDI 62.** Characterization of small molecule inhibitors of HPV E6. **J.L. Krstenansky,** S. Kolluru

**MEDI 63.** Identification of ACY-1083: A novel, potent, and highly selective HDAC6 inhibitor. **A. Molina**

**MEDI 64.** Development of glutaminase inhibitors for cancer therapeutics.

**S. Zimmermann,** E. Wolf, A. Luu, A. Thomas, J. Alt, B. Poore, A. Le, R. Rais, B. Slusher, T. Tsukamoto

**MEDI 65.** Type IIb prodrugs of riluzole for the treatment of melanoma and ALS. **H. Bian,** S. Chen, J.C. Pelletier, R. Shah, J.E. Wrobel, M.E. McDonnell, B.E. Blass, M.D. Vera, G.R. Smith, A.B. Reitz

**MEDI 66.** 2,3-dehydrostilbinin derivatives: Design, synthesis, and biological evaluation in human prostate cancer cell models. **S. Zhang,** B. Vae, X. Zhang, T. Lee, M. Huang, Q. Chen

**MEDI 67.** Discovery and optimisation of 2,8-disubstituted naphthyridine and 4,6-disubstituted isoquinoline series as modulators of the mediator complex-associated kinases CDK8 and CDK19.

**A. Mallingner,** K. Schiemann, C. Rink, J. Seiberger, M. Honey, M. Stubbs, O. Poeschke, M. Busch, P. Czodrowski, R. Schneider, D. Musil, D. Schwarz, M. Ortiz-Ruiz, P. Workman, K. Urbahns, D. Wienke, P. Clarke, C. Esdar, F. Raynaud, s. Eccles, F. Rohdich, J. Blagg

**MEDI 68.** Withdrawn.

**MEDI 69.** Role of water in the DNA doxorubicin intercalation mechanism. **J. Finan**

**MEDI 70.** Disruption of the Mcl-1-Bak-BH3 protein-protein interaction with 2,6-disubstituted nicotines. **B. Drennen,** J. Scheenstra, J. Yap, P. Wilder, L. Chen, M.E. Lanning, S. Fletcher

**MEDI 71.** Withdrawn.

**MEDI 72.** Novel CDK8 inhibitors with long residence time new opportunities for cancer treatment. **J. Benningshof,** P. van Meurs, E. Damen, J. Veerman, H. Weber, F. Totzke, J. Ehler, C. Schächtele, M. Kubbutat, G. Mueller

**MEDI 73.** Discovery of novel cleavable linkers for site-specific antibody drug conjugates containing non oncology payloads. **J.C. Kern,** R. Garbaccio, M. Cancilla, D. Dooney, K. Kwasiujuk, R. Zhang, S. Antonenko, M. Beaumont, I. Figueroa, S. Hsieh, L. Liang, D. Tomazela, J. Zhang, S. Zhang, Y. Zhang, P.E. Brandish, A. Palmieri, P. Stivers, M. Cheng, G. Feng, P. Geda, S. Shah, A. Beck, D. Breeson, J. Firdos, D. Gately, N. Knudsen, A. Manibusan, Y. Sun

**MEDI 74.** Structure-based design, synthesis, and activity studies of small hybrid molecules targeting G9a and HDAC enzymes. **M. Kondengaden,** P.G. Wang

**MEDI 75.** Exploring EGFR kinase-ligand interactions for optimizing dual action inhibitors. **H. Shadnia,** C. Williams, J. Bertrand

**MEDI 76.** Structural approach to elucidating metalloenzyme inhibitor selectivity. **B. Dick,** S. Cohen

**MEDI 77.** Design and synthesis of novel probes for irreversible binding to glutathione S-transferase (GST) and uridine 5'-diphospho-glucuronosyl transferase (UGT) enzymes. **R.N. Nair,** R. Corley, A.T. Wright

**MEDI 78.** Synthesis and medicinal chemistry optimization of CK2 kinase inhibitors. **J. Dowling**

**MEDI 79.** Synthesis and DNA binding studies of heterocyclic amidines designed to target DNA mixed sequences containing guanine. **R. Abou-Elkhair,** A. Paul, P. Guo, D.W. Boykin, **W. Wilson**

**MEDI 80.** Novel quaternary ammonium cucuminoinds as potential anticancer agents. **S. Gurrappu,** L. Solano, G.L. Nelson, S.K. Jonnalagadda, C. Ronayne, E.A. Lueth, M. Hill, V.R. Mereddy

**MEDI 81.** Targeting protein kinases in DFG-out conformation for cancer poly-pharmacology. **P. Ung,** A. Schlessinger

**MEDI 82.** Design and synthesis of small molecule HDAC inhibitors equipped with ER $\alpha$  activity for selective targeting of the breast cancer. **V. Khodaverdian**

**MEDI 83.** Withdrawn.

**MEDI 84.** DNA shape influences minor groove binding of a synthetic small molecule. **S. Laughlin-Toth,** E.K. Carter, Y. Chai, I.N. Ivanov, D.W. Boykin, W. Wilson

- MEDI 85.** CDK8/19 inhibitors: 3-benzylindazoles. **K. Schiemann**, A. Mallinger, D. Wienke, C. Esdar, O. Poeschke, M. Busch, F. Rohdich, s. Eccles, R. Schneider, F. Raynaud, P. Czodrowski, D. Musil, D. Schwarz, K. Urbahns, J. Blagg
- MEDI 86.** Synthesis of 5-BDBD analogues as new potential P2X4 receptor antagonists. **M. Wang**, **M. Gao**, J. Meyer, J. Peters, H. Zarrinmayeh, P. Territo, Q. Zheng
- MEDI 87.** Design and evaluation of naphthyridones as novel KDM5A inhibitors. **S.S. Labadie**, P.S. Dragovich, L. Ackerman, R. Cummings, G. Deshmukh, A. Gustafson, J. Harmange, J.R. Kiefer, J. Liang, B.M. Liederer, Y. Liu, W. Mao, W. Manieri, L. Murray, D.F. Ortwine, P. Trojer, E. VanderPorten, M. Vinogradova
- MEDI 88.** Discovery of novel (2-(substituted benzylsulfonyl) ethyl) substituted benzenes as highly potent anti-cancer agents. **M. Reddy**, **M.R. Mallireddigari**, S.C. Cosenza, B. Akula, D. Subbaiah, E. Bharathi, V. Pallela, S. Divakar, P. Reddy
- MEDI 89.** Synthesis, synthesis and biological evaluation of DS-5272: A potent p53-MDM2 interaction inhibitor possessing a dihydromidazothiazole scaffold. **M. Miyazaki**, K. Uoto, Y. Sugimoto, H. Naito, K. Yoshida, T. Okayama, H. Kawato, H. Shimizu, M. Miyazaki, M. Kitagawa, T. Seki, S. Fukutake, M. Aonuma, T. Soga
- MEDI 90.** New metformin analogues for the treatment of triple-negative breast cancer. **E. Diers**, G. Deng, D. Márquez-Garban, R. Pietras, M.E. Jung
- MEDI 91.** Optimisation of RET inhibitors with improved KDR selectivity. **R. Newton**, S. Fritzl, A.M. Jordan, N. McDonald, H. Small, I. Waddell, B. Waszkowycz, A. Watson, D. Ogilvie
- MEDI 92.** Histone deacetylase inhibitors equipped with selective estrogen receptor modulator to fight against breast cancer. **S. Fathi**, L. Szymczak, M. Mirksich, A.K. Oyeler
- MEDI 93.** Synthesis and biological characterization of novel CD3254 analogs. **C.E. Wagner**, P.W. Jurutka, P.A. Marshall, I. Kaneko, P. Shahani, D.H. Seto, J. Varkey, C.L. Hum, J.T. Sarnowski, M.R. Wentzel, C. Chhun
- MEDI 94.** Synthesis and biological characterization of novel NEI-TMN analogs. **C.E. Wagner**, P.W. Jurutka, P.A. Marshall, M.C. Heck, P. Shahani, S. Bains, M. MacNeill, M. Shimabuku, N.M. Robinson, D.H. Seto, J. Varkey, C.L. Hum
- MEDI 95.** Synthesis, SAR, and combination study of novel third-generation taxoids. **X. Wang**, C. Wang, S. Lee, I. Ojima
- MEDI 96.** Batch-flow approach to levomilnacipran. **R. Pineda**, S. Matsuda, A.C. Evans
- MEDI 97.** Synthesis and biological evaluation of cyclopentaquinoline derivatives as nonsteroidal glucocorticoid receptor antagonists. **M. Edda**, T. Kuroda, S. Kaneko, Y. Aoki, O. Chieko, T. Ohbora, M. Sakae, N. Koyama, K. Aritomo
- MEDI 98.** Discovery of KATII inhibitors via a fragment-based approach. **Y. Han**, S.M. Stachura, A. McClure, C.L. Cavallaro, C. Allard, R. Rajamani, W. Yong, H. Lewis, J. Muckelbauer, D.A. Loughney, W. Metzler, D. Nirschi, H.N. Weller, S.W. Gerritz
- MEDI 99.** Design and synthesis of potential CNS-permeable inhibitors of *T. gondii* Cathepsin L. **N. Diaz**, J. Zwicker, S.D. Larsen, V. Carruthers
- MEDI 100.** Structure-based design of selective calpain-2 inhibitors. **Y.L. Luo**, P. Chatterjee, A. Alsamrah, D. Kent, M. Baudry
- MEDI 101.** Coumarin analogues as potential inhibitors of acetylcholinesterase: Synthesis, molecular docking, and biological studies. **S. Singla**, P. Piplani
- MEDI 102.** Natural product galangin is an APP-Selective BACE inhibitor and is a potential agent to treat Alzheimer's disease. **B. Jagodzinska**, J. Campagna, P. Spilman, D. Bai, V. John
- MEDI 103.** Identification of a conformationally restricted analog of GABA as the first highly selective BGT-1 inhibitor based on the three-dimensional structural diversity-oriented strategy. **A. Suemasa**, T. Kobayashi, H. Fukuda, A. Igawa, S. Ide, M. Minami, S. Shuto
- MEDI 104.** Withdrawn.
- MEDI 105.** Development of a drug candidate for Alzheimer's disease. **J. Pham**, J. Campagna, P. Spilman, M. Alam, B. Jagodzinska, D. Bredesen, M.E. Jung, V. John
- MEDI 106.** Probing the muscarinic pharmacophore with novel and functionally selective M<sub>1</sub>/M<sub>2</sub> non-competitive antagonists. **J.F. Boulos**, J. Momirov
- MEDI 107.** Design, synthesis and biological evaluation of novel dual-acting, non-brain penetrant inhibitors of inducible nitric oxide synthase (iNOS) and cannabinoid (CB1) receptors. **M.R. Iyer**, R. Cinar, G. Kunos
- MEDI 108.** Exploring the biochemical effects of methylene blue on a triple transgenic mouse model of Alzheimer's disease. **L.S. Webb**, **B.C. Genovese**, S.E. Fink, Q.E. Pace, N. Khan, H.J. Grauf, D. Mitran
- MEDI 109.** Design and evaluation of inhibitors of A $\beta$ <sub>42</sub> aggregation. **S. Veliyath**, S. Kantham, S. Dighe, G. Deora, S. Chan, R. McGeary, B. Ross
- MEDI 110.** Withdrawn.
- MEDI 111.** Synthesis of novel  $\beta$ -carbolines as a GABA<sub>A</sub> subtype selective agents for the treatment of alcohol abuse. Regiospecific solution to the problem of 3,6-disubstituted  $\beta$ - and aza- $\beta$ -carboline specificity. **V. Tiruveedhula**, K. Warnock, X. Simeone, M. Ernst, M. Gondre-Lewis, J.M. Cook
- MEDI 112.** Problem-based learning in drug discovery with MOE. **A. Bonin**
- MEDI 113.** Privileged scaffolds and frequent hitters in drug discovery. **P. Schneider**, G. Schneider
- MEDI 114.** Evaluating docked poses using SAR data. **D.W. Moreland**
- MEDI 115.** CDD vault: A modern approach for drug research project team informatics. **B.A. Bunin**
- MEDI 116.** Rationalizing non-standard interactions in ligand design: The duality of halogens. **E. Metwally**, A. Ajamian, C. Williams
- MEDI 117.** Highly functionalized spirohydantoin as 3-dimensional templates for fragment screening. **H. Prevet**, M. Filipo, O. Sperandio, B. Deprez, N. Willand
- MEDI 118.** PHGDH: A case study for the structural rationalization of thermodynamics and kinetics of protein-ligand binding. **I. Lukac**, A. Leach, J. Madden, G. Holdgate, G. Davies
- MEDI 119.** Generating accessible, novel R-groups in lead optimization. **T. Cheeseright**, **R. Lawrence**, M. Mackey, G. Tedesco
- MEDI 120.** Application of 3D-RISM to water placement and scoring. **A. Ajamian**
- MEDI 121.** Towards more explicit understanding of the binding molecular aspects: hydrophobic-based cooperativity among series of thrombin inhibitors. **A.M. Said**, D.G. Hangauer
- MEDI 122.** Novel biologically performance-based compounds. **J. Zoller**, O.O. Verho, Z.V. Boskovic, M. Wawer, S. Dandapani, S.L. Schreiber
- MEDI 123.** Design and characterization of high quality, chemically diverse fragment libraries to support orthogonal fragment screening campaigns and rapid hit identification, validation, and follow up. **P.S. Tanis**, D. Cole, R. Kamran, D. Lawson, P. Schwartz, C. Smith, S. Swann, S. Wang, X. Wang, S. Woodhead, H. Wu
- MEDI 124.** Withdrawn.
- MEDI 125.** Novel self-patented gold nanoparticles for antineoplastic activity. **J. Payne**, R. Dakshinamurthy
- MEDI 126.** Novel self-patented gold nanoparticle synthesis, characterization, and antibacterial susceptibility testing. **H. Moolani**, J. Payne, R. Dakshinamurthy
- MEDI 127.** Development and impact of the medicinal chemistry sub-team of the ACS GCJ pharmaceutical roundtable. **D.T. Richter**, J.B. Manley, M.C. Bryan, P. Richardson, L.E. Shuster, F. Gallou, I.T. Raheem, M. Grist, H. Sneddon
- MEDI 128.** New fluoroquinolone hydroxamic acids as antibacterial and urease inhibitors: Design, synthesis and molecular docking studies. **M.A. Ali**, G.A. Abuorahmaa, R.M. Abdelbaky, E.M. Abdel Hafez, H.A. Hassan
- MEDI 129.** Design, synthesis, and structure activity evaluations of broad spectrum antibacterial activity of quinoline-based bisarylimidazole motifs. **M. Semreen**, R. Abu Odeh, R. Al-Qawasmeh, M. Abu-Zarga, B. Bani Huthail, H. Tarazi, T.H. Altel
- MEDI 130.** Lead optimization of a thienopyridine scaffold possessing pan-serotype antiviral activity against dengue virus. **J. Burgeson**, D. Dai, A. Berhanu, D. Grosenbach, K. Jones, C. Lovejoy, S. Tyavanagimatt, R. Jordan, C. Byrd, D. Hruby
- MEDI 131.** Evaluation of functional carb-pharmacophores as a potential inhibitors of *Tubercle bacilli*. **Z.J. Witzcak**, M. Korycka-Machala, A. Brzostek, J. Dziaadek
- MEDI 132.** New series of bisphosphonate inhibitors of geranylgeranyl diphosphate synthase. **B.J. Foust**, C. Allen, S.A. Holstein, D.F. Wiemer
- MEDI 133.** Enantioselective synthesis of 2-aziridinyl phosphonates and studies of their biological activities. **O. Dogan**, S. Polat Cakir, N. Beksultanova, N. Altanlar, D. Simsek
- MEDI 134.** Oxadiazole-based cell permeable macrocyclic transition state inhibitors of norovirus 3CL protease. **V. Damalanka**, Y. Kim, K. Alliston, P. Weerawarna, A. Galasiti Kankanamalage, G. Lushington, N. Mehzabeen, B. Kevin, S. Lovell, K. Chang, W. Groutas
- MEDI 135.** Boceprevir as a viable HCV treatment: Making dosage more manageable. **C. Santori**, **M.G. Fritsche**, **A. Andes**, I.J. Kresse, G. Jones
- MEDI 136.** Withdrawn.
- MEDI 137.** Construction and validation of the 3D-structure of *T. cruzi* siriuin-2 by modeling threading. **G.M. Monteiro Ferreira**, V.G. Maltarollo, F.S. Emery, G. Trossini
- MEDI 138.** Design, synthesis, and antimicrobial activity of ATP-binding site inhibitors of N<sup>5</sup>-CAIR synthetase. **Q. Lin**, S.M. Firestone
- MEDI 139.** Discovery and preclinical characterization of the P1 *bi*-cyclopropane BMS-890068, a potent inhibitor of HCV NS3 protease. **L. Sun**, E. Mull, Q. Zhao, S.V. D'Andrea, Z. Zheng, A.X. Wang, S. Sit, Y. Chen, J. Chen, N. Shin, B.L. Venables, J. Zhu, F. Yu, D. Hernandez, A. Sheaffer, J. Friberg, P. Falk, S. Levine, C. Chen, J.O. Kniepe, K. Mosure, M.I. Cockett, F. McPhee, N.A. Meanwell, P.M. Scola
- MEDI 140.** Use of trehalose-derived probes to visualize *Mycobacterium tuberculosis*. **S. Zeiders**, G.A. Marriner, E.V. Nazarova, S. Tan, D. Russell, Y. Ahn, C.E. Barry
- MEDI 141.** Adenosine/guanosine nucleoside ribohydrolase is a distinct and drug-gable antitrichomonal target. **S. Beck**, S.N. Muellers, A. Benzie, D.W. Parkin, B.J. Stockman
- MEDI 142.** Discovery of GSK2818713, a novel second generation HCV NS5A replication complex inhibitor. **W.M. Kazmierski**, G.M. Adjabeng, S. Baskaran, J. Cooper, R. Grimes, R. Hamatake, M.T. Leivers, R. Meesala, M. Nagaraju, J.R. Walker
- MEDI 143.** Multicationic quaternary ammonium cations (multiQAQCs): Simple amphiphile scaffolds with antimicrobial, anti-biofilm, and anti-resistance properties. **M. Forman**, S. Al-khalifa, M. Jennings, M. Fletcher, S. Duggan, W.M. Wuest, K.P. Minbiole
- MEDI 144.** Potent influenza endonuclease inhibitors developed from metal-binding pharmacophore library screen. **C.V. Credille**, S. Cohen
- MEDI 145.** Avoiding antibiotic inactivation in *Mycobacterium tuberculosis* through strategic nucleoside modification. **M. Bockman**, S. Dawadi, C.C. Aldrich
- MEDI 146.** 8-hydroxyquinoline as a scaffold for the development of New Delhi metallo- $\beta$ -lactamase-1 inhibitors. **R. Adamek**, C.V. Credille, P.W. Thomas, W. Fast, S. Cohen
- MEDI 147.** Synthesis of some new benzo[d][1,3]dioxoles and their antimicrobial activity. **P.S. Achanta**, **R. Akkinepally**, R. Bobbala, A.V. Achanta
- MEDI 148.** Synthesis of some new benzo[d][1,3]dioxoles and their antibacterial activity. **P.S. Achanta**, R. Akkinepally, R. Bobbala, A.V. Achanta
- MEDI 149.** Thermal degradation of the antiviral dinucleoside phosphorothioate analogs: Novel fragmentation pathway results in the formation of cyclonucleosides. **R.H. Gimi**, A. Sheri, S. Padmanabhan, D. Cleary, R. Vaidyanathan, S. Khedkar, R. Iyer
- MEDI 150.** Structure optimization of small molecule inhibitors of bacterial transglycosylase. **L. Krasnova**, X. Wang, T. Cheng, C. Wong
- MEDI 151.** Investigation of unique sulfonamides on *Leishmania* cell viability and pathway of inhibition. **J. Katinas**, R. Eppllin, C. Hamaker, M.A. Jones
- MEDI 152.** Optimization of a peptidomimetic for the nucleoprotein E339...R416 salt bridge of the influenza virus. **J. Woodring**, T. Cheng, C. Wong
- MEDI 153.** Design of triazole-based macrocyclic inhibitors of norovirus 3CL protease: Synthetic, in depth X-ray crystallographic, NMR, and antiviral studies. **P. Weerawarna**, Y. Kim, A. Galasiti Kankanamalage, V. Damalanka, G. Lushington, N. Mehzabeen, K.P. Battaille, S. Lovell, K. Chang, W. Groutas
- MEDI 154.** Substituted bisaryl benzamide derivatives to inhibit HIV-1 replication. **N. Malik**, G. Schiltz, C. Song, R. D'Aquila

**MEDI 155.** Identification of whole-cell active inhibitors of *Mycobacterium tuberculosis* FadD32. **E. Alexander**, K.D. Grimes, C. Shi, C.C. Aldrich

**MEDI 156.** Withdrawn.

**MEDI 157.** SAR study of natural isoflavone as interleukin-5 antagonist for novel anti-asthmatic drug. **S. Jung**, P. Boggio, M. Manickam, E. VenkateswaraRao, Y. Kim

**MEDI 158.** Identification of novel imidazole-lactone derivatives as potential antischistosomal agents. **A.M. Omar**, M. Mahran, M. Ghatge, N. Chowdhury, F. Bamane, M.E. El-Araby, O. Abdulmalik, M. Safo

**MEDI 159.** Stereoccontrolled total synthesis of the DHA-derived protectin-related epoxide and sulfido-conjugates. **N. Vlasenko**, S. Glynn, C.M. DeAngelo, T.F. Lam, **N.A. Petasis**

**MEDI 160.** Stereoccontrolled total synthesis of macrophage-derived specialized pro-resolving lipid mediators. **S. Glynn**, N. Vlasenko, C.M. DeAngelo, R. Nshimiyimana, **N.A. Petasis**

**MEDI 161.** Recent advances in potent heterocyclic modulators of complement C3a receptor. **J. Rowley**, R.C. Reid, M. Hallil, A.M. Yau, J. Lim, R. Lohman, D.P. Fairlie

**MEDI 162.** Synthesis, SAR, and pharmacological characterization of novel potent and selective EP4 antagonists triaryl scaffold. **T.N. Vetman**, M.J. Blanco-Pillado, S.L. Kuklish, P.R. Manninen, D.R. Mudra, A. Warshawsky, X. Yu, M.J. Fisher, S. Chandrasekhar, A. Harvey, M.G. Chambers, C. Lin, J.L. Oskins, X. Wang

**MEDI 163.** Discovery of 4-(1-benzoyl-1H-imidazol-3-yl) benzoic acids as potent and selective allosteric inhibitors of ROR $\gamma$ t for the treatment of autoimmune diseases. **H. Zhang**, K.J. Barr, C. Correll, H. Ferguson, L. Hedge, R. Miller, G. Parthasarathy, B.W. Trotter

**MEDI 164.** Optimization of substituted cinnoline Bruton's tyrosine kinase inhibitors. **P. Vu**

**MEDI 165.** Towards a continuous flow synthesis of levomilnacipran. **M. Nguyen**, C. Ayoub, A.C. Evans

**MEDI 166.** Development of hypoxia inducible factor prolyl hydroxylase domain inhibitor as orally available therapeutic agents against chronic kidney disease anemia. **S. Kim**, C. Im, S. Lee, G. Park, H. Hwang, M. Song, S. Yoon, Y. Hong, C. Park, S. Kwon, D. Jung, S. Ahn, J. Cho

**MEDI 167.** Novel strategy for the treatment of asthma by targeting the  $\alpha_4$  subunit of GABA $_A$  receptors in airway smooth muscle. **R. Jahan**, M. Stephen, G.T. Youcum, G. Gallos, Y. Zhang, Z. Varagic, R. Puthenkalam, M. Ernst, A. Arnold, D. Stafford, C. Emala, J.M. Cook

**MEDI 168.** Discovery of 1-[4(5)-(hydroxymethyl)-1H-imidazol-2-yl] ethanone: Novel oral active sphingosine 1-phosphate lyase inhibitor. **J. Chiba**, F. Muro, J. Watanabe, R. Inoue, M. Ohtoyo, K. Hagihara, H. Yuita, M. Tamura, R. Hashimoto, T. Shimozato, N. Machinaga

**MEDI 169.** Photochemistry and cell phototoxicity of hexa thio glycosylated fused diporphyrins. **A. Aggarwal**

**MEDI 170.** Discovery, design, and synthesis of peroxisome proliferator-activated receptor  $\delta$  agonists. **J. Chin**, G. Lee, H. Hwang, H. Kang

**MEDI 171.** Optimization of CH5447240; the discovery of an orally active small molecule PTH1R agonist, PCO371 (Part II). **Y. Nishimura**, T. Esaki, Y. Isshiki, Y. Furuta, A. Mizutani, T. Kotake, T. Emura, Y. Watanabe, M. Ohta, T. Nakagawa, K. Ogawa, S. Arai, H. Noda, M. Shimizu, H. Kitamura, T. Tamura, H. Sato

**MEDI 172.** From an HTS hit to CH5447240; the discovery of an orally active small molecule PTH1R agonist, PCO371 (Part I). **T. Esaki**, Y. Nishimura, Y. Isshiki, N. Okamoto, Y. Furuta, T. Kotake, T. Emura, Y. Watanabe, M. Ohta, T. Nakagawa, S. Arai, H. Noda, M. Shimizu, H. Saito, T. Tamura, H. Sato

**MEDI 173.** Synthesis of carbon-11-labeled purine and imidazo[4,5-b]pyridine analogues as new PET tracers for imaging of NPP1. **M. Gao**, M. Wang, Q. Zheng

**MEDI 174.** Discovery of 1,2,4-oxadiazolidine-3,5-dione derivatives as novel GPR40 agonists. **K. Negoro**, F. Iwasaki, Y. Yonetoku, K. Ohnuki, T. Kurosaki, K. Kuramoto, S. Yoshida, H. Tanaka, M. Hayashi, H. Kayakiri

**MEDI 175.** Spermine: Its biochemical use in tissue processing. **J. Neff**, D. Nochebuena

**MEDI 176.** Next generation high throughput screening. **K. Elison**, G. Copeland, H. Muradyan, J. Berlin

**MEDI 177.** Design and synthesis of nuclear receptor antagonists targeting RAR $\alpha$  for male contraception. **J. Kyzer**, Y. Chen, N. Cheryala, R.A. Cuellar, T.A. Holth, E. Schonbrunn, G.I. Georg

**MEDI 178.** Identification and exploitation of diverse GPCR allosteric small-molecule binding sites. **J. Christopher**, S. Andrews, A.H. Baig, A.J. Brown, S.H. Brown, K.A. Bennett, A. Bortolato, R.K. Cheng, M. Congreve, R.M. Cooke, A.S. Doré, J.C. Errey, A. Jazayeri, J. Kean, M. Koglin, D. Lamb, A. O'Brien, K. Okrasa, J.C. Patel, N.J. Robertson, M. Serrano-Vega, S.M. Southall, B.G. Tehan, I. Teobald, G.R. Wiggan, F.H. Marshall

**MEDI 179.** Ring fused thiazolo-2-pyridones as modulators of disordered protein aggregation. **A.G. Cairns**, N. Jain, E. Chorell, M. Chapman, F. Almqvist

**MEDI 180.** Magnetically vectored delivery of cancer drug using remotely on-off switchable NanoCapsules. **S.D. Kong**, S. Jin

**MEDI 181.** Computational structure-based design of fatty acid binding proteins (FABPs) inhibitors as anti-nociceptive and anti-inflammatory agents. **L. Wei**, S. Tong, M.J. Rebecchi, H. Hsu, M. Kaczocha, H. Li, R.C. Rizzo, D. Deutsch, I. Ojima

**MEDI 182.** Structure-activity relationship studies of guanidine-based aminothiazole inhibitors of sphingosine kinase. **E.S. Childress**, Y. Kharel, A. Brown, D.R. Bevan, K.R. Lynch, W.L. Santos

### My Comments to the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

### My Experience with & Advice for Improving Diversity in Chemistry

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### My Experiences in & Advice for Organic Chemistry Courses

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## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 6F

### Neuroactive Steroids: New Drugs with Old Scaffolds

S. Runyon, *Organizer, Presiding*

**9:00 MEDI 183.** Neurosteroids and oxysterols: Big targets and potentially big payoffs. **C.F. Zorumski**

**9:30 MEDI 184.** *ent*-Neurosteroids: Their use as experimental tools and potential as drugs. **D.F. Covey**

**10:00 MEDI 185.** Novel 17-substituted neuroactive steroids for the potential treatment of neurological disorders. **S. Runyon**

**10:30 MEDI 186.** 17 $\beta$ -heteroaryl-3 $\alpha$ -hydroxyandrostanes: Allosteric modulators of  $\gamma$ -aminobutyric acid $_A$  (GABA $_A$ ) receptors with anxiolytic and anti-convulsant activity. **D.J. Hogenkamp**

**11:00 MEDI 187.** Novel GABA $_A$  positive allosteric modulator 2nd generation neuroactive steroids as potential therapies for epilepsy, seizure, and GABAergic dysfunction. **G. Martinez Botella**, F.G. Salituro, A.J. Robichaud

**11:30 MEDI 188.** Novel sterols as modulators of the NMDA receptor. **G. Martinez Botella**, F.G. Salituro, A.J. Robichaud

### Section B

San Diego Convention Center  
Room 6E

### Medicinal Chemistry Challenges in the Development of Countermeasures to Highly Lethal Chemicals & Biologicals

A. J. Duplantier, *Organizer, Presiding*

**9:00 MEDI 189.** Challenges to the development of countermeasures to chemical and biological warfare agents. **R. Fisher**

**9:30 MEDI 190.** Multidisciplinary approach for the treatment of botulinum intoxication. **K.D. Janda**

**10:00 MEDI 191.** Discovery of clinical candidate GS-5734, a novel nucleotide prodrug for the treatment of Ebola virus disease (EVD). **D. Siegel**, T. Warren, R. Jordan, V. Soloveva, A. Ray, R. Bannister, R. Mackman, M. Clarke, B.S. Ross, M. Perron, K. Stray, J. Feng, Y. Xu, J. Wells, K. Stuthman, L. Welch, E. Doerfler, L. Zhang, K. Chun, H. Hui, S. Neville, W. Lew, Y. Park, D. Babusis, R. Strickley, P. Wong, S. Swaminathan, W.A. Lee, D. Mayers, T. Cihlar, S. Bavari

**10:30 MEDI 192.** Dynamic mapping of acetylcholinesterase for structural-dynamics based reactivator design. **G. Santoni**, E. de la Mora, J. Colletier, L. Jean, Y. Xu, J. Sussman, I. Silman, R. Baati, P. Renard, F. Nachon, **M. Weik**

**11:00 MEDI 193.** Reactivation and tissue disposition mechanisms affecting the efficacy of oximes in averting toxicity from organophosphate (OP) exposure. **P. Taylor**, Z. Radic, L. Zhang, P. Marchot, Y. Bourne, V. Fokin, R. Sit, K.B. Sharpless

**11:30 MEDI 194.** Spectinomycin analogs as novel therapeutics for bacterial infections. **J. Liu**, S.L. Waidyarachchi, D. Bruhn, L. Douglas, M.M. Butler, J. Rosch, T.L. Bowlin, R.G. Panchal, R.E. Lee

### Section C

San Diego Convention Center  
Room 6D

### Young Investigator Symposium

T. E. Prisinzano, *Organizer, Presiding*

**9:00 MEDI 195.** Beta-secretase (BACE1) inhibitors for Alzheimer's disease. **C. Butler**, M.A. Brodney, K. Ogilvie, L.A. Martinez-Alsina, C.J. Helal, C.E. Nolan, K. Parris, F.F. Vajdos, C. Gonzales, A. Robshaw, S.D. Doran, E.M. Beck, G. Barreiro, D. Riddell

**9:30 MEDI 196.** Discovery of highly potent, selective, and brain-penetrant GluN2A-selective NMDA receptor positive allosteric modulators (PAMs). **M. Volgraf**, B.D. Sellers, Y. Jiang, P. Reynen, C.O. Ly, E. Villemure, P. Yuen, G. Wu, A. Liu, P. Lupardus, H. Wallweber, B.M. Liederer, G. Deshmukh, J. Hanson, D.H. Hackos, K. Scearce-Lavie, J.B. Schwarz

**10:00 MEDI 197.** Discovery of a pan-genotype HCV NS5B polymerase primer grip inhibitor. **K.J. Eastman**, K.E. Parcella, K. Yeung, K. Grant-Young, T. Wang, Z. Zhang, Z. Yin, D. Parker, K. Mosure, Y. Wang, H. Fang, J. Lemm, X. Zhuo, U. Hanumegowda, M. Liu, K. Rigat, M. Donoso, M. Tuttle, T. Zvyaga, Z. Haarhoff, N.A. Meanwell, M. Soars, S. Roberts, J.F. Kadow

**10:30 MEDI 198.** Atypical inactive-state inhibitors of spleen tyrosine kinase (SYK). **M.D. Altman**

**11:00 MEDI 199.** Discovery, characterization and optimization of sodium-coupled citrate transporter (NaCT or SLC13A5) inhibitors for the treatment of metabolic diseases. **K. Huard**, G.E. Aspnes, K. Bahnck, J.A. Brown, S. Cabral, J.J. Calloway, D. Canterbury, L. Di, D. Erion, K. Futatsugi, C.N. Garcia-Irizarry, N.E. Genung, A.M. Gilbert, M.F. Gorgoglione, J. Gosset, M.M. Hayward, D. Hepworth, M. Herr, B. Khunte, A. Lanba, Q. Li, Z. Li, P.M. Loria, T.V. Magee, J.I. Montgomery, M. Niosi, J.A. Pfefferkorn, D. Pirman, J. Polivkova, J. Purkal, K.A. Riccardi, T. Rolph, J. Siderewicz, D.P. Uccello, N.B. Vera, C. Vernochet, A. Wolford

**11:30 MEDI 200.** Leveraging pre-competitive risk sharing to accelerate understanding of LRRK2 kinase inhibition. **J.M. Ellis**

### Global Initiatives in Research Data Management & Discovery

#### Role of Community & Standards

Sponsored by CINF, Cosponsored by ANYL, COMP, MEDI and PHYS

#### Is There a Crisis in Organic Chemistry Education?

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:

[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## MONDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 6F

## Medicinal Chemistry Driven by Phenotypic Assays

J. Barrow, G. McGaughey, *Organizers, Presiding*

**2:00 MEDI 201.** Integrating design, analysis and visualization into the phenotypic drug discovery workflow. G. McGaughey

**2:30 MEDI 202.** Chemogenomic screening identifies small molecule up-regulators of MBNL1 for the treatment of type 1 myotonic dystrophy. L.H. Jones

**3:00 MEDI 203.** *In vivo* phenotypic screening and optimization for antipsychotic drug candidates. S. Kolczewski

**3:30 MEDI 204.** Optimization of pyrrolo[2,3-d]pyrimidines to block the metastatic transformation of tumor cells using a high content assay. N. Southall, K.J. Frankowski, S. Patnaik, F.J. Schoenen, S. Huang, C. Wang, S. Titus, C. Dextras, M. Ferrer, W. Zheng, J. Aubé, J.J. Marugan

**4:00 MEDI 205.** Identifying novel mechanisms for regulating brain apolipoprotein E levels using phenotypic screens. M. Pettersson, E.A. LaChapelle, G. Ramaswamy, F. Vincent, K.R. Bales

**4:30 MEDI 206.** Discovery of CFTR modulators for the treatment of cystic fibrosis. S.S. Hadida-Ruah

## Section B

San Diego Convention Center  
Room 6E

## Design of Radioligands &amp; Molecular Probes

Financially supported by EFMC

Y. P. Auberson, *Organizer, Presiding*

**2:00 MEDI 207.** PET ligand discovery: A fully integrated medicinal chemistry strategy is essential for success. J. Andres

**2:30 MEDI 208.** Identification of CNS PET tracer candidates using the target-bound fraction in brain. M. Schou

**3:00 MEDI 209.** Tau PET imaging: Discovery of [<sup>18</sup>F]MK-6240 for human *in vivo* quantification of neurofibrillary tangles (NFTs). A.M. Walji

**3:30 MEDI 210.** Application of LC-MS/MS techniques to the selection of PET tracers and determination of receptor occupancy in preclinical studies. C.D. Jesudason, V.N. Barth, A.B. Need

**4:00 MEDI 211.** *In vivo* chemistry for cancer imaging and therapy. M. Robillard

**4:30 MEDI 212.** Human serum albumin-based molecular probes for molecular imaging. Z. Cheng

## Section C

San Diego Convention Center  
Room 6D

## Discovery, Pharmacology &amp; Medicinal Chemistry of Rapidly Acting Antidepressants

Financially supported by Janssen

R. J. DeVita, *Organizer, Presiding*

**2:00** Introductory Remarks.

**2:05 MEDI 213.** Discovery and clinical update: Ketamine and other NMDAR antagonists. J. Murrough

**2:35 MEDI 214.** Intranasal esketamine in treatment-resistant depression. N.I. Carruthers, J. Singh

**3:05 MEDI 215.** Critical review of the “ketamine paradigm” as an approach to the development of new neurotherapeutics. I.W. Wainer

**3:35 MEDI 216.** Preclinical pharmacology of rapid acting antidepressants. T. Gould

**4:05 MEDI 217.** Design of novel NR2B-selective NMDA negative allosteric modulators for treatment-resistant depression. L.A. Thompson

**4:35 MEDI 218.** Discovery and Characterization of Selective GluN2A PAMs. J.B. Schwarz, M. Volgraf, B.D. Sellers, C.Q. Ly, E. Villemure, Y. Jiang, P. Yuen, G. Wu, A. Liu, P. Lupardus, H. Wallweber, B.M. Liederer, G. Deshmukh, C. Chan, R. Carano, J. Elstrott, D.H. Hackos, J. Hanson, P. Reynen, K. Searce-Levie, M. Weber

## Diversity-Quantification-Success?

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

## Global Initiatives in Research Data Management &amp; Discovery

## Technical Infrastructures: Enabling Cultural Shifts

Sponsored by CINF, Cosponsored by ANYL, COMP, MEDI and PHYS

## LGBT Chemists' Symposium on Chemical Biology

Sponsored by PROF, Cosponsored by BIOL, BIOT, MEDI, ORGN, PRES and WCC

## Undergraduate Research Posters

## Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

## MONDAY EVENING

## Section A

San Diego Convention Center  
Hall D/E

## Sci-Mix

W. B. Young, *Organizer*

## 8:00 - 10:00

64-65, 70, 72, 76, 78, 81, 109, 145, 155, 163. See previous listings.

312, 328, 349, 358, 366, 380, 385. See subsequent listings.

## TUESDAY MORNING

## Section A

San Diego Convention Center  
Room 6F

## MEDI Award Symposium

Financially supported by GSK

W. B. Young, *Organizer*

T. D. Bannister, *Presiding*

**9:00 MEDI 219. Award Address** (George and Christine Sosnovsky Award for Cancer Research sponsored by the George and Christine Sosnovsky Endowment Fund). Resurgence of covalent drugs. J. Singh

**9:40 MEDI 220. Award Address** (ACS Award for Team Innovation sponsored by ACS Corporation Associates). Discovery of Xeljanz™ (tofacitinib): A first-in-class JAK inhibitor for the treatment of rheumatoid arthritis. M.F. Brown, P. Changelian, M.E. Flanagan, M.J. Munchhof, C. Subramanyam

**10:20 MEDI 221.** Ligand-targeted imaging and therapeutic agents for cancer, autoimmune, and infectious diseases. P.S. Low

**11:00 MEDI 222.** Expanding genetic code. P.G. Schultz

**11:40 MEDI 223. Award Address** (Alfred Burger Award in Medicinal Chemistry sponsored by Gilead Sciences, Inc.). Chemical biotechnology applied to metabolic diseases. R. Dimarichi

## Section B

San Diego Convention Center  
Room 6E

## Progress &amp; New Approaches in the Ongoing Battle against Multidrug-Resistant Bacteria

Financially supported by Paraza Pharma Inc.

T. S. Haque, R. I. Higuchi, *Organizers, Presiding*

**8:30 MEDI 224.** What have we learned from traditional antibiotic research and what are our alternatives? S.J. Baker

**9:15 MEDI 225.** Explorations of siderophore-based antibacterial strategies. E.M. Nolan

**9:50 MEDI 226.** Cyclic boronic acid beta-lactamase inhibitors. S.J. Hecker, K.R. Reddy, M. Totrov, O. Lomovskaya, D. Griffith, R. Tsivkovski, D. Sun, M. Sabet, Z. Tarazi, T. Nolan, M. Clifton, M. Dudley

**10:25 MEDI 227.** Improving our understanding of porin permeability in gram-negative bacteria. T.F. Durand-Reville, A.J. Campbell, M. Sylvester, S. Patey, A. Nayar, S. Sriram, M. Huband, A. Miller, J. Manchester, G.S. Bisacchi, R.A. Tommasi

**10:55 MEDI 228.** Fully synthetic tetracyclines: Increasing chemical diversity to combat multidrug-resistant bacteria. C. Sun

**11:30 MEDI 229.** Catalytic site-selective alterations of complex glycopeptide antibiotics. S.J. Miller

## Computer-Aided Drug Design

## Free Energy Calculations

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

## Driving Change: Impact of Funders on the Research Data &amp; Publications Landscape

Sponsored by CINF, Cosponsored by MEDI and ORGN

## TUESDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 6F

## Blood-Brain Barrier in Drug Discovery

L. Di, E. H. Kerns, Z. Rankovic, *Organizers, Presiding*

**2:00** Introductory Remarks.

**2:05 MEDI 230.** Pharmacokinetics and free drug hypothesis for CNS drug candidates. A. Reichel

**2:35 MEDI 231.** Designing CNS drugs for optimal brain exposure. Z. Rankovic

**3:05 MEDI 232.** Discovery of lorlatinib (PF-06463922), a brain penetrant ALK inhibitor with broad spectrum ALK potency. T.W. Johnson

**3:35 MEDI 233.** Case study on DLK inhibitors for the treatment of neurodegenerative diseases. M. Siu

**4:05 MEDI 234.** Designing peripheral drugs for minimal brain exposure. S.K. Bagal

**4:35 MEDI 235.** P-gp matters: PET imaging for measuring CNS drug exposure. H.G. Selnick

## Section B

San Diego Convention Center  
Room 6E

## Advances in the Development of Type II Kinase Inhibitors

A. C. Hart, D. Marcoux, *Organizers, Presiding*

**2:00 MEDI 236.** Modeling protein kinase structures for the discovery of type-II kinase inhibitors. A. Schlessinger

**2:30 MEDI 237.** Allosteric modulation of protein kinases with small molecule inhibitors. D.J. Maly

**3:00 MEDI 238.** Identifying putative type II inhibitors from HTS campaigns: Importance of high-throughput mechanism studies in the hit triage process. L.M. Abell

**3:30 MEDI 239.** Fragment-based approaches to type 2 kinase inhibitors. C. Johnson

**4:00 MEDI 240.** Mining kinase type II inactive conformations: Switch control inhibition as an advanced platform for increasing inhibitor durability and selectivity. D.L. Flynn, M.D. Kaufman, B.D. Smith, W. Lu, S.C. Wise, Y. Ahn, G.E. Brandt, T. Caldwell, C.L. Ensinger, M.M. Hood, C.B. Leary, W.C. Patt, T. Rutkoski, T.B. Samarakoon, H. Telikepalli, B.A. Turner, L. Vogeti, K. Yates, M. Clare, L. Chun, L. Stewart

**4:30 MEDI 241.** Discovery of novel and selective pan-Trk inhibitors for chronic pain: Maximizing diversity from a kinase screen through structure and computation. S. Stachel, J. Sanders, D. Henze, M.T. Rudd, H. Su, Y. Li, K. Nanda, M.S. Egbertson, P. Manley, K. Jones, E.J. Brnardic, A. Green, J. Grobler, B. Hanney, M. Leitl, M. Lai, V. Munshi, D. Murphy, K. Rickert, D. Riley, A. Krasowska-Zoladek, C. Daley, P. Zuck, S.A. Kane, M.T. Bilodeau

## Section C

San Diego Convention Center  
Room 6D

## General Orals

W. B. Young, *Organizer*

R. J. DeVita, *Presiding*

**1:30 MEDI 242.** Get “RIP”ped: Discovery of a lean & mean atypical kinase scaffold for the selective inhibition of RIP1. B. King

**1:55 MEDI 243.** Use of an S1-S3 triaryl motif to obtain CNS penetrant BACE inhibitors with robust central *in vivo* activity. E.J. Gilbert, C. Huang, J. Cumming, A.W. Stamford, D. Burnett, R. Hodgson, L. Hyde, U. Iserloh, M. Kennedy, J. Misiaszek, P. Orth, E. Parker, J.D. Scott, C. Strickland, H. Wang, W. Wu, Y. Yu



**2:20 MEDI 244.** Structure-activity-relationship (SAR) optimization of a pyrazolo[1,5-*a*]pyrimidin-7(4*H*)-one scaffold that led to potent, selective and cellularly-active KDM5 inhibitors with excellent pharmacokinetic profile suitable for *in vivo* biological studies. **J. Liang**

**2:45 MEDI 245.** Clinical candidate FP-208, a novel mTOR inhibitor with tolerable activity on PI3K. **Q. Ji, Z. Du, L. Wang, C. Gao, L. Gong, B. Chen, Y. Li, X. Zhang**

**3:10 MEDI 246.** Highly selective and cell-potent ASK1 inhibitors. **C. Zapf, F.E. Lovering, N. Papaioannou, D. Hepworth, C. Allais, S.W. Kortum, J.W. Coe, J. Jasti, R. Kurumbail, R. Frisbie, F. Vincent, M. Fleming, P. Morgan, J. Brodfehrer, H. Dowty, K.L. Lee**

**3:35 MEDI 247.** Challenging the central tenet: "Greasy targets like greasy molecules" improving physicochemical properties of wall teichoic acid early stage inhibitors for gram positive MRSA infections. **M.B. Mandal, J. Su, J.P. Caldwell, Z. Tan, C.B. Madsen-Duggan, S.H. Lee, C.M. Tan, M.A. Labroli**

**4:00 MEDI 248.** How to design cell permeable non-peptidic macrocycles. **B. Over, P. Matsson, C. Tyrchan, P. Artursson, B.C. Doak, M.A. Foley, C. Hilgendorf, S.E. Johnston, M.D. Lee, R.J. Lewis, P.R. McCarran, G. Muncipinto, M.W. Perry, J.R. Duvall, J. Kihlberg**

**4:25 MEDI 249.** Discovery of a potent, highly selective, and efficacious RAF kinase inhibitor to treat non-small lung cancers (NSCLC). **S. Ramurthy, G.A. Nishiguchi, A.C. Rico, B.R. Taft, R. Aversa, P. Barsanti, K. Briner, M.T. Burger, M.P. Dillon, T.A. Dineen, E. Ginn, J.M. Jansen, Y. Lou, M. Mamo, V.R. Polyakov, V. Rauniyar, S. Subramanian, H.R. Tanner, L. Wan, B. Appleton**

**4:50 MEDI 250.** Discovery and structure-based optimization of substituted 4-hydroxy-5,6-dihydropyran/dihydropyridin-2-ones as potent inhibitors of human lactate dehydrogenase **A. B. Wei, K.D. Robarge, S.S. Labadie, A. Zhou, B.P. Fauber, P.S. Dragovich, Z. Gao, C. Ding, T. Lai, L. Corson, A. Hitz, M. Ultsch, C. Eigenbrot, I. Yen, L. Salphati, T. O'Brien, H.E. Purkey**

**Computer-Aided Drug Design**

**Computational Biophysics**

*Sponsored by MPPG, Cosponsored by BIOL, CINP, COMP, MEDI and PHYS*

**Driving Change: Impact of Funders on the Research Data & Publications Landscape**

*Sponsored by CINP, Cosponsored by MEDI and ORGN*

**WEDNESDAY MORNING**

**Section A**

San Diego Convention Center Room 6F

**First Time Disclosures**

L. A. Thompson, *Organizer, Presiding*

**9:00 MEDI 251.** Discovery of a potent and selective phosphoinositide-3-kinase- $\gamma$ -inhibitor, IPI-549, as an immuno-oncology clinical candidate. **C. Evans, T. Liu, A. Lescarbeau, S. Nair, L. Grenier, J. Pradeilles, Q. Glenadel, T. Tibbitts, M. Tremblay, J.P. Dinitto, E. Brophy, E. Murphy, J. Ali, N. Hurst, S. Goldstein, C. Martin, J. Hoyt, J. Soglia, C. Cheung, M. Pink, N. Kosmider, J. Proctor, K. Mogovern, J. Adams, V. Palombella, J. Kutok, A.C. Castro**

**9:40 MEDI 252.** Discovery of AZD7594, an inhaled non-steroidal selective glucocorticoid receptor modulator (SGRM) in clinical development for treatment of asthma. **M. Hemmerling, K. Edman, M. Lepistö, T.G. Hansson**

**10:20 MEDI 253.** Discovery of VX-984: A novel, selective DNA-PK inhibitor for the treatment of cancer. **J.P. Maxwell, K.M. Cottrell, J. Xu, R. Arimoto, B. Boucher, K. Chandupatla, J.E. Cochran, V. Damagnez, J. Engtrakul, P. Ford, B. Furey, S. Giroux, J. Green, L. Henry, S. Hillier, J.K. Hogan, R. Hoover, K.L. Jackson, W. Markland, C.S. Moody, M. Morris, A.C. Pierce, D.E. Shannon, R. Stearns, N. Waal, Y. Wang, M. Wood, D.M. Boucher, P.S. Charifson**

**11:00 MEDI 254.** Discovery of GLPG1690: A first-in-class autotoxin inhibitor in clinical development for the treatment of idiopathic pulmonary fibrosis. **N. Desroy, A. Joncour, X. Bock, C. Housseman, C. Peixoto, N. Bienvenu, V. Labeguere, L. Cherel, D. Annoot, T. Christophe, K. Conrath, N. Triballeau, P. Mollat, A. Wohlkonig, R. Blaque, C. Cottereaux, B. Hrvacic, M. Borgonovi, A. Monjardet, E. Van der Aar, R. Brys, B. Heckmann**

**Section B**

San Diego Convention Center Room 6E

**Accelerating Medicinal Chemistry by Trusting Genetics**

J. J. Crawford, A. A. Estrada, *Organizers, Presiding*

**9:00 MEDI 255.** Genetics and drug discovery. **A. Kamb**

**10:00 MEDI 256.** Impact of genetic insights on the development of BTK inhibitors. **A. Johnson, L. Belmont, R. Burton, R. Choy, J.J. Crawford, C. Everett, A. Katewa, P. Kohli, D.F. Ortwine, E. Penuel, W.B. Young**

**10:40 MEDI 257.** Discovery and SAR evolution of potent and selective ROMK inhibitors: Strategies for improved selectivity over the hERG channel. **S.P. Walsh, E. Kim, A. Shahipour, H. Tang, R. DeJesus, Y. Zhu, N. Teumelson, J. Frie, L. Yang, E. Parmee, B. Priest, B. Thomas-Fowlke, A. Swenson, G. Kaczorowski, M. Garcia, A. Weinglass, M. Alonso-Galicia, X. Zhou, L. Pai, C. Hampton, J. Kunkel, O. Price, M. Hernandez, C. Gill, M. Dajee, K. Shah, J. Metzger, M. Forrest, J. Ormes, M. Hu, K. Owens, K. Samuel, R. Miller, V. Tong, T. Bateman, S. Roy, K. Sullivan, A. Pasternak**

**11:20 MEDI 258.** Discovery of PF-05089771: A potent, subtype selective Na<sub>v</sub>1.7 inhibitor for the treatment of pain. **N. Swain**

**From mAb to ADCs: Tailored Antibodies & Dedicated Chemistry Technologies for Site Specific ADCs**

*Sponsored by CARB, Cosponsored by MEDI*

**Computer-Aided Drug Design**

**Real World Dynamics**

*Sponsored by MPPG, Cosponsored by BIOL, CINP, COMP, MEDI and PHYS*

**WEDNESDAY AFTERNOON**

**Section A**

San Diego Convention Center Room 6F

**First Time Disclosures**

*Financially supported by Genentech*

L. A. Thompson, *Organizer, Presiding*

**2:00 MEDI 259.** Discovery of GDC-0853: A highly potent, selective, and non-covalent Btk inhibitor. **W.B. Young**

**2:40 MEDI 260.** GPR40 agonists for the treatment of type 2 diabetes: From the laboratory to the patient. **C. Hamdouchi**

**3:20 MEDI 261.** Discovery of clinical candidate PF-06650833: A potent, selective, and efficient inhibitor of IRAK4 from fragment-based drug design. **K.L. Lee, C. Allais, C. Ambler, D. Anderson, B. Boscoe, A. Bree, J. Brodfehrer, M. Bunnage, C. Choi, S. Chung, K. Curran, J. Day, C. Dehnhardt, A. Dermenci, S. Drozda, R. Frisbie, L. Gavrin, J. Goldberg, S. Han, M. Hege, D. Hepworth, B. Jacobson, I. Kilty, S.W. Kortum, A. Lee, F.E. Lovering, M.D. Lowe, J. Mathias, E.A. Murphy, N. Papaioannou, A. Patry, B. Pierce, S. Ramsey, V. Rao, E. Saiah, J. Shin, H. Soutter, J.W. Strohbach, P. Symanowicz, S. Thaisrivongs, J.R. Thomson, J. Trzupek, R. Vargas, F. Vincent, X. Wang, A. Winkler, S.W. Wright, J. Yan, C. Zapf**

**4:00 MEDI 262.** Therapeutic targeting the NOTCH3 receptor with antibody drug conjugates. **A. Maderna**

**4:40 MEDI 263.** Discovery of a first-in-class PAR4 antagonist as a novel antithrombotic. **E.S. Priestley, J. Banville, M. Callejo, D. Deon, L. Dube, M. Gagnon, V. Guarino, J. Guy, J. Guay, T. Harper, J. Lavallee, A. Martel, S. Posy, R. Remillard, E.H. Ruediger, F. Tremblay, C.A. Watson, P.C. Wong, M. Bouvier, D. Gordon, J. Yang, R.R. Wexler, A. Marinier**

**Section B**

San Diego Convention Center Room 6E

**General Orals**

W. B. Young, *Organizer*

K. Leftheris, *Presiding*

**1:30 MEDI 264.** Reaction-driven design of viral protease inhibitors from covalently binding fragments. **R. Schulz, G. Wolber**

**1:50 MEDI 265.** Parallel medicinal chemistry (PMC) in current drug discovery paradigm. **Z. Shi**

**2:10 MEDI 266.** Identification of novel, *in vivo* active Chk1 inhibitors utilizing structure guided drug design. **S. Stokes**

**2:30 MEDI 267.** Activation and inhibition of MAPK-interacting kinase 2 (Mnk2): A conformational perspective using *in silico* models. **M. Kumarasiri, W. Shudong**

**2:50 MEDI 268.** Discovery of QBE170: An inhaled ENaC blocker with a reduced potential to induce hyperkalemia. **N.J. Smith, S. Collingwood, H. Danahay, K. Coote, S. Czarniecki, M. Kabra, R. Lock, D. Paisley, R. Robinson, H. Watson, B. Abrahams**

**3:10 MEDI 269.** Design of novel GPCR family-targeted scaffolds: Synthetic and cheminformatic exploration of novel medicinal chemistry space. **J. Benningshof, P. van Meurs, S. van Assema, G. Mueller, D. Stumpfe, A. de la Vega de León, N. Furtmann, D. Dimova, J. Bajorath**

**3:30 MEDI 270.** Triazolopyridine inhibitors of myeloperoxidase. **N. Wurtz, A. Viet, S. Shaw, A. Dilger, M. Valente, J. Khan, S. Jusuf, R. Narayanan, G. Fernando, F. Lo, X. Liu, G. Locke, L.M. Kopcho, L. Abell, P. Slep, M. Basso, L. Zhao, R. Wexler, F. Duclos, E.K. Kick**

**3:50 MEDI 271.** Design and synthesis of early stage inhibitors targeting wall teichoic acid biosynthesis. **J.P. Caldwell, J. Su, S. Yang, M.A. Labroli, C. Yang, M.B. Mandal, Z. Tan, C.B. Madsen-Duggan, G.D. Ho, S.H. Lee, C.M. Tan, T. Roemer**

**4:10 MEDI 272.** Discovery of a novel potent selective SMYD3 inhibitor with oral bio-availability. **L.H. Mitchell**

**4:30 MEDI 273.** Identification of small molecule translesion synthesis inhibitors that target Rev1 protein-protein interactions. **M.K. Hadden, V. Sail, E.N. Thompson, A. Rizzo, D. Korzhnev**

**4:50 MEDI 274.** New splice modulators targeting the human spliceosome. **M.D. Burkart**

**Computer-Aided Drug Design**

**New Modalities RNA**

*Sponsored by MPPG, Cosponsored by BIOL, CINP, COMP, MEDI and PHYS*

**WEDNESDAY EVENING**

**Section A**

San Diego Convention Center Hall F

**General Posters**

*Financially supported by Genentech*

W. B. Young, *Organizer*

**7:00 - 9:00**

**MEDI 275.** Anticancer potential of novel ferrocene based urea derivatives: Synthesis, modal studies, and cell line investigations. **A. Badshah, A. Altaf, B. Lal, S. Ullah, D.C. Crans**

**MEDI 276.** Rational design, synthesis and evaluation of small molecule IL-6/GP130 inhibitors as anticancer agents. **L. Mao, G. Shi, C. Li**

**MEDI 277.** Identification and characterization of potential BRDT inhibitors by fragment-based screening using differential scanning fluorimetry, PrOF-NMR, and protein crystallography. **A. Wisniewski, C. Gee, J. Cai, X. Zong, W.C. Pomerantz, S. Ember, E. Schonbrunn, J. Hawkinson, G.I. Georg**

**MEDI 278.** Novel "trigger and release" strategy for imaging tumor hypoxia *in vivo*. **S. Banister, B. Shen, M. Rafat, M. Vivalta, M. Brown, E. Graves, A. Srinivasan, F.T. Chin**

**MEDI 279.** Cancer-preventive isothiocyanate forms irreversible adducts with glutathione S-transferase (GST): Consequences on GST activity. **V. Kumari, E. Hamm, R.J. Holland, A.E. Maciag, L.K. Keefer, S.V. Singh, X. Ji**

**MEDI 280.** Design and synthesis of drugs that reduce  $\beta$ -catenin and attenuate cell proliferation. **A. Jelowicki, A. Vis, M. Young, C. Bunye, E. Guglielmo, R. Nguyen, S. Guzman, C. Wen, C. Ott, N. Patel, P. de Lijser**

- MEDI 281.** Soluble epoxide hydrolase and peroxisome proliferator-activated receptors in polypharmacology: An efficient appliance for the treatment of complex diseases. **R. Bloecher**, C. Lamers, S. Wittmann, D. Merk, M. Hartmann, O. Diehl, A. Brueggerhof, C. Angioni, M. Wurglics, A. Kahnt, M. Boss, B. Bruene, L. Weizel, D. Steinhilber, M. Schubert-Zsilavecz, J. Imig, E. Proschak, G. Geisslinger, B.D. Hammock
- MEDI 282.** Properties-based optimization of *in vitro* and *in vivo* clearance of a series of DNA-PK inhibitors. **J. Xu**, R. Arimoto, K.M. Cottrell, S. Giroux, K.L. Jackson, D.J. Lauffer, M. Morris, N. Waal, D.M. Boucher, P.S. Charifson, J.P. Maxwell
- MEDI 283.** Discovery of VX-984: Mitigation of aldehyde oxidase metabolism through the use of targeted deuteration. **K.M. Cottrell**, B. Boucher, R. Arimoto, J. Engtrakul, J. Xu, S. Giroux, A.C. Pierce, R. Stearns, D.M. Boucher, P.S. Charifson, J.P. Maxwell
- MEDI 284.** Improving solubility, permeability, and cellular potency of a series of DNA-PK inhibitors. **M. Strohmeier**, **J.P. Maxwell**, J. Xu, K.M. Cottrell, A.C. Pierce, B. Song, P.W. Snyder, N. Waal, P.S. Charifson
- MEDI 285.** Discovery of novel chiral 3<sup>o</sup>-SMe pyrrolidine as extracellular regulated kinase (ERK) inhibitors. **S.B. Boga**, A. alhassan, A.B. Cooper, R. Doll, N. Shih, Y. Deng, G.W. Shippis, R. Sun, J. Desai, H. Zhu, M. Patel, K. Muppalla, L. Zhu, Y. Nan, J. Wang, X. Gao, S. Gudipati, J. Kelly, A.M. Siddiqui, A.A. Celebi, Y. Wu, S. Paliwal, H. Tsui, L. Xiao, A. Hruza, V.S. Madison, A. Buevich, D. Heska, A. Samatar, D. Carr, B. Long, S. Black, P. Dayananth, W. Windsor, P. Kirschmeier, R. Bishop
- MEDI 286.** Withdrawn.
- MEDI 287.** Design and synthesis of Rpn11 inhibitors, prodrugs, and probe molecules. **Y. Ma**, J. Li, C. Perez, R. Deshaies, S. Cohen
- MEDI 288.** Scaffold replacement and 3D ligand optimization applied to the discovery of tyrosine kinase inhibitors. **R. Alvarez**, A. Ajamian
- MEDI 289.** Exploration of new structural motifs for the design and synthesis of anti-cancer drugs that regulate intracellular levels of  $\beta$ -catenin. **R. Nguyen**, A. Jelowicki, A. Vis, M. Young, C. Bunye, E. Guglielmo, S. Guzman, C. Wen, C. Ott, N. Patel, P. De Lijser
- MEDI 290.** Identification of chromosome based anticancer agents for ovarian cancer. **A. Kulshrestha**, K. Beaman, **S. Patil**
- MEDI 291.** Design, synthesis, and biological evaluation of flufenamic acid derived bioisosteres as inhibitors of aldo-keto reductase 1C3 (AKR1C3) expressed in prostate cancer. **M.L. Lolli**, C. Cena, A. Giraudou, E. Marini, A.C. Pippione, S. Oliaro-Bosso, T. Ferrante, M. Sadiq, K. Pors, D. Boschi, R. Braga, C. Andrade
- MEDI 292.** Studies on the selectivity of metalloprotein inhibitors and their effects on cellular metal ion homeostasis. **Y. Chen**, B. Lai, S. Cohen
- MEDI 293.** Toward next-generation cancer chemotherapy: Targeting cancer stem cells, as well as bulk tumor cells with novel biotin- and hyaluronic acid-taxoid conjugates. **Y. Zhang**, A. Gupta, K. Xie, A. Vaynrub, J.G. Vineberg, T. Wang, G.I. Botchkina, I. Ojima
- MEDI 294.** Design, synthesis of diamino Hx-amides (Hx-I\*P and Hx-IP\*): DNA binding properties and controlling expression of the topoisomerase II alpha gene. **V. Satam**, P. Patil, B. Babu, M. Gregory, M. Bowerman, K. Olson, M. Savagian, M. Lee, L. Pett, K. Kiakos, J. Hartley, **M. Lee**
- MEDI 295.** Design, synthesis, structural characterization, and *in vitro* cytotoxic activity of mononuclear Ru(II) complexes. **S. Thota**
- MEDI 296.** Structure based design with modulation of known ligands leading to switch in mode of inhibition of human topoisomerase II $\alpha$ . **S.M. Amrutkar**, S.K. Guchhait, U.C. Banerjee
- MEDI 297.** Interrogating panobinostat's binding kinetics for the development of novel HDAC inhibitors to be used in the treatment of proteasome inhibitor resistant multiple myeloma. **J. McClure**, C. Zhang, E. Inks, C. Chou
- MEDI 298.** Non-traditional methods in targeting sphingosine kinase 2: Using bisubstrate inhibitors to improve potency and selectivity. **T.K. Dawson**, R. Dyer, Y. Kharel, K.R. Lynch, T.L. Macdonald
- MEDI 299.** Using polyethylene glycol derivatives to stabilize a selective anti-cancer agent. **K.G. Earnest**, A. Kizhakkakkara Vadukoot, J. Mulloy, E.J. Merino
- MEDI 300.** Ligand-receptor binding study of site specific dendrimer with PEG 3350 and folic acid and its interaction with folate receptor. **D. Sampogna**, I.D. Araya, J.A. Valencia-Gallegos, V. Márquez, F.D. González-Nilo
- MEDI 301.** Development of isoform-selective compounds for Grp94 inhibition. **S.J. Mishra**, S. Ghosh, A. Stothert, C.A. Dickey, B.S. Blagg
- MEDI 302.** Isatin derived spirocyclic analogs with  $\alpha$ -methylene- $\gamma$ -butyrolactone as anticancer agents: A structure activity relationship study. **S. Rana**, E. Blowers, J. Contreras, R. Rattan, A. Natarajan
- MEDI 303.** Synthesis, cytotoxic activities and cell cycle arrest profiles of benzimidazole - 1,3,4-oxadiazole conjugates. **B. Mochona**, E. Mazzi, R. Jean, N.N. Mateeva, K. Redda
- MEDI 304.** Novel multi-target agents: COX-2/sEH dual inhibitors. **S. Hwang**, J. Yang, K. Wagner, G. Zhang, C. Morisseau, J. Imig, B.D. Hammock
- MEDI 305.** Identification of inhibitors of HIF2 $\alpha$  as modulators of the hypoxia response for the treatment of cancer. **S. Johnstone**, J. Albert, B.B. Masek, L. Wang, S. Brothers, S. Bourgault, E. Grazinni, M. Coupal
- MEDI 306.** Structure-based design, synthesis, and evaluation of novel peptides allosteric inhibitors of Hsc70. **C.C. Clement**, E.L. Ewul, J. Gonzalez, M. Philipp
- MEDI 307.** Stimuli-responsive nanomedicine for synergistic leukemia therapy. **J. Kemp**, C.A. Hong, J. Edson, Y.J. Kwon
- MEDI 308.** Metal-binding pharmacophores yields a potent inhibitor of the proteasome subunit Rpn11. **C. Perez**, J. Li, S. Cohen, R. Deshaies
- MEDI 309.** Withdrawn.
- MEDI 310.** Fragment-based drug discovery of potent and selective MKK3/6 inhibitors. **S. Bigi**, M. Adams, T. Kobayashi, D. Lawson, M. Saitoh, K. Shimagawa, M. Hixon, C. Smith, T. Tatamiya, M. Goto, J. Russo, C. Grimshaw, S. Swann
- MEDI 311.** Combinatorial approach to auron synthesis. **Z. Taylor**, E. Conley, S. Handy
- MEDI 312.** Targeted screening library for the identification of ATX fragment hits. **M.C. Lanier-Gross**, D. Cole, J. Cowden, **J. Demeo**, M. Hixon, M. Klein, P. Schwartz, R. Tjhen
- MEDI 313.** Withdrawn.
- MEDI 314.** Development of imidazo[1,2-c]quinazolin-5-ones as neuroprotective agents through 18kDa translocator protein (TSPO) activation. **F. Halle**, I. Lejri, C. Klein, M. Schmitt, A. Eckert, G. Mensah, J. Bourguignon, F. Bihel
- MEDI 315.** Redesigned inhibitors of soluble epoxide hydrolase with improved drug-like properties and better target occupancy for the treatment of diabetic neuropathic pain. **K.S. Lee**, J. Liu, K. Wagner, S. Pakhomova, M.E. Newcomer, J. Yang, C. Ng, J. Niu, B.D. Hammock
- MEDI 316.** Natural product lead for the design and synthesis of selective inhibitors of kainate receptors. **L. Recnik**, D.E. Jane, C.L. Willis
- MEDI 317.** Discovery and *in vitro* and *in vivo* profiles of N-ethyl-N-[2-[3-(5-fluoro-2-pyridinyl)-1H-pyrazol-1-yl]ethyl]-2-(2H-1,2,3-triazol-2-yl)-benzamide (TASP0428980) as a novel class of dual orexin receptor antagonist. **R. Suzuki**, D. Nozawa, A. Futamura, R.N. Shimonono, M. Abe, N. Hattori, H. Ohta, Y. Araki, D. Kambe, M. Ohmichi, S. Tokura, T. Aoki, N. Ohtake, H. Kawamoto
- MEDI 318.** Novel controlled deactivation cannabinoid receptor agonists. **S. Kulkarni**, S. Nikas, R. Sharma, C. Paronis, S. Jiang, C. Honrao, S. Mallpeddi, O. Benchama, T. Jarbe, J. Bergman, A. Makriyannis
- MEDI 319.** Serotonin (5-HT) 5-HT<sub>2C</sub> receptor (5-HT<sub>2C</sub>R) positive allosteric modulators as novel neurotherapeutics. **C. Wild**, C. McAllister, E. Wold, C. Ding, N. Anastasio, R. Fox, S. Stutz, H. Chen, S.M. Tomlinson, K.A. Cunningham, J. Zhou
- MEDI 320.** Search for water soluble  $\alpha$ -6 Bz/GABA(A) receptor subtype selective ligands in order to determine their *in vivo* activity. **R.S. Verma**
- MEDI 321.** Design and synthesis of novel bis-imidazole carbonic anhydrase activators as potential nootropics. **J. Musco**, B. Draghici, U.K. Mondal, M.A. Ilies
- MEDI 322.** Synthesis of novel A<sub>2A</sub> selective xanthine derivatives as antiparkinsonian agents. **R. Bansal**, S. Rohilla, P. Chauhan, K. Klotz
- MEDI 323.** Synthesis of N-substituted 3-hydroxyphenylpyrrolidines and their evaluation as selective D<sub>3</sub> receptor ligands. **S. Eslamimehr**, A.M. Crider, W.L. Neumann
- MEDI 324.** Development of a positron emission tomography (PET) tracer to evaluate phosphodiesterase 10A (PDE10A) target engagement. **M. Chappell**, A.E. Tripp, D.M. Bender, D.R. Benesh, S.A. Monk, E. Chernet, K. Rash, L. Phebus, L.J. Sliker, H. Kuwabara, R.F. Dannals, H. Valentine, H.T. Ravert, D.F. Wong, V.N. Barth
- MEDI 325.** Potential novel targets for schizophrenia: Stereospecific GABA<sub>A</sub> receptor subtype selective imidazobenzodiazepines. **G. Li**, M.M. Poe, N.J. Raddatz, D.A. Baker, M. Ernst, J.M. Cook
- MEDI 326.** Non-peptidic inhibitors of insulin-regulated aminopeptidase (IRAP). **J. Savmarker**, S.R. Borhade, T. Lundbäck, S.Y. Chai, M. Hallberg
- MEDI 327.** Blind and visually impaired-accessible investigation of hydration propensities of biologically relevant  $\alpha$ -ketoamides. **H.B. Wedler**, T. Palazzo, R.P. Pemberton, **C.S. Hamann**, M. Kurth, D.J. Tantillo
- MEDI 328.** Computer-aided rational drug design: Develop novel antibiotics to treat drug-resistant bacteria. **L. Hokama**, K. Mortelmans, C. Green, D. Sahner, M.J. Tanga, **L. Jiong**
- MEDI 329.** Modeling molecular recognition: Free energy calculations for ligand-protein binding. **W. Chen**, Z. Tang, C. Chang
- MEDI 330.** Increasing lipase activity through computational modelling: Structure-activity relationship of *Candida antarctica* lipase B and its mutants in various solvents. **H. Kim**, Y.G. Yingling
- MEDI 331.** Basic computational analysis and molecular conformational prediction of quaternary and neutral oximes with potential activity for reactivation of nerve agent-inhibited human acetylcholinesterase. **J. Valle da Silva**, L. Costa, M. Koning, **T. Costa Franca**, I.B. Junior
- MEDI 332.** Discovery of novel Ebola virus entry inhibitors enabled by QSAR-based approaches. **S. Capuzzi**, A. Tropsha, E. Muratov
- MEDI 333.** Improving antibiotic drug discovery through bacterial co-culture and synthetic chemistry. **A.L. Wolfe**, S.C. Seaton
- MEDI 334.** Dipicolinic acid derivatives as inhibitors of New Delhi metallo- $\beta$ -lactamase-1. **Y. Chen**, P.W. Thomas, W. Fast, S. Cohen
- MEDI 335.** Development of novel non-nucleoside HCV NS5B polymerase inhibitors: QSAR, molecular docking directed synthesis and *in vitro* studies. **V. Patil**, N. Masand, S. Gupta
- MEDI 336.** Strategies to improve pharmacokinetic properties of SAL-AMS, a potent nucleoside drug effective against *Mycobacterium tuberculosis*. **S. Dawadi**, H.I. Boshoff, C.E. Barry, C.C. Aldrich
- MEDI 337.** Staggered localization of the TriA and TriB periplasmic proteins in the TriABC-OpmH efflux pump of *Pseudomonas aeruginosa*. **A.T. Ntreh**, J.W. Weeks, L.M. Nickels, H.I. Zgurskaya
- MEDI 338.** Natural product engineering enabled by a YcaO-domain bottommycin macrocyclase. **C. Schwalen**, P.M. Blair, K. Dunbar, D. Mitchell
- MEDI 339.** Discovery of the potent and selective fungal CYP51 inhibitor VT-1129. **S.M. Sparks**, E.P. Garvey, R.J. Scholzinger, S.R. Shaver, W.J. Hoekstra
- MEDI 340.** HCV NS5A inhibitors excellent with pan-genotypic picomolar potency and better stability. **Z.J. Zhan**, H. Yan, Q. Li
- MEDI 341.** Bolstering the antibacterial arsenal: Propargyl linked antifolates for gram negative pathogens. **N. Gummundipundi Dayananand**, M.N. Lombardo, A.C. Anderson, D.L. Wright
- MEDI 342.** Essential oils and methylglyoxal: A possible effective alternative treatment for antibiotic resistant bacterial infections. **E. Cieslak**, J. Mack
- MEDI 343.** Novel quinolone-class antibiotics designed to overcome resistance to fluoroquinolones. **C. Kulkarni**, T.R. Towle, R.J. Kerns
- MEDI 344.** Structure-guided cap-centered optimization of potency and pharmacokinetics of norovirus 3CL protease inhibitors. **A. Galasiti Kankanamalage**, Y. Kim, S.T. Doyle, A.F. Alsoudi, P. Weerawarna, V. Damalanka, N. Mehzabeen, B. Kevin, S. Lovell, K. Chang, W. Groutas

- MEDI 345.** Property-guided synthesis of  $\beta$ -lactam adjuvants for methicillin resistant *Staphylococcus aureus*. **P.M. Barbour**, X. Wang
- MEDI 346.** Small molecules against tick-borne flaviviruses. **D.I. Osolodkin**, E.V. Dueva, A.A. Orlov, L. Kozlovskaya, V.A. Palyulin, G. Karganova, N.S. Zefirov
- MEDI 347.** In silico investigation of phytochemicals as antiviral agents against dengue fever. **C.N. Powers**, W.N. Setzer
- MEDI 348.** Design, synthesis, and NDM-1 inhibitory potency of indoline sulfonamides. **T. Heath**, A. Stewart, P.W. Thomas, W. Fast, D.P. Becker
- MEDI 349.** Flexible nucleosides as potential Ebola inhibitors. **M. Shirley**, N. Steenrod, T. Ku, Z.S. Zhou, K.L. Seley-Radtke
- MEDI 350.** Withdrawn.
- MEDI 351.** Design, synthesis, and evaluation of heterocyclic chalcones and their derivatives. **S. Zingales**, M.Z. Wallace, M.E. Moore, J. Futch, K. Brown
- MEDI 352.** Airway macrophage black carbon as a marker of indoor air pollution in former smokers with COPD. **A.J. Belli**, S. Bose, **C.O. DaSilva**, L.A. Grammer, N.N. Hansel
- MEDI 353.** Synthesis and evaluation of benzoxaborole-metronidazole based compounds for *Clostridium difficile*. **S.K. Jonnalagadda**, D. Imitiaz, S. Gurrapu, C. Ronayne, G.L. Nelson, L. Solano, E.A. Lueth, V.R. Mereddy
- MEDI 354.** Characterization of bioactive compounds obtained from halophilic bacteria in the Oklahoma salt plains. **O.O. Oyewole**, A. Jorski, R. Sheaff
- MEDI 355.** Synthesis of amphiphilic linear and cyclic peptides containing arginine and hydrophobic residues as potent antibacterial agents. **N. Riahifard**, A. Shirazi, J. Yamaki, K. Parang, R.K. Tiwari
- MEDI 356.** Structure-activity relationships for a series of benzimidazole derivatives as cruzain inhibitors. **A.D. Andricopulo**, I. Pauli, M. Souza, R. Ferreira, M. Dessoay, G. Oliva, L.C. Dias
- MEDI 357.** Keeping antibiotics off your mind: Beta-lactam conjugates of D-cycloserine and other neuroleptic agents effective against *Mycobacterium tuberculosis*. **J. Buonomo**, C.C. Aldrich
- MEDI 358.** Discovery of fluorobenzimidazole HCV NS5A inhibitors. **J.T. Randolph**, C.A. Flentge, S.V. Patel, L. Nelson, R. Mondal, N. Mistry, T. Reisch, T. Dekhtyar, P. Krishnan, T. Pilot-Matias, D.W. Beno, R. Wagner, W.M. Kati
- MEDI 359.** Orally bioavailable and *in vivo* efficacious antimalarial 4(1H)-quinolones. **C. Lichorowic**, J.R. Maignan, R. Neelapur, A. Monastyrskiy, J.V. Giarrusso, T. Mutka, L. Dong, D. Casandra, A. LaCrue, D. Kyle, R. Manetsch
- MEDI 360.** Profiling of bacterial cell wall peptidoglycan pathway inhibitors using LC-MS/MS-based quantification of cytoplasmic pathway intermediates. **W.G. Guthel**, H. Vemula, N. Ayon
- MEDI 361.** Synthesis and characterization of menaquinone (MK) analogs and other substrate analogs for the novel *Mycobacterium tuberculosis* hydrogenase, MenJ. **J.T. Koehn**, X. Wu, C.D. Rithner, D.C. Crick, **D.C. Crans**
- MEDI 362.** Chemical desialylation in the life process. **M. Wei**, T. Li, J. Li, P.G. Wang
- MEDI 363.** Synthesis, optical resolution, and optimization of novel  $\alpha$ -truxillic acid derivatives as anti-nociceptive and anti-inflammatory agents, targeting fatty acid binding protein (FABP). **S. Tong**, M.W. Elmes, H. Hsu, M. Kaczocha, H. Li, R.C. Rizzo, D. Deutsch, I. Ojima
- MEDI 364.** Discovery of gemilukast (ONO-6950), a dual CysLT<sub>1</sub> and CysLT<sub>2</sub> antagonist as a therapeutic agent for asthma. **J. Takeuchi**, S. Itadani, K. Yashiro, H. Egashira, Y. Aratani, T. Sekiguchi, A. Kinoshita, H. Moriguchi, N. Ohta, S. Takahashi, A. Ishida, Y. Tajima, M. Ima, K. Hisaichi, J. Ueda, T. Sekioka, M. Kadode, Y. Yonetomi, T. Nakao, A. Inoue, H. Nomura, T. Kitamine, M. Fujita, T. Nabe, Y. Yamaura, N. Matsumura, A. Matsumura, Y. Nakayama, K. Ohmoto
- MEDI 365.** DSP-1363, a novel orally available human neutrophil elastase inhibitor for the treatment of inflammation. **K. Tojo**, M. Tobe, T. Tanaka, Y. Takanashi, T. Nakamura, K. Kubota, K. Ikeda, M. Isobe, H. Nishimuta, K. Suzuki, T. Shiro
- MEDI 366.** Structure-based design and synthesis of potent and selective inhibitors of PI3K $\delta$  for autoimmune diseases: A medicinal chemistry approach to reduce aldehyde oxidase (AO) metabolism. **T. Gibson**, J. Brown, E. Chang, B. Lam, S. Murphy, F. Zhou
- MEDI 367.** Binding affinity and biological activity evaluation of novel C-type lectin Mincle ligands. **T. Matsumaru**, A. Furukawa, R. Ikeno, Y. Shuchi, K. Maenaka
- MEDI 368.** Rational design and stereoselective synthesis of novel naturally derived PDE4 inhibitors. **M. Helal**, E. Habib, K. Darwish
- MEDI 369.** Synthesis and biological evaluation of benzofuran ring containing compound BRL-37959 and its analogs. **S.A. Ahmed**, D. Hiji, M. Jellen, M. Hossain
- MEDI 370.** Structure-based computer-aided IL-6/GP130 protein-protein interaction (PPI) inhibitor design. **G. Shi**, L. Mao, C. Li
- MEDI 371.** Withdrawn.
- MEDI 372.** Incorporation of phosphonate into benzonaphthyridine TLR7 agonists for adsorption onto aluminum hydroxide. **T.Y. Wu**, A. Cortez
- MEDI 373.** Structural activity relationship of lipopeptide TLR2 agonist. **T.Y. Wu**, Y. Zou
- MEDI 374.** SAR expansion and drug-like in-silico property assessment of novel quinoline and naphthalene EP4 antagonists. **S.L. Kuklish**, T.N. Vetman, P.R. Manninen, S. Chandrasekhar, M.J. Fisher, A. Harvey, M.G. Chambers, C. Lin, D.R. Mudra, J.L. Oskins, X. Wang, X. Yu, A. Warshawsky, M.J. Blanco-Pillado
- MEDI 375.** Discovery of novel ursolic acid derivatives as ROR-gamma inhibitors. **R. Sharma**, **R. Anupindi**, R. Husain, B. Sahu, A. Almeida, N. Chakor
- MEDI 376.** Design and synthesis of multi-target inhibitors for soluble epoxide hydrolase (sEH) and fatty acid amide hydrolase (FAAH). **S.D. Kodani**, S. Hwang, C. Morrisseau, B.D. Hammock
- MEDI 377.** Modification and characterization of TLR4 and TLR7 ligands obtained by high throughput screening. **Y. Kakitsubata**, M. Wakao, Y. Suda, M. Chan, H.B. Cottam, T. Hayashi, D. Carson
- MEDI 378.** Synthesis of tetra-substituted cyclobutane derivatives with potential biological activity using green chemistry and studies of substrate scope. **K. Banerjee**, **S. Herson**, T. Schmit, A. Hanna, D. Mobley, **M. Collins**, **S. Slack**, **J. Randall**
- MEDI 379.** Discovery of a liver-directed glucokinase activator having anti-hyperglycemic effect without hypoglycemic potential. **A.M. Deshpande**, D. Bhuniya, S. De, D. Umrani, V. Madgula, A. Chugh, V. Palle, K. Mookhtiar
- MEDI 380.** Discovery of 5-substituted-2,4-oxazolinediones as potent GPR40 agonists for treatment of type II diabetes. **S. Lin**
- MEDI 381.** Design and synthesis of novel coumarin analogues by Mannich type reaction for spermicidal and anti-microbial actions: A dual approach for contraception. **S. Gupta**, B. Kushwaha, G. Gupta, A.K. Dwivedi
- MEDI 382.** Antidote of cyanide (sodium and hydrogen cyanide) poison and rectification of vitamin B<sub>12</sub> deficiency (production of drugs and injection). **S.N. Olatunji**
- MEDI 383.** Synthesis and biological evaluation of 20S,23S- and 20S,23R-dihydroxyvitamin D3 isomers together with their 1 $\alpha$ -hydroxyl derivatives. **Z. Lin**, S. Marepally, D. Ma, C. Cheng, L. Myers, A. Postlethwaite, T. Kim, R. Tuckey, A. Slominski, D.D. Miller, W. Li
- MEDI 384.** Synthetic approaches to a [1.1.1] bicyclopentane and its incorporation into darlapladib as a phenyl bioisostere. **N. Meason**, K. Down, D. Hirst, C. Jamieson, E. Manas, V. Patel, D. Somers
- MEDI 385.** Discovery of novel building blocks to facilitate drug discovery. **P.K. Mykhailiuk**
- MEDI 386.** Design, synthesis and application of novel building blocks to "escape the flatland" in medicinal chemistry. **P.K. Mykhailiuk**
- MEDI 387.** Synthesis of novel unique pyrrolidines by [3+2]-cycloaddition of azomethine ylides with electron-deficient alkenes. **I. Yavnyik**
- MEDI 388.** Synthesis of conformationally restricted scaffolds by double-Mannich reaction of cyclic ketones. **I. Yavnyik**
- MEDI 389.** Design, synthesis and application of novel morpholine analogues: Valuable building blocks for drug discovery. **I. Yavnyik**
- MEDI 390.** Synthesis and application of unnatural proline analogues: advanced building blocks for medicinal chemistry. **D. Lonergan**
- MEDI 391.** Protecting group strategies in the synthesis of DNA-encoded libraries. **S. Chilakapati**, D. Young, E.L. Samuels, N. Simmons, C. Santini
- MEDI 392.** Efficient synthesis of fused imidazole containing ring systems via dual oxidative amination of C(sp<sup>3</sup>)-H bonds. **G. Castanedo**
- MEDI 393.** New approaches to the carbon-13 nuclear magnetic resonance spectral properties of cholest-4-en-3-one and cholest-5-en-3-one. **E.J. Parish**, **H. Honda**, T. Wei, Y. Lo
- MEDI 394.** Design and synthesis of novel fluorinated amines: promising building blocks for drug discovery. **D. Lonergan**
- MEDI 395.** Monobocyclization of diamines in continuous flow. **A. Ku**, D.J. Sarmiento, D. Scheel, A. Evans
- MEDI 396.** Direct H/D exchange of pharmaceuticals using an NHC-amidate Pd(II) catalyst in D<sub>2</sub>O. **N. Zargari**, **K. LaCroix**, G. Ahn, R. Narain, J. Lee, K.W. Jung
- MEDI 397.** Synthesis of oleonic acid derivatives for inducing hair restoration. **M. Kang**, H. Choi, C. Kim, Y. Kwak
- MEDI 398.** Development of a novel amide coupling strategy for aminoisobutyric acid using magnesium amidate. **M. Jo**, S. Won, J. Lee, Y. Kwak
- MEDI 399.** Design and utilisation of a poised fragment library in the search for inhibitors of PHIP(2), an atypical bromodomain. **O.B. Cox**, J. Spencer, P. Brennan

## THURSDAY MORNING

### Big Data Science

#### Accessing Chemical Space & Better Modeling

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

### Computer-Aided Drug Design

#### New Modality Therapeutics

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

## THURSDAY AFTERNOON

### Big Data Science

#### Interpreting Pharmacology

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS

## NUCL

## Division of Nuclear Chemistry and Technology

A. Hixon, Program Chair

### OTHER SYMPOSIA OF INTEREST:

**Frontiers in Heavy Element Inorganic Chemistry** (see INOR, Mon, Tue)

**Adsorption of Metals by Geomedia** (see GEOC, Mon, Tue, Wed, Thu)

**Separations for the Nuclear Fuel Cycle in the 21st Century Revisited** (see I&EC, Tue, Wed)

### SOCIAL EVENTS:

**Social Hour**, 6:00 PM: Tue

### BUSINESS MEETINGS:

**Executive Committee Meeting**, 5:00 PM: Sun

**Business Meeting**, 5:00 PM: Tue

## SUNDAY MORNING

### Section A

San Diego Convention Center  
Room 15A

**Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Matthew J. Polinski & Thomas E. Albrecht-Schmitt**  
Cosponsored by INOR

T. E. Albrecht-Schmitt, Organizer, Presiding

**8:15 NUCL 1. Award Address** (Nobel Laureate Signature Award for Graduate Education in Chemistry sponsored by Avantor™ Performance Materials, Inc.). Berkelium. **T.E. Albrecht-Schmitt**

**8:45 NUCL 2. Award Address** (Nobel Laureate Signature Award for Graduate Education in Chemistry sponsored by Avantor™ Performance Materials, Inc.). Unusual covalent bonding observed in a californium borate. **M. Polinski**

**9:15 NUCL 3.** Actinide redox chemistry in the gas phase: From Cf(II) to Np(VII). **J.K. Gibson**, P.D. Dau, D.K. Shuh, R. Maurice, R. Eric

**9:35 NUCL 4.** Theoretical study of the complexation of curium, berkelium, and californium. **P. Yang**

**9:55** Intermission.

**10:15 NUCL 5.** Opportunities in using actinide  $L_{3-}$  edge resonant x-ray emission spectroscopy (RXES) to determine 5f orbital occupancy and localization. **C. Booth**

**10:35 NUCL 6.** Thermodynamics of heavy actinide interactions with dipicolinic acid. **J. Braley**

**10:55 NUCL 7.** Energetics and electronic structures of actinide clusters. **D.A. Dixon**, M. Vasiliiu, H. Arnold, S. Polansky, W. Layfield

**11:15 NUCL 8.** ACS 2016 Nobel Signature awardees and their quest for actinide borates. **D.E. Hobart**

**11:35 NUCL 9.** Fine-tuning ligand platforms for specific recognition of actinides in solution. **R.J. Abergel**, I. Yakovlev, D. An

## SUNDAY AFTERNOON

### Section B

San Diego Convention Center  
Room 15A

#### Tackling the Challenging Electronic Structure of Actinides: Symposium in honor of Richard Martin

E. R. Batista, *Organizer*

A. E. Clark, *Organizer, Presiding*

**1:15** Introductory Remarks.

**1:20 NUCL 10.** On the application of density functional theory to heavy elements: Density functionals for two- and four-component methods. **G. Scalmani**, M.J. Frisch

**1:40 NUCL 11.** Novel physics of  $UO_2$ . **T. Durakiewicz**

**2:00 NUCL 12.** Using attosecond pulses to control the electron dynamics in atoms and molecules. **B. Schneider**, X. Guan, K. Bartschat

**2:20 NUCL 13.** Evaluation of electronic coupling in solids with DFT and PBC calculations. **A. Biancardi**, M. Barclay, **M. Caricato**

**2:40 NUCL 14.** Understanding technetium. **A.P. Sattelberger**, F. Poineau, K. Czerwinski, W.M. Kerlin

**3:00** Intermission.

**3:20 NUCL 15.** Transition metal-like lanthanide and actinide ions. **F.U. Furche**, G. Chen, A. Chan, H. Choi

**3:40 NUCL 16.** Integration of theory and experiment with Rich Martin. **D.L. Clark**

**4:00 NUCL 17.** Actinide chemistry using singlet-paired coupled cluster and its combinations with density functionals. **G.E. Scuseria**

**4:20 NUCL 18.** Effects of spin-orbit coupling, non-collinear spins, and solvation on actinide-water complexes. **M.J. Frisch**, J.L. Sonnenberg, G. Scalmani, F. Egidi, X. Li

**4:40 NUCL 19.** Strategies toward reliable, structural, and energetic properties for the heavy elements. **A.K. Wilson**, G. Schoendorff, D.A. Penchoff, C. Peterson

## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 15A

#### Francis P. Garvan-John M. Olin Medal: Symposium in honor of Annie Kersting Environmental Chemistry of Actinides

*Cosponsored by ENVR*

M. Zavarin, *Organizer*

J. Begg, *Organizer, Presiding*

R. M. Tinnacher, *Presiding*

**8:00** Introductory Remarks.

**8:10 NUCL 20.** Science-based cleanup of Rocky Flats: Ten years later, what have we learned? **D.L. Clark**

**8:40 NUCL 21.** Influence of kinetics on nanoparticle migration in fractured rocks: Experiences from URL work. **T. Schäfer**, F. Huber, F. Quinto, M. Lagos, S. Heck, I. Blechschmidt, U. Noseck, T. Reiche

**9:00 NUCL 22.** Controls on neptunium behaviour in the environment. **G. Law**, S. Shaw, J. Lloyd, F. Livens, R. Patrick, P. Bots, A. Rizoulis, D. Brookshaw, C. Thorpe, A. Williamson, N. Master-Waage, F. Mosselmans, K. Morris

**9:20 NUCL 23.** Controls on radionuclide distribution in the Sellafield near-shore. **D. Ray**, A. Kersting, M. Zavarin, J. Begg, C. Joseph, P. Zhao, G. Law

**9:35 NUCL 24.** Desorption of plutonium from altered nuclear melt glass: Flow-cell experiments. **C. Joseph**, M. Zavarin, A. Kersting

**9:55** Intermission.

**10:10 NUCL 25.** Redox impact on radionuclide mobility. **H. Geckeis**

**10:40 NUCL 26.** Uranium(VI) diffusion in sodium-montmorillonite at alkaline pH. **R.M. Tinnacher**, J. Davis, C. Tournassat, J. Birkholzer

**11:00 NUCL 27.** Evaluating phosphonate-modified mesoporous silica for the sequestration of U(VI). **E.C. Uribe**, H. Mason, J. Shusterman, A. Bruchet, H. Nitsche

**11:15 NUCL 28.** Plutonium sorption to goethite at sub-femtomolar to micromolar concentrations: Redox transformations and surface precipitation. **P. Zhao**, J. Begg, M. Zavarin, S. Turney, R. Williams, Z. Dai, R. Kips, A. Kersting

**11:35 NUCL 29.** Understanding plutonium sorption to pure mineral phases: A review of recent progress. **A.E. Hixon**

### Section B

San Diego Convention Center  
Room 24A

#### Tackling the Challenging Electronic Structure of Actinides: Symposium in honor of Richard Martin

E. R. Batista, A. E. Clark, *Organizers*

M. Caricato, *Presiding*

**8:00 NUCL 30.** Water adsorption on  $AnO_2$  ( $An = U, Np, Pu$ ) surfaces. **J. Wellington**, A. Kerridge, **N. Kaltsoyannis**

**8:20 NUCL 31.** Quantum chemical modelling of the separation of Am(III) from Eu(III) by liquid-liquid extraction with Cyanex 272 and 301. **M.F. Dolg**, X. Cao, J. Zhang, N. Heinz, D. Weissmann

**8:40 NUCL 32.** Computational investigations of actinyl hydroxide complexes. **H. Schreckenbach**, S.O. Odoh

**9:00 NUCL 33.** Solvation of  $Cm^{3+}$  in binary water/methanol solutions. **M. Kelley**, P. Yang, S.B. Clark, A.E. Clark

**9:20 NUCL 34.** Activation of molecular oxygen by transition metal complexes. **J.M. Keith**, D. Kim, H. Kwon, H. Wei, S. Holland, F. Evans, Y. Ye

**9:40 NUCL 35.** New generation, quantum-based molecular dynamics. **A.M. Niklasson**

**10:00** Intermission.

**10:20 NUCL 36.** Linear response Douglas-Kroll-Hess theory for calculating excited-state, fine structure splittings of heavy elements. **X. Li**, F. Egidi, J.J. Goings

**10:40 NUCL 37.** Some research inspired by Martin's papers. **E.R. Davidson**

**11:00 NUCL 38.** Spectroscopic signatures of geometric phase effects in nonadiabatic dynamics near conical intersections. **A.F. Izmaylov**

**11:20 NUCL 39.** Computational studies of hydrolysis reactions of cationic and anionic actinide complexes. **D.A. Dixon**, M. Vasiliiu, H. Arnold, K.A. Peterson, J.K. Gibson

## MONDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 15A

#### Francis P. Garvan-John M. Olin Medal: Symposium in honor of Annie Kersting Environmental Chemistry of Actinides

*Cosponsored by ENVR*

J. Begg, *Organizer*

M. Zavarin, *Organizer, Presiding*

Y. Jiao, *Presiding*

**1:30 NUCL 40.** Tetravalent actinides in aqueous solutions. **L. Soderholm**, S. Skanthakumar

**2:00 NUCL 41.** Characterization of aqueous actinide complexes from first-principles molecular dynamics simulations. **C. Lo**, M. Vu, M. Massey, **P. Huang**

**2:20 NUCL 42.** High-pressure  $^{13}C$  NMR of  $[NpO_2(CO_3)_3]^{4+}$  to measure exchange rates with free carbonate anion. **C. Pilgrim**, M. Zavarin, W.H. Casey

**2:35 NUCL 43.** Interactions of Np with clay and mineral surfaces at high temperatures and high ionic strengths. **D.L. Wang**, D.T. Olive, B.A. Powell, H. Nitsche

**2:50 NUCL 44.** Structural incorporation of Np(V) and U(VI) in carbonate and sulfate minerals. **E. Balboni**, J. Morrison, Z. Wang, M. Engelhard, P.C. Burns

**3:10** Intermission.

**3:25 NUCL 45.** Characterization of reaction energies and speciation changes underlying strong actinide sorption to mineral surfaces. **B.A. Powell**

**3:55 NUCL 46.** Mechanistic sorption models: Species, thermodynamics, and application. **V. Brendler**, C. Richter, M. Stockmann

**4:15 NUCL 47.** Does the presence of a second mineral enhance Cs desorption? **C. Durrant**, J. Begg, M. Zavarin, K. Ünlü, A. Kersting

**4:30 NUCL 48.** Comparing plutonium redox and sorption reactions on organic- and inorganic-based substrates. **E.M. Wylie**, B.A. Powell

**4:50 NUCL 49.** Plutonium interactions with Suwannee River fulvic acid. **N.A. Conroy**, B.A. Powell, M. Zavarin, A. Kersting

**5:05 NUCL 50.** Microbe-mediated uranium transformation and mineralization. **D.M. Park**, M. Yung, L.N. Lammers, **Y. Jiao**

**5:25 NUCL 51. Award Address** (Francis P. Garvan-John M. Olin Medal sponsored by the Francis P. Garvan-John M. Olin Medal Endowment). **Francis P. Garvan-John M. Olin Medal**. A. Kersting

### Section B

San Diego Convention Center  
Room 24A

#### Tackling the Challenging Electronic Structure of Actinides: Symposium in honor of Richard Martin

E. R. Batista, A. E. Clark, *Organizers*

N. Kaltsoyannis, *Presiding*

**1:00 NUCL 52.** Transition states in siderophore, metal-binding mechanisms. **J.L. Sonnenberg**, Z. Greeley, M.F. Skaro, M. Hughey

**1:20 NUCL 53.** Search for the vacuum ultra-violet  $^{229}Th$  nuclear isomeric transition in  $MgF_2$ . **X. Zhao**, Y. de Escobar, A. Roman, B. Barker, E. Meyer, J. Ellis, R. Rundberg, E. Bond, R. Martin, T. Bredeweg, M. Wilkerson, S. Kozimor

**1:40 NUCL 54.** Soft x-ray synchrotron radiation spectroscopy of actinide materials: Theory-enabling experiment. **D.K. Shuh**, S.G. Minasian, J.M. Keith, E.R. Batista, D.L. Clark, S.A. Kozimor, R.L. Martin, S. Butorin, J. Vegelius, M. Suzu, Y. Yun, J. Nor, P. Oppeneer

**2:00 NUCL 55.** Calculating magnetic resonance parameters of f-element complexes. **J. Autschbach**

**2:20 NUCL 56.** Predicting the redox potentials of actinide complexes using first-principles. **P. Yang**

**2:40 NUCL 57.** Bonding and magnetism in tris-cyclopentadienyl neodymium, uranium complexes, and their isocyanide adducts. **W.W. Lukens**, M. Speldrich, P. Yang

**3:00** Intermission.

**3:20 NUCL 58.** Synthesis, spectromicroscopy, and theory of lanthanide and actinide oxide materials. **S.G. Minasian**, A.B. Altman, E.R. Batista, C. Booth, J.M. Keith, W.W. Lukens, S.A. Kozimor, R.L. Martin, J. Pacold, D.K. Shuh, X. Wen

**3:40 NUCL 59.** Toward controlling the inter-system crossing in Fe(II)-polypyridines. **E. Jakubikova**

**4:00 NUCL 60.** New insights from XPS and XAS. **P.S. Bagus**, C.J. Nelin

**4:20 NUCL 61.** Modeling electron detachment in metal oxide clusters using efficient electronic structure methods. **H.P. Hratchian**

### Adsorption of Metals by Geomeedia

#### Theory & Modeling after Twenty Years

*Sponsored by GEOG, Cosponsored by ENVR, MPPG† and NUCL*

**Frontiers in Heavy Element Inorganic Chemistry**

Sponsored by INOR, Cosponsored by NUCL

**TUESDAY MORNING**

**Section A**

San Diego Convention Center  
Room 15A

**Young Investigators in Nuclear & Radiochemistry**

Cosponsored by YCC

L. C. Shuller-Nickles, *Organizer*

A. E. Hixon, *Organizer, Presiding*

**9:00** Introductory Remarks.

**9:05 NUCL 62.** Stability constant determinations for technetium (IV) complexation with selected carboxylic ligands in sodium nitrate. **T. Omoto**, N. Wall

**9:25 NUCL 63.** Oxidation of actinyl(V) by addition of nitrogen dioxide revealed via replacement of acetate by nitrite. **P.D. Dau**, J.M. Carretas, J. Marçalo, W.W. Lukens, J.K. Gibson

**9:45 NUCL 64.** Trace-level neptunium (V) sorption to different aluminum (hydr)oxide minerals. **T. Baumer**, A.E. Hixon, P. Kay

**10:05** Intermission.

**10:25 NUCL 65.** Strontium interactions and colloid silica in the presence and absence of humic acids. **K. Swearingen**, N. Wall

**10:45 NUCL 66.** Supramolecular assembly, structure, and spectroscopic properties of Np complexes with pyridinium ions. **K.L. Pellegrini**, R.G. Surbella, G. Sigmon, P.C. Burns, B. McNamara, C.L. Cahill, J.M. Schwantes

**11:05 NUCL 67.** Uranyl peroxide formation in the absence of light. **A.S. Jayasinghe**

**11:25 NUCL 68.** Synthesis and structural comparison of *f* element-carbonato species for nuclear material analysis. **J.F. Corbey**, L.E. Sweet, B. McNamara, J. Schwantes

**Section B**

San Diego Convention Center  
Room 24A

**Tackling the Challenging Electronic Structure of Actinides: Symposium in honor of Richard Martin**

A. E. Clark, *Organizer*

E. R. Batista, *Organizer, Presiding*

**8:00 NUCL 69.** Electronic structure of actinide oxides from hybrid functionals and photoemission. **J. Joyce**, T. Durakiewicz, R.L. Martin, B. Scott, T.M. McCleskey, Q. Jia, M. Beaux, X. Wen, K. Graham, E. Bauer, L.E. Roy, A.K. Burrell, G.E. Scuseria

**8:20 NUCL 70.** Prediction of screened hybrid functional on actinide oxides and transition metals oxides.

**X. Wen**, R.L. Martin, E.R. Batista, S. Rudin, G.E. Scuseria, Y. Yang, H. Jiao, Y. Li

**8:40 NUCL 71.** Cuprates from quantum chemistry. **G.K. Chan**

**9:00 NUCL 72.** Computational studies of *f*-element complexes with high-nitrogen-containing ligands for separations processes. **N. Henson**, J.M. Veauthier, J.L. Kiplinger, R.L. Martin

**9:20 NUCL 73.** Magnetic trends in actinide oxides. **L. Soderholm**, S. Skanthakumar, G. Jin

**9:40 NUCL 74.** Actinide organometallic chemistry: A meeting with Rich Martin at the bottom of the periodic table. **J.L. Kiplinger**

**10:00** Intermission.

**10:20 NUCL 75.** Coordination chemistry of trivalent actinides. **S.A. Kozimor**, E.R. Batista, J.M. Berg, E. Birnbaum, J. Cross, J. Engle, M.G. Ferrier, H. La Pierre, J. Lezama, B. Stein, P. Yang

**10:40 NUCL 76.** Cp<sub>2</sub>U(=NR)<sub>2</sub>: Simple organoactinide compounds with surprisingly complicated electronic structures. **J.M. Boncella**, N.C. Tomson, A. Tondreau, M. Winston, B. Scott

**11:00 NUCL 77.** Challenging the metal-ligand bifunctional mechanism. **J.C. Gordon**, P. Dub, B. Scott

**11:20 NUCL 78.** Metal-ligand bifunctional mechanism and metal-ligand cooperation: Critical analyses of catalytic cycles involving H<sub>2</sub>. **P.A. Dub**, J.C. Gordon

**11:40 NUCL 79.** Journey to the land of excited-state dynamics in organic semiconductors. **S. Tretiak**

**Adsorption of Metals by Geomedia Thermodynamics & Kinetics Experimental Study**

Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL

**Frontiers in Heavy Element Inorganic Chemistry**

Sponsored by INOR, Cosponsored by NUCL

**TUESDAY AFTERNOON**

**Section A**

San Diego Convention Center  
Room 15A

**Young Investigators in Nuclear & Radiochemistry**

Cosponsored by YCC

A. E. Hixon, *Organizer*

L. C. Shuller-Nickles, *Organizer, Presiding*

**1:45 NUCL 80.** Lanthanide harvesting from mixed-bed ion exchange resin at the Facility for Rare Isotope Beams. **M.D. Scott**, J. Gilkey, J.D. Robertson

**2:05 NUCL 81.** Separation of technetium from aqueous media with surface-modified materials. **S.C. Bortorff**, T.R. Hayes, L.R. Martin, P.D. Benny

**2:25 NUCL 82.** Separation of americium in high-oxidation states from curium utilizing sodium bismuthate. **J.M. Richards**, R. Sudowe

**2:45 NUCL 83.** Molecular and crystal structures of uranyl nitrate complexes bearing *N*-substituted 2-pyrrolidone derivatives: Towards a new aspect of nuclear fuel reprocessing. **K. Takao**, Y. Ikeda

**3:05** Intermission.

**3:25 NUCL 84.** Quantum-mechanical calculations of iodine incorporation into Ag(NO<sub>3</sub>). **J. Buff**, L.C. Shuller-Nickles

**3:45 NUCL 85.** Synthesis and characterization of 1,1,1,5,5,5-hexafluoroacetyl-acetate compounds for rapid thermochromatographic separations of light nuclear fission products. **A. Jones**, J.D. Auxier, E. Barrowclough, H.L. Hall

**4:05 NUCL 86.** Dissolution methods for simulated, urban debris samples formed from nuclear weapons explosions.

**R.K. Springs**, R. Sudowe

**4:25 NUCL 87.** Accurate mass and mobility speciation of metal complexes: Uranium, barium, cesium, and lanthanum. **A. Davis**, B. Clowers

**Separations for the Nuclear Fuel Cycle in the 21st Century Revisited**

Sponsored by I&EC, Cosponsored by NUCL

**Adsorption of Metals by Geomedia**

**Thermodynamics & Kinetics Experimental Study**

Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL

**Frontiers in Heavy Element Inorganic Chemistry**

Sponsored by INOR, Cosponsored by NUCL

**WEDNESDAY MORNING**

**Section A**

San Diego Convention Center  
Room 15A

**Young Investigators in Nuclear & Radiochemistry**

Cosponsored by YCC

L. C. Shuller-Nickles, *Organizer*

A. E. Hixon, *Organizer, Presiding*

**9:00 NUCL 88.** <sup>77</sup>As complexes for potential PET and radiotherapy. **Y. Feng**, A. DeGraffenreid, M. Gott, A. Ketring, C. Cutler, S.S. Jurisson

**9:20 NUCL 89.** Development of PDT/PET theranostics: Synthesis and biological evaluation of a 18F-radiolabeled, water-soluble porphyrin. **G.M. Entract**, R.W. Boyle, F. Bryden, J. Domarkas, H. Savoie, L. Allott, C. Cawthorne, S.J. Archibald

**9:40 NUCL 90.** Synthesis and evaluation of an <sup>18</sup>F-labeled pyrimidine-pyridine amine for targeting CXCR4 receptors in gliomas with intact blood-brain barriers. **D.W. Demoin**, M. Shindo, H. Zhang, I. Serganova, K.J. Edwards, N. Pillarsetty, J.S. Lewis, R.G. Blasberg

**10:00** Intermission.

**10:20 NUCL 91.** Development of a copper sulfide (CuS) immunconjugate nanoparticle for targeted radiotherapy. **L. Sutherland**, J.D. Robertson, P. Pevsner

**10:40 NUCL 92.** <sup>177</sup>Lu-doped lanthanide phosphate nanoparticles (<sup>177</sup>LuGdPO<sub>4</sub>@Au) for targeted radiotherapy. **N. Sobol**, P. Pevsner, J.C. Lattimer, E. Cedrowska, J. Schorp, J.D. Robertson

**11:00 NUCL 93.** Development of a new solid-phase method for the production of high-specific activity *fac*-[M(CO)<sub>3</sub>]<sup>+</sup> (M = Re, <sup>99m</sup>Tc) radiopharmaceuticals. **T.R. Hayes**, A.S. Powell, P.D. Benny

**11:20 NUCL 94.** Alpha-particle spectroscopy coupled with gas-phase separations. **M.T. Cook**

**11:40** Concluding Remarks.

**Section B**

San Diego Convention Center  
Room 24A

**Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger**

Cosponsored by INOR‡

D. L. Clark, D. K. Shuh, *Organizers*

L. Soderholm, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 NUCL 95.** Recent advances in uranium-pnictide multiple-bond chemistry. **S.T. Liddle**, D. King, B. Gardner, P. Cleaves, A. Woolles, J. McMaster, G. Balazs, M. Scheer, F. Tuna, E. McInnes, W. Lewis, A. Blake

**8:25 NUCL 96.** Preparation and characterization of actinide nitrides. **K. Czerwinski**, A.P. Sattelberger

**8:45 NUCL 97.** Chemistry behind the radiation release at WIPP. **D.L. Clark**

**9:05 NUCL 98.** Heavy element chemistry using synchrotron radiation. **D.K. Shuh**, S. Butorin, A. Modin, J. Vegelius, M. Suzu, P. Oppeneer, D. Andersson

**9:25 NUCL 99.** Technetium binary halides: A tribute to Al Sattelberger. **F. Poineau**

**9:45 NUCL 100.** Chemical predictive modeling in actinide chemistry. **P. Yang**

**10:05** Intermission.

**10:25 NUCL 101.** U-mediated electrocatalytic H<sub>2</sub> production from water with a molecular uranium coordination complex. **K. Meyer**

**10:45 NUCL 102.** Nanostructured, bilayered uranium oxide: Metal oxide films for solar hydrogen production. **J. Leduc**, T. Fischer, S. Mathur

**11:05 NUCL 103.** Theoretical studies of covalency in *f*-element materials. **E.R. Batista**, S.A. Kozimor

**11:25 NUCL 104.** Thinking small: Plutonium separations and processing at the microscale. **R.M. Chamberlin**, N. Xu, J. Gao, S.L. Yarbrough, Q. McCulloch

**Adsorption of Metals by Geomedia**

**Radionuclides: Uranium & Transuranium - Extension of ACS Garvan-Olin Medal Session**

Sponsored by GEOC, Cosponsored by ENVR, MPPG‡ and NUCL

**Separations for the Nuclear Fuel Cycle in the 21st Century Revisited**

Sponsored by I&EC, Cosponsored by NUCL

**WEDNESDAY AFTERNOON**

**Section B**

San Diego Convention Center  
Room 15A

**Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger**

Cosponsored by INOR‡

D. L. Clark, L. Soderholm, *Organizers*

D. K. Shuh, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 NUCL 105.** Heteroditopic, soft donor ligands: Emerging opportunities for actinide/lanthanide separations. **S.R. Daly**, A.V. Blake, G. Durgaprasad

**1:55 NUCL 106.** Synthetic investigations towards a *cis*-uranyl complex. **T.W. Hayton**

**2:15 NUCL 107.** Chemical speciation for forensic science of nuclear materials. **M.P. Wilkerson**

**2:35 NUCL 108.** Fluorido complexes of low-valent technetium. **S. Mariappan Balasekaran**, A. Hagenbach, U. Abram, F. Poineau

**2:55 NUCL 109.** Towards new molecular functionalities for neptunium and plutonium. **A. Gaunt**, B. Scott, J. Brown, T.W. Hayton, E.R. Batista, S.T. Liddle, D.E. Smiles, S.D. Reilly, S.A. Kozimor, J.M. Boncella

3:15 Intermission.

**3:35 NUCL 110.** Accurate solution phase thermochemistry for actinide solvation, complexation, and transport from aqueous to organic phases. **A.E. Clark**

**3:55 NUCL 111.** Energetic studies of different uranyl nanoclusters. **M. Sharifronzi, J. Szymanski, P.C. Burns**

**4:15 NUCL 112.** Covalency in Ce<sup>III</sup> and Ce<sup>IV</sup> complexes: What a difference an electron makes. **R.L. Martin**

**4:35 NUCL 113.** Technetium separations and waste-form development for advanced nuclear fuel cycles. **G.D. Jarvinen, E. Mausolf, F. Poineau, K. Czerwinski**

#### Adsorption of Metals by Geomedia

##### X-ray Spectroscopy

Sponsored by GEOC, Cosponsored by ENVR, MPPG† and NUCL

#### Separations for the Nuclear Fuel Cycle in the 21st Century Revisited

Sponsored by I&EC, Cosponsored by NUCL

## WEDNESDAY EVENING

#### Adsorption of Metals by Geomedia

Sponsored by GEOC, Cosponsored by ENVR and NUCL

## THURSDAY MORNING

### Section B

San Diego Convention Center  
Room 15A

#### Heavy Element Inorganic Chemistry: A Tribute to Al Sattelberger

Cosponsored by INOR†

D. L. Clark, D. K. Shuh, L. Soderholm,  
*Organizers*

D. E. Hobart, *Presiding*

8:30 Introductory Remarks.

**8:35 NUCL 114.** Technetium chemistry at Los Alamos National Laboratory in the early 90s. **J.C. Bryan**

**8:55 NUCL 115.** Synthesis and chemistry of novel actinide complexes in the gas phase. **J.K. Gibson**

**9:15 NUCL 116.** Computational studies of lanthanide and actinide fluorides and hydroxides. **D.A. Dixon, Z. Lee, T. Mikulas, Z. Fang, M. Vasiliiu, K.A. Peterson, L. Andrews, T. Vent-Schmidt, S. Riedel**

**9:35 NUCL 117.** Actinide science research capabilities at Florida State University. **D.E. Hobart**

**9:55 NUCL 118.** Structural characterization and microfluidic spectroscopy of salphenazine complexes for detection of copper and uranyl. **A.E. Gordon, B.A. Maynard, E.E. Hardy, J.E. Brooks, C.J. Easley**

**10:15 NUCL 119.** Electronic structure studies of radioactive solids by NMR and NQR spectroscopy. **H. Cho**

10:35 Intermission.

**10:55 NUCL 120.** Electronic structure in actinide materials and alloys containing aluminum. **S.G. Minasian, A.B. Altman, E.D. Bauer, C. Booth, S. Pemmaraju, J. Pacold, D. Prendergast, D.K. Shuh, T. Tyliczszak**

**11:15 NUCL 121.** Blending nitrogen-rich chemistry with f-elements for the development of new, high-purity routes to actinide nitrides. **J.M. Veauthier, J.L. Kiplinger, K. Browne, K.A. Maerzke, N.E. Travia, B.C. Tappan, N.J. Henson, P. Yang, A.H. Mueller, B. Scott, D.E. Chavez**

**11:35 NUCL 122.** Putting the AI in Allyl: A summary of our adventures with Ir-, Rh- and other allyl complexes. **K. John**

**11:55 NUCL 123.** Actinide chemistry with soft donor ligands: Picking up where Sattelberger left off. **J.R. Walensky, A. Behrle**

12:15 Concluding Remarks.

#### Adsorption of Metals by Geomedia

##### Biosorption: Metal & Bacteria

Sponsored by GEOC, Cosponsored by ENVR, MPPG† and NUCL

## THURSDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 15A

#### General Topics in Nuclear & Radiochemistry

D. E. Hobart, *Organizer, Presiding*

**1:00 NUCL 124.** Study of cesium extraction using novel ligands for the development of a supercritical, carbon dioxide decontamination process. **S. Montel, E. Andreiadis, A. Dartiguelongue, A. Leybros, M. Miguirditchian**

**1:15 NUCL 125.** Determination of <sup>3</sup>H and <sup>14</sup>C of radwaste oils and radwaste ion exchange resins from nuclear power plants using a dry oxidation method. **Y. Ko, C. Kim, G. Choi, K. Chung, M. Kang**

**1:30 NUCL 126.** Optimization of selective separations of lanthanides: An integrated computational and experimental study. **D.A. Penchoff, C. Peterson, J.D. Auxier, H.L. Hall, A.K. Wilson**

**1:45 NUCL 127.** Electrochemically modulated extraction of neodymium. **S. Anderson, E.E. Kalu, C. Clark, M. Nilsson**

**2:00 NUCL 128.** Rapid and selective production and separation of volatile metal fluorides via nitrogen trifluoride fluorination for mass spectrometry. **R. Clark, B. McNamara, C. Barinaga, J. Peterson, N. Govind, A. Andersen, D. Abrecht, J. Schwantes, N. Ballou**

2:15 Intermission.

2:35 NUCL 129. Withdrawn.

**2:50 NUCL 130.** Enriched B-10 benzene molecules for thermal neutron detection and overdeveloped p-terphenyl derivatives for pulse shape discrimination. **H. Yemam, A. Mahl, U. Greife, A. Sellinger**

**3:05 NUCL 131.** Development of a chemical system for rutherfordium using TEHA and TEHP. **J. Roifes, J. Despotopulos, N. Gharibyan, R. Henderson, D.A. Shaughnessy, R. Sudowe**

**3:20 NUCL 132.** Results of an international interlaboratory comparison of NBL CRM 124-3 material. **L.P. Colletti, L. Tandon, E. Noriyuki, M. Sumi, H. Okazaki, S. Mitsuhiro, M. Kayano, M. Kazutomi, T. Kageyama, S. Nobuo**

**3:35 NUCL 133.** Development of pre-detonation nuclear forensic signatures in metallic structures. **J.D. Auxier, C. Eley, D.R. Brocklehurst, M. Lang, H.L. Hall**

3:50 Intermission.

**4:10 NUCL 134.** Targeting breast cancer with NOTA-derivatized pH (low) insertion peptide (pHLIP) complexes with <sup>64</sup>Cu and <sup>18</sup>F: Conjugation strategies change everything. **D.W. Demoin, K.J. Edwards, L.C. Wyatt, D. Abdel-Atti, M. Sarparanta, J. Blower, N. Pillarsetty, O.A. Andreev, Y.K. Reshetnyak, N. Viola-Villegas, J.S. Lewis**

**4:25 NUCL 135.** Nickel-based alloys from VDM Metals® for molten-salt, nuclear fast-reactor (MSNFR) applications. **I.B. Polovov, V.V. Karpov, A.V. Abramov, A.F. Gibadullina, A.Y. Zhilyakov, S.V. Belikov, V.A. Volkovich, O.I. Rebin**

**4:40 NUCL 136.** Identification of basic processes influencing radiation-field generation in water-cooled nuclear reactors through multivariate statistics. **C.A. Gregorich**

**4:55 NUCL 137.** Separation of actinium from lanthanum for targeted alpha therapy. **L.H. Delmau, R.A. Boll, C.O. Reynolds, C. Hindman**

## ORGN

### Division of Organic Chemistry

**R. Broene and M. McIntosh, Program Chairs**

#### OTHER SYMPOSIA OF INTEREST:

**Alpha Olefin Catalysis: Production & Transformations** (see I&EC, Sun)

**Discussions with the President's Task Force on Employment** (see PRES, Sun)

**Is There a Crisis in Organic Chemistry Education** (see PRES, Mon)

**Diversity-Quantification-Success?** (see PRES, Mon)

**LGBT Chemists' Symposium on Chemical Biology** (see PROF, Mon)

**Start-up Businesses in Drug Discovery** (see SCHB, Mon)

#### SOCIAL EVENTS:

**Social Hour, 8:30 PM: Wed**

## SUNDAY MORNING

### Section A

San Diego Convention Center  
Room 6A

#### Peptides, Proteins & Amino Acids

M. C. McIntosh, *Organizer*

A. A. Fuller, *Presiding*

**8:00 ORGN 1.** Densely N-alkylated peptides: Unexplored rigid and chiral peptides. **R. Kaminker, W. Gutekunst, I. Kaminker, Y. Luo, J. Niu, S. Lee, M. Markmann, S. Han, C.J. Hawker**

**8:20 ORGN 2.** Spontaneous, templated synthesis of peptide nucleic acids. **L. Leman, Y. Masaki, M. Ghadiri**

**8:40 ORGN 3.** Novel protecting and activating group for reactive cysteines. **O. Schaefer, D. Huesmann, M. Barz**

**9:00 ORGN 4.** Synthesis and study of diversely functionalized mimics of peptide-derived azole-containing natural products. **A.A. Fuller, A. Koh, G. Gate, A. Mohan, K. McCormas**

**9:20 ORGN 5.** X-ray crystallographic structure of oligomers formed by a toxic  $\beta$ -hairpin derived from  $\alpha$ -synuclein: Trimers and higher-order oligomers. **P. Salveson, J.S. Nowick**

**9:40 ORGN 6.** Solid-phase peptide synthesis (SPPS) of bulky  $\alpha$ ,  $\beta$ -dehydroamino acid-containing peptides to assess their stabilities to proteolysis. **A. Jalan, S.L. Castle**

**10:00 ORGN 7.** Biophysical characterization of reflectin isoforms from squid and cuttlefish. **L. Phan, D. Ordinario, E. Leung, W. Walkup, A.A. Gorodetsky**

**10:20 ORGN 8.** Serine peptide ligations. **R. Schreihsans, M.C. Pirrung**

**10:40 ORGN 9.** Aza-glycine induces collagen hyperstability. **Y. Zhang, R.M. Malamakal, D.M. Chenoweth**

**11:00 ORGN 10.** Modulate protein aggregation and amyloid toxicity by structure-based computational approaches. **L. Jiang, Q. Cao, D. Eisenberg**

### Section B

San Diego Convention Center  
Room 6B

#### Nanomaterials

M. C. McIntosh, *Organizer*

A. Yang, *Presiding*

**9:00 ORGN 11.** Syntheses of organic cage molecules via alkyne metathesis. **A. Yang, S. Lee, T. Money Penny, J.S. Moore**

**9:20 ORGN 12.** Efficient aerobic oxidation of amines to imines by cesium-promoted, mesoporous manganese oxide. **S. Biswas, B. Dutta, K. Mullick, C. Kuo, S.L. Suib**

**9:40 ORGN 13.** High mobility semiconducting discotic liquid crystals. **B. Gomez-Lor, C. Ruiz, A. Benito**

**10:00 ORGN 14.** Secondary structure controlled self-assembly and conservation of polypeptidic nanoparticles by dynamic covalent bonds. **O. Schaefer, D. Huesmann, M. Barz**

**10:20 ORGN 15.** Controllable fabrication of high-quality, one-dimensional graphene configuration and as electrode materials in supercapacitor. **T. Fan, Z. Xiao, Y. Feng, F. Guo, H. Tang, Y. Liu, H. Meng, Y. Min**

**10:40 ORGN 16.** Investigation of up-conversion enhancement of PbS nanocrystals with tetracene derivatives. **D. Simpson, M. Mahboub, Z. Huang, M. Tang**

**11:00 ORGN 17.** Extended periacenes: Synthesis from novel bisacenes and characterization by scanning probe microscopy. **C. Rogers, F.R. Fischer**

**11:20 ORGN 18.** Degradable, clinically transplantable, enzyme-responsive, polymeric nanoparticles. **N. Collins**

**11:40 ORGN 19.** Water-soluble organic nanoparticles with functionalized, molecularly imprinted hydrophobic binding pockets. **L. Hu, Y. Zhao**

### Section C

San Diego Convention Center  
Room 6C

#### Biolegally-Related Molecules & Processes

M. C. McIntosh, *Organizer*

M. Hammers, *Presiding*

**8:30 ORGN 20.** Novel synthesis of ribonucleic guanidine. **R.H. Trude, G. Tolentino, A.M. Awad**

**8:50 ORGN 21.** Development of new fluorescent G-quadruplex ligands. M. Livendahl, E. Chorell

**9:10 ORGN 22.** Withdrawn.

**9:30 ORGN 23.** Abyssomicin 2 reactivates latent HIV-1 by a PKC- and HDAC-independent mechanism.

**B. Leon,** G. Navarro, B.J. Dickey, G. Stepan, A. Tsai, G.S. Jones, M.E. Morales, T. Barnes, S. Ahmadyar, M. Tsiang, R. Gelezizunas, T. Cihlar, N. Pagratis, Y. Tian, H. Yu, R.G. Linington

**9:50 ORGN 24.** Full-spectrum fluorogenic tetrazine bioorthogonal probes for live-cell imaging. H. Wu, S. Alexander, C. Cole, N.K. Devaraj

**10:10 ORGN 25.** Fluorescent dyes for multicolor STED microscopy in living cells. **A.N. Butkevich,** G.Y. Mitronova, S. Sidenstein, J.L. Klocke, D. Kamin, D.N. Meineke, E. D'Este, J.G. Danzl, V.N. Belov, S.W. Hell

**10:30 ORGN 26.** Discovery of quino-line-derived trifluoromethyl alcohols, and determining their *in vivo* toxicity and anticancer activity in zebrafish embryo model. **M.A. Lnu**

**10:50 ORGN 27.** Bright fluorescent probe enables analyte responsive, 3D imaging of H<sub>2</sub>S in live zebrafish using light-sheet fluorescence microscopy. **M. Hammers,** M.D. Pluth

**11:10 ORGN 28.** Synthesis of a tri-agonist compound library used to evaluate innate and adaptive immune responses. **J. Tom,** T.J. Albin, A. Esser-Kahn

**11:30 ORGN 29.** Development of ratiometric photoacoustic probes. **P. Zhang,** J. Chan

## Section D

San Diego Convention Center  
Room 5B

### Asymmetric Reactions & Syntheses

M. C. McIntosh, *Organizer*

D. Bandyopadhyay, *Presiding*

**8:00 ORGN 30.** Palladium-catalyzed, enantioselective aziridine desymmetrization. **J.B. Morgan**

**8:20 ORGN 31.** Synthesis of enantio-enriched alkylfluorides by the fluorination of boronate complexes. **C. Sandford,** R. Rasappan, V.K. Aggarwal

**8:40 ORGN 32.** Transition metal-catalyzed synthesis of chiral amino acids and their synthetic applications. **Y. Tahara,** M. Ito, S. Obinata, M. Michino, K. Kanyiva, T. Shibata

**9:00 ORGN 33.** Vinylogous iminium-ions in asymmetric organocatalysis. **P.H. Poulsen,** K.A. Jorgensen

**9:20 ORGN 34.** Control of stereoselectivity in amino-acid-derived, phosphine-catalyzed annulations through intermolecular hydrogen bonds. **M.C. Holland,** R. Gilmour, K.N. Houk

**9:40 ORGN 35.** Recent progress in the enantioselective synthesis of  $\alpha$ -tosyloxy ketones using iodine(III) reagents. **C. Legault**

**10:00 ORGN 36.** Computational approach to develop phosphoramidite ligand applied to Rh-catalyzed asymmetry cycloisomerization and Cu-catalyzed asymmetry conjugate addition. **Q. Peng,** R.S. Paton

**10:20 ORGN 37.** Vanadium complex catalyzed enantioselective synthesis of oxa[9] helicenes. **S. Takizawa,** M. Sako, H. Sasai

**10:40 ORGN 38.** Enantioselective propargyl and allyl Claisen rearrangements catalyzed by chiral nickel(II)/*N,N'*-dioxide complex. **Y. Liu,** X. Feng

**11:00 ORGN 39.** Chiral magnesium(II) complex-catalyzed asymmetric  $\alpha$ -hydroxylation of  $\beta$ -keto esters or  $\beta$ -keto amides and asymmetric [3 + 2] cycloaddition of methyleneindolinones with cyclic azomethine imines. **C. Yin,** X. Feng

**11:20 ORGN 40.** Asymmetric ring-opening of cyclopropyl ketones with nitrogen, oxygen, and sulfur-containing nucleophile. **Y. Xia,** X. Liu, L. Lin, X. Feng

**11:40 ORGN 41.** Chemical development of a novel antiviral at Merck. **M. McLaughlin**

## Section E

San Diego Convention Center  
Room 1A

### Metal-Mediated Reactions & Syntheses

M. C. McIntosh, *Organizer*

T. Newhouse, *Presiding*

**8:00 ORGN 42.** Pd/C and Ru/C-catalyzed conversion of 5-hydroxymethylfurfural (HMF) to fuel additives. **J. Francis,** D.G. Kovacs

**8:20 ORGN 43.** Efficient hydrogenation of olefins using water as the hydrogen atom source. **S. Cummings,** T.T. Le, G. Fernandez, L. Quiambao, L.M. Gong, B.J. Stokes

**8:40 ORGN 44.**  $\pi$ -allyl palladium catalysis beyond allylation. **T. Newhouse**

**9:00 ORGN 45.** Synthesis of arylated spiro phosphonates. **R.A. Stockland**

**9:20 ORGN 46.** Organometallic aluminum azomethine ylides meet visible light: Unique reactivity for direct syntheses of heterocycles. **A. Mendoza,** J. Otero, S. Suarez-Pantiga, K. Colas

**9:40 ORGN 47.** Mechanistic elucidation of amine directed aliphatic C-H bond aziridination and the development of a chiral process. **A. Smalley,** M. Gaunt

**10:00 ORGN 48.** Platinum-mediated ring opening of 2,3-cyclopropanated *N*-tosylpiperidines. **V. Barat,** S. Kasinathan, R. Bates

**10:20 ORGN 49.** Iridium-catalyzed borylation of unactivated alkyl C-H bonds directed by a hydrosilyl group. **M.A. Larsen,** S. Cho, J.F. Hartwig

**10:40 ORGN 50.** Pre-transmetalation intermediates in the Suzuki-Miyaura reaction revealed: Evidence for "the missing links". **A.A. Thomas,** S.E. Denmark

**11:00 ORGN 51.** Nickel-catalyzed regio-specific functionalization of 8-methylquinolines. **X. Lei,** Z. Guo, F. Hu

**11:20 ORGN 52.** Oxyboration: Addition of B-O sigma bonds to C-C pi bonds. **K.T. Tu,** J. Hirner, S.A. Blum

**11:40 ORGN 53.** Catalysis under confinement: Towards new chemistries and selectivities. **V.O. Rodionov**

## Section F

San Diego Convention Center  
Room 1B

### New Reactions & Methodology

M. C. McIntosh, *Organizer*

R. A. Altman, *Presiding*

**8:00 ORGN 54.** Oxazolone cycloadducts as versatile frameworks for alkaloid synthesis. **R.C. Lapo**

**8:20 ORGN 55.** Enantioselective photocatalytic [3+2] cycloadditions of aryl cyclopropyl ketones. **A. Amador,** E. Sherbrook, T.P. Yoon

**8:40 ORGN 56.** Highly diastereoselective synthesis of substituted cyclopentenones through multicomponent reactions of phosphines, enynediates, and benzylidene malononitriles via an unexpected phosphine  $\alpha$ -addition- $\delta$ -evolution of an anion pathway. **S. Chuang,** S. Sung

**9:00 ORGN 57.** Metal-catalyzed strategies for decarboxylative fluoralkylation. **R.A. Altman**

**9:20 ORGN 58.** Modeling of organic reactions as they traverse time with automated platforms. **V.W. Rosso,** J. Selekman, V. Vydra, B. Mack, J. Tabora, J. Janey

**9:40 ORGN 59.** Copper-catalyzed oxidative decarboxylative C-H arylation reactions. **J.M. Hoover,** K. Bustin, L. Chen, L. Ju, E. Aguilera

**10:00 ORGN 60.** New reactions with a simple, versatile, and metal-free photoredoxocatalyst. **S.O. Poelma,** G.L. Burnett, K.M. Mattson, N.J. Treat, E. Discekici, Z. Hudson, P. Clark, B.E. Barton, S. Mukhopadhyay, C.J. Hawker, J. Read De Alaniz

**10:20 ORGN 61.** Palladium/phosphadamtane catalyst enables an exclusively *trans*-selective chlorocarbonylation of alkynes. **C. Le,** X. Hou, T. Sperger, F. Schoenebeck, M. Lautens

**10:40 ORGN 62.** Ligand-controlled, regio-divergent hydrothiolation: A [Rh]-catalyzed pathway to selectively form 1,2- and 1,3-amino thioethers. **J.L. Kennemur,** G. Kortman, K.L. Hull

**11:00 ORGN 63.** Palladium-catalyzed transfer hydrogenation reactions of alkenes and alkynes with water mediated by diboron reagents. **S.P. Cummings,** T.T. Le, G. Fernandez, L. Quiambao, L. Gong, **B.J. Stokes**

**11:20 ORGN 64.** Synthesis of spirodienone lactams through 5-*endo*-dig cyclization of phosphorylated allenes. **P. Adler,** A. Fadel, N. Rabasso

## SUNDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 6A

#### ACS Award for Creative Work in Synthetic Organic Chemistry: Symposium in honor of Scott J. Miller

M. S. Sigman, *Organizer, Presiding*

**1:00 ORGN 65.** Synthesis of complex guanidinium alkaloids. **S. Herzon**

**1:45 ORGN 66.** Recent advances in olefin metathesis. **R.H. Grubbs**

**2:30** Intermission.

**2:35 ORGN 67.** Bringing big data tools to physical organic chemistry. **M.S. Sigman**

**3:20 ORGN 68.** Nickel-catalyzed stereospecific cross-coupling and reductive coupling reactions. **E.R. Jarvo**

**4:05** Introductory Remarks.

**4:10 ORGN 69. Award Address** (ACS Award for Creative Work in Synthetic Organic Chemistry sponsored by Aldrich Chemical Company, LLC). Searching for selective catalytic reactions in complex molecular environments. **S.J. Miller**

### Section B

San Diego Convention Center  
Room 6B

#### Lewis Base Catalyzed Asymmetric Transformations

D. W. Piotrowski, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 70.** Lewis-base catalysis of asymmetric acylation, sulfonylation, and phosphorylation processes. **A.C. Spivey**

**1:45 ORGN 71.** Regio- and enantioselective synthesis of azole hemiaminal esters by Lewis-base-catalyzed dynamic kinetic resolution. **A.S. Kamlet**

**2:15 ORGN 72.** Development of chiral pyridine catalysts. **R. Kluga,** A. Kinens, E. Vedejs, E. Suna

**2:55** Intermission.

**3:05 ORGN 73.** Amidine-based catalysts and their applications. **V. Birman**

**3:45 ORGN 74.** Lewis-base catalyzed, dynamic kinetic resolution in the synthesis of a complex nucleoside. **G. Beutner,** T. Benkovic, A. Ortiz, C. Sfougataakis

**4:15 ORGN 75.** Chiral phosphines and asymmetric phosphinocatalysis. **O. Kwon**

**4:55** Concluding Remarks.

### Section C

San Diego Convention Center  
Room 6C

#### Molecularly-Related Biocatalysis & Processes

M. C. McIntosh, *Organizer*

C. W. Littlefield, *Presiding*

**1:30 ORGN 76.** Chemiluminescent imaging agents for nitroreductase and tissue oxygenation in living animals. **J. Cao,** A. Lippert

**1:50 ORGN 77.** Functionally modifying triazabutadienes. **F. Kimani,** J.C. Jewett

**2:10 ORGN 78.** Artificial membrane fusion via copper-free click chemistry. **S. Whitehead,** S. Alam, M. Best

**2:30 ORGN 79.** Amphiphilic fluorescent foldamers as membrane-curvature sensors. **R.W. Gunasekara,** Y. Zhao

**2:50 ORGN 80.** Toward the fluorescent sensing of glycolipids. **C.W. Littlefield,** C. Ren, T.E. Glass

**3:10 ORGN 81.** Binding and biomimetic cleavage of the RNA by synthetic deoxypolypeptides/peptoids (DOPPs). **L. Cheng,** R. Breslow

**3:30 ORGN 82.** Controlling photophysics and the fidelity of DNA synthesis using substituted cytidine analogues. **D.D. Burns,** B. Rodgers, R. Lee, G. Stengel, R.D. Kuchta, **B.W. Purse**

**3:50 ORGN 83.** Probing chemical space of oridonin-inspired diterpenoids to identify biologically important molecules. **Y. Ding,** C. Ding, Y. Zhang, H. Chen, N. Ye, C. Wild, Z. Liu, H. Chen, M. White, Q. Shen, **J. Zhou**

**4:10 ORGN 84.** Green by design for process evolution: Asymmetric syntheses of vibegron. **F. Xu,** B. Kosjek, R. Desmond, Z. Liu, J. Park

**4:30 ORGN 85.** Fine feathers make fine birds: Diastereoselective design of privileged structures for phenotypic screening. **T.H. Altel**

## Section D

San Diego Convention Center  
Room 5B

## Asymmetric Reactions &amp; Syntheses

M. C. McIntosh, *Organizer*  
N. Kerrigan, *Presiding*

**1:00 ORGN 86.** Asymmetric catalytic synthesis of thiochromenes. N.A. Ahlemeyer, V. Birman

**1:20 ORGN 87.** Nickel catalyzed, stereospecific cross-coupling: Novel approaches to optically enriched triarylimethanes. L. Hanna

**1:40 ORGN 88.** Nickel-catalyzed cross-electrophile coupling reactions of benzylic esters with aryl halides. M. Konev, E.R. Jarvo

**2:00 ORGN 89.** Asymmetric synthesis of polyketide building blocks from ketenes. N. Kerrigan, S. Chen, A. Ibrahim, M. Mondal, K.A. Wheeler

**2:20 ORGN 90.** New phosphine oxide type organocatalysts for the asymmetric synthesis of organic compounds. O. Dogan, S. Polat Cakir, N. Beksultanova

**2:40 ORGN 91.** Computational investigation of the mechanism and stereoselectivity of the asymmetric organocatalytic azaelectrocyclizations of aza-ortho-quinone methides. A. Patel, M. Rueping, K.N. Houk

**3:00 ORGN 92.** Co(II)-based metalloradical catalysis for radical cyclopropanation with  $\alpha$ -halodiaoacetates: Enantioselective construction and applications of  $\alpha$ -halocyclopropylcarboxylates. Q. Cheng, S. Lopez De Mesa, P.X. Zhang

**3:20 ORGN 93.** Asymmetric bicyclization of diazoketones via Co(II)-based metalloradical catalysis. Q. Cheng, P.X. Zhang

**3:40 ORGN 94.** Catalytic asymmetric [3 + 2] cycloaddition of azomethine imines with ketenes. M. Mondal, N. Kerrigan

**4:00 ORGN 95.** Asymmetric synthesis of  $\gamma$ -lactones from vinyl sulfoxonium salts. N. Peraino, N. Kerrigan

**4:20 ORGN 96.** Enantioselective synthesis of contiguous quaternary stereocenters by organocatalytic allylboration. M. Alam, T. Vollgraff, K. Szabo

**4:40 ORGN 97.** Dearomatization of electron-deficient nitrogen heterocycles via cobalt-catalyzed asymmetric cyclopropanation. Y. Chen

## Section E

San Diego Convention Center  
Room 1A

## Metal-Mediated Reactions &amp; Syntheses

M. C. McIntosh, *Organizer*  
N. Selander, *Presiding*

**1:00 ORGN 98.** Stereospecific nickel-catalyzed cross-coupling reactions of benzylic ethers: Investigations of novel nucleophiles and electrophiles. D. Dawson, E. Tollefson, C. Osborne, E.R. Jarvo

**1:20 ORGN 99.** Diastereoselective nickel-catalyzed ring contraction reactions for cyclopropane synthesis. E. Lucas, L.W. Erickson, E. Tollefson, E.R. Jarvo

**1:40 ORGN 100.** Nickel-catalyzed, stereospecific, intramolecular, reductive cross-electrophile coupling of allylic and benzylic ethers with alkyl halides. L.W. Erickson, E. Tollefson, E. Lucas, E.R. Jarvo

**2:00 ORGN 101.** Functionalization of aryl-nitroso compounds mediated by copper(II)-halides. N. Selander, A. van der Werf

**2:20 ORGN 102.** Thermal and metal-mediated cycloaromatization reactions of conjugated tri- $\pi$  systems. K.M. Veccharelli, J.M. O Connor

**2:40 ORGN 103.** Development of tandem deoxydehydration/C-C bond-forming reactions. C. Boucher-Jacobs, K.M. Nicholas

**3:00 ORGN 104.** Tandem approach to carbazoles and alpha-carbolines from indoles and 7-azaindoles via successive Fujiwara-Moritani reactions followed by cyclization. J. Laha

**3:20 ORGN 105.** Triazole-gold promoted intermolecular propargyl alcohol addition to alkyne: Chemo and stereoselective reaction cascade for the synthesis of allene and substituted furan. S. Hosseyini

**3:40 ORGN 106.** Selective Negishi coupling of secondary alkylzinc reagents to aromatic and heteroaromatic substrates. B. Atwater, M. Pompeo, N. Chandrasoma, R. Froese, M. Rodriguez, D. Mitchell, M.G. Organ

**4:00 ORGN 107.** Mono arylation of primary amines, chiral secondary amines, and ammonia using specially designed Pd-NHC complexes. S. Sharif, R.P. Rucker, R. Froese, M.J. Rodriguez, D. Mitchell, M.G. Organ

## Section F

San Diego Convention Center  
Room 1B

## New Reactions &amp; Methodology

M. C. McIntosh, *Organizer*  
T. G. Minehan, *Presiding*

**1:00 ORGN 108.** Cascade reactions of nitrogen-substituted isocyanates: A new tool in heterocyclic chemistry. J. Vincent-Rocan, R.A. Ivanovich, J.S. Derasp, A.M. Beauchemin

**1:20 ORGN 109.** Engaging  $\alpha$ -oxy radicals in nickel-catalyzed cross coupling. K. Arendt, A.G. Doyle

**1:40 ORGN 110.** Stereospecific connective synthesis of alkenes by eliminative cross-coupling of enantioenriched carbenoids. Z. Wu, P.R. Blakemore

**2:00 ORGN 111.** Synthesis of complex fluorinated heterocycles. N. Frueh, J. Charpentier, A. Togni

**2:20 ORGN 112.** Rhodium-catalyzed, carbon-carbon bond-activation of unstrained ketones. R. Zeng, G. Dong

**2:40 ORGN 113.** Iodide-mediated  $\delta$  C-H amination. E. Wappes, S. Fosu, D.A. Nagib

**3:00 ORGN 114.** Extending the utility of ynoles for carbon-carbon bond formation: Synthesis of  $\alpha$ -alkylidene-,  $\alpha$ -benzylidene-,  $\alpha$ -methylene- $\gamma$ -butyrolactones, and  $\delta$ -valerolactones. T.G. Minehan, K. Ng

**3:20 ORGN 115.** Chemoselective Brown-type oxidation of aryl di-boron systems enabled by speciation control. T. Clohessy, J.J. Molloy, N. Anderson, G.C. Lloyd-Jones, A.J. Watson

**3:40 ORGN 116.** Oxidative activation of dihydropyridine amides to reactive acyl donors. J.B. Trads, E.D. Funder, K.V. Gothelf

**4:00 ORGN 117.** Catalytic hydroalkylation and hydroarylation of alkynes and alkenes using gold and gallium  $\pi$ -acids. V. Gandon

**4:20 ORGN 118.** Tandem metathesis-dihydroxylation and metathesis-oxidative cyclization reactions. P.K. Dornan, Z.K. Wickens, D. Lee, C. Blumenfeld, R.H. Grubbs

## Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## SUNDAY EVENING

## Section A

San Diego Convention Center  
Hall D

## Chemistry &amp; Computers

R. D. Broene, *Organizer*

8:00 - 10:00

**ORGN 119.** Rationally and computationally guided development of inhibitors targeting deoxyhypusine synthase for the treatment of cancer. J.M. Alburger, S. Nakanishi, J. Cleveland, W.R. Roush

**ORGN 120.** Electro-optical and charge transport properties of trans-3-(3,4-dimethoxyphenyl)-2-(4-(nitrophenyl)prop-2-enitrile): A DFT approach. A.G. Alsehem

**ORGN 121.** Structure elucidation of organic compounds by NMR: DP4 made easy. K. Ermanis, J.M. Goodman

**ORGN 122.** Investigations of a bisbenzylguanidine proton sponge and a ring-closed guanidine proton sponge. A. Zuo, D.M. Birney

**ORGN 123.** Computational study of the enantioselectivity of an intramolecular alkylation by doubly quaternized cinchona-based phase transfer catalysts. C.Q. He, A. Simon, C. Lam, K.N. Houk

**ORGN 124.** Monosaccharide shapes vary with oxidation state at the 6-position: A systematic computational investigation. A. Vickman, N.L. Pohl

**ORGN 125.** Investigating sterically congested dimethoxybenzenes using computational methods. J.D. Zehr, C.S. Hamann

**ORGN 126.** Quantifying the strengths of dual hydrogen bonding organocatalyst. J. Shea, S.E. Wheeler

**ORGN 127.** Unraveling the origin of enantioselectivity in SPINOL-phosphoric acid catalyzed syntheses of 2,3-dihydroquinazolinones. C.J. Laconsay, T. Seguin, S.E. Wheeler

## Section B

San Diego Convention Center  
Hall D

## Asymmetric Reactions &amp; Syntheses

R. D. Broene, *Organizer*

8:00 - 10:00

**ORGN 128.** Withdrawn.

**ORGN 129.** Asymmetric [3 + 2]-cycloaddition reactions of enamine with electrophilic metalloenolcarbene intermediates. Y. Deng, M.P. Doyle

**ORGN 130.** Chiral organocatalysts-mediated asymmetric reactions. S.K. Mangawa, S.K. Awasthi

**ORGN 131.** Palladium-catalyzed enantioselective Heine reaction. K. Kennedy, M. Punk, C.P. Merkley, J.B. Morgan

**ORGN 132.** Diastereoselective formation of butyrolactones from donor-acceptor cyclopropane 1,1-diester. M. Smith, E. Finney

**ORGN 133.** Enantioselective Diels-Alder of yrones and functionalized dienes towards chiral 1,4-cyclohexadiene products. M. Walley, J.A. Horton, D. Reilly, W. Chalfoux

**ORGN 134.** Catalytic asymmetric synthesis of oxazole derivatives. W. Luo, X. Feng

**ORGN 135.** Enantioselective [5+2] cycloaddition of oxidopyrylium ylides by iminium catalysis. K.N. Fuhr, S.E. Brenner-Moyer, R.P. Murelli

**ORGN 136.** Catalytic, asymmetric fluorination of oxindoles and ring-opening of meso-aziridines with primary alcohols. J. Li, X. Feng

**ORGN 137.** Asymmetric dearomatization of indoles through Michael/Friedel-Crafts-type cascade to construct polycyclic spiroindolines. X. Zhao, X. Feng

**ORGN 138.** Asymmetric catalytic 1,3-dipolar cycloaddition reaction of nitrile imines for the synthesis of chiral spiro-pyrazoline-oxindoles. G. Wang, X. Feng

**ORGN 139.** Enantioselective  $\beta$ -protonation by a cooperative catalysis strategy. M. Wang, D.T. Cohen, C.B. Schwamb, R.K. Mishra, K. Scheidt

**ORGN 140.** Fused imidazole ligands: Design and application to asymmetric catalysis. N.A. Ahlemeyer, V. Birman

**ORGN 141.** Axially chiral N-heterocyclic carbene: Design and application to asymmetric catalysis. K. Sharmah Gautam, V. Birman

**ORGN 142.** Chiral  $N,N'$ -dioxide-scandium(III)-catalyzed asymmetric dearomatization of 2-naphthols through an amination reaction. X. Lian, X. Feng

**ORGN 143.** Catalytic asymmetric (hetero)-Diels-Alder reaction of silyloxydienes. J. Zheng, X. Feng

**ORGN 144.** 3-Benzylidenecamphor derivatives and their conversion into chiral auxiliaries and organocatalysts. P.J. Hartfield, M.K. Kennedy, D.E. Lewis

**ORGN 145.** Stereoselective synthesis of fused polycyclic ethers: Exo-mode oxacyclizations of vinylloxiranes. N. Setterholm, F.E. McDonald

**ORGN 146.** Enantioselective synthesis of polysubstituted benzopyrano[3,4-c]pyrrolidine for C-C/C-N bond formation via Cinchona alkaloid scaffold. G. Chang, W. Lin

**ORGN 147.** Harnessing ammonium/F-C bond attraction in enantioselective catalysis. K. Lee, D.L. Silverio, S. Torker, F. Haeflner, D. Robbins, A.H. Hoveyda

**ORGN 148.** Asymmetric total synthesis of (+)-O-methylasparvenone. R. Lafleur-Lambert, J. Boukouvalas

**ORGN 149.** Catalytic asymmetric synthesis of ketene heterodimer  $\beta$ -lactones. S. Chen, A. Ibrahim, D. Nalla, M. Mondal, N. Kerrigan

**ORGN 150.**  $N,N'$ -dioxide-scandium(III) catalyzed asymmetric Michael addition of  $\beta,\gamma$ -unsaturated butenolides to  $\alpha,\beta$ -unsaturated- $\gamma$ -keto esters. J. Ji, X. Feng

**ORGN 151.** Organocatalytic Friedel-Crafts reaction of  $N$ -methylindole: An unusual selectivity reversal. M.C. Holland, J.B. Metternich, R. Gilmour

**ORGN 152.** Desymmetrization of 4-substituted cyclohexanones to novel axially chiral oximes. S. Nimmagadda, J.C. Antilla

**ORGN 153.** Optimization of the Leighton allylation of aldehydes: Application for the synthesis of SIA7248. B. Lindquist-Kleissler, J. Zheng, G. O'Doherty



**ORGN 154.** Unexpected, high-yielding synthesis of an excellent Michael acceptor and its application in synthesis of substituted tryptophan. **R.N. Nair**, J. Rosnow, S. Lindemann

**ORGN 155.** Development of a C-selective alkylation of cycloalkanediones via alkylation of dimethylhydrazones. **R.A. Velez-Pena**, R.J. Sharpe, J.S. Johnson

**ORGN 156.** Developing an organocascade methodology to achieve  $\alpha,\alpha$ -chloro-fluoroalcohols. **M. Rodriguez-Alvarado**, S.E. Brenner-Moyer

**ORGN 157.** Catalysis control in multi-component aziridination of chiral aldehydes. **Y. Dai**, Y. Zhou

**ORGN 158.** NMR study of organocatalyst-transition state analogue complexes for enantioselective anhydride desymmetrization reactions. **N.G. Rockey**, D.G. Alberg, G.E. Hofmeister

**ORGN 159.** Preparation and characterization of 4-thiophenyl-1,1,1-trifluoro-2-butanone and its sulfoxide. **W. Powell**, S. Purrington

**ORGN 160.** Syntheses of transition-state analogues for mechanistic studies of organocatalytic desymmetrization reactions. **C.A. Leahy**, D.G. Alberg, G.E. Hofmeister

**ORGN 161.** Bisphosphorylimides as organocatalysts for asymmetric Friedel-Crafts reactions. **R.G. Iafe**, L. Ahlberg, M. Dean, G. Diaz, B. Klasic, J. Maynard, L. Abrous

**ORGN 162.** Withdrawn.

**ORGN 163.** Towards the synthesis of tubotaiwine analogues and stemmadenine alkaloids. **S.J. Kim**

**ORGN 164.** Novel approaches to the chemical synthesis of oxazolidinone and the related derivatives with the attachment of imidazole molecules. **E.J. Parish**, W. Huang, H. Honda, T. Wei

**ORGN 165.** Determining absolute configuration of chiral epoxides using the competing enantioselective conversion method. **G. Suryn**, S.D. Rychnovsky

**ORGN 166.** New improvements in the synthesis tetralol-related chiral auxiliaries. **J. Gatignol**, F. Gelat, J.L. Montchamp

## Section C

San Diego Convention Center  
Hall D

### Flow Chemistry & Continuous Processes

R. D. Broene, *Organizer*

8:00 - 10:00

**ORGN 167.** Facile cyclocondensation in a microfluidic reactor for continuous synthesis of thiazoles/selenazoles/oxazoles. **M. Alam**, B. Jagodzinska, J. Campagna, P. Spilman, V. John

**ORGN 168.** Use of a "catalytic" co-solvent, N,N-dimethyl octanamide, allows the flow synthesis of Gleevec with no solvent switch. **J. Yang**, D. Niu, S.L. Buchwald

**ORGN 169.** Development of a continuous-flow, high-pressure nitro reduction using a trickle-bed reactor. **M. Laurila**, B. Campbell, K.P. Cole, J.R. Martinelli, R. Cope, M.D. Johnson, M. Paul

**ORGN 170.** Gold nanoparticle-catalyzed alkyne activation: Hydration under basic conditions and hydroamination. **S. Liang**, L.C. Hammond, B. Xu, G.B. Hammond

**ORGN 171.** Flow process for a stereoselective aldol/epoxidation reaction and subsequent chemistry. **J.A. Hansen**

## Section D

San Diego Convention Center  
Hall D

### Materials, Devices & Switches

R. D. Broene, *Organizer*

8:00 - 10:00

**ORGN 172.** Photo-responsive molecular switch for regulating transmembrane proton-transfer kinetics. **Y. Li**, S.C. Zimmerman, A.A. Gewirth

**ORGN 173.** Molecular breakwater-like tetrapods for organic solar cells. **J. Yang**, Y. Qin

**ORGN 174.** Fabrication of tunable graphene/polyaniline composite via laser printing for high performance supercapacitor. **C. Ma**, S. Wang, Y. Wang, Z. Lv, Y. Yu, Y. Liu, Y. Min

**ORGN 175.** Smartphone-based, chemiluminescent, point-of-care imaging device for asthma using exhaled breath condensate. **M.E. Quimbar**, A. Lippert

**ORGN 176.** Functionalized tetracene organic field effect transistors. **D.J. Ventre**, M. Tang, D. Simpson

**ORGN 177.** Tricyclic nonclassical thiophenes: Synthesis of new fused-ring thiophene monomers and their application to conjugated materials. **E. Culver**, K. Konkol, S.C. Rasmussen

**ORGN 178.** Electrochemical and photophysical structure-property relationship investigation for 1,2,5-triarylpyrroles and their synthetic precursor 1,4-diaryl-1,3-butadiynes. **C.J. Seibert**, R.G. Garibyan, S.T. Collins, K. Ogawa

## Section E

San Diego Convention Center  
Hall D

### Nanomaterials

R. D. Broene, *Organizer*

8:00 - 10:00

**ORGN 179.** New approaches to the chemical synthesis of polycyclic electron-donor for nanomaterials study. **E.J. Parish**, H. Honda, T. Wei, M. Hsiao

**ORGN 180.** Highly porous, N-confused porphyrin-based metal-organic frameworks. **Y. Yang**, R. Sakashita, M. Ishida, H. Furuta

**ORGN 181.** Click synthesis of bifunctional ionic liquids via thiol-ene chemistry for surface coating applications. **M. Sanchez Zayas**, J.C. Gaitor, S.T. Nestor, S. Minkowicz, Y. Sheng, A. Mirjafari

**ORGN 182.** Functionalization of hydroxylated nanoparticles with cyclic azasilanes: Experimental and computational studies. **O.A. Mazyar**, R. Suresh, V.N. Khabashesku

**ORGN 183.** Nanoporous membranes from a polymerizable discotic liquid crystal. **J.C. Buttrick**, H.D. Root, B.T. King

**ORGN 184.** Library of fluorinated electrophiles for chemical tagging: Toward a multifunctional  $^{19}\text{F}$  MRI contrast agent based on mesoporous silica nanoparticles. **S. Fitzgerald**, J. Rutowski, J.L. Steinbacher

**ORGN 185.** Cyclohexane rings reduce small ion membrane permeability in archaea-inspired tetraether lipids. **T. Koyanagi**, G. Leriche, M. Mayer, J.C. Yang

**ORGN 186.** Thermodynamics study of absorption of aromatic organic compounds to carbon nanotubes. **M. Watanabe**, L.J. Lozenski

**ORGN 187.** Investigation of graphene oxide fiber. **D. Zhang**, S. Mo, J. Shen, Y. Liu, Y. Min

## Section F

San Diego Convention Center  
Hall D

### Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

R. D. Broene, *Organizer*

8:00 - 10:00

**ORGN 188.** Improving photocatalytic activity by appending a DABCO ring and a quinone to ruthenium polypyridyl complex. **A.N. James**, T. Nguyen, N. Zheng

**ORGN 189.** Nucleophile, radical trap, or both? The potential dual reactivity of alkenes in the intramolecular reactions of iminoxyl radicals and oxime ether radical cations. **N. Armada**, S. Pham, L. Marsalla, P. de Lijser

**ORGN 190.** Synthesis and photophysical studies of lophine derivatives with polycyclic aromatic hydrocarbon moieties and electron-donating groups. **T. Hamada**, L. Lien, R.A. Isovitsch

**ORGN 191.** Preparation of water-soluble perylene monoimides, and studies of photophysical properties and biocompatibility. **G.H. Aryal**, S.A. Dupre, L. Huang, K.W. Hunter

**ORGN 192.** Kinetic and competition studies of oxygen atom transfer reactions with a corrole-manganese(V)-oxo species. **H. Jeddi**, W. Luo, R. Zhang

**ORGN 193.** Withdrawn.

**ORGN 194.** Inducing oxidative cyclization reactions of benzaldehyde oximes with built-in heteroaromatic nucleophiles via photochemical and metal catalysis. **A.S. Alshreimi**, J. Dang, P. De Lijser

**ORGN 195.** Complete kinetic study of the aminolysis of *N*-aryl-4-chloro-1,8-naphthalimides. **S.M. Anderson**, S.D. Mitchell, D.E. Lewis

**ORGN 196.** Computational comparisons of intramolecular Diels-Alder transition states leading to fused and bridged tetracycles. **K.J. Kron**, R.J. Cave, D.A. Vosburg

**ORGN 197.** Role of noncovalent interactions in asymmetric catalysis involving chiral phosphoric acids. **T. Seguin**, S.E. Wheeler

**ORGN 198.** Distortion and hyperconjugative aromaticity/antiaromaticity determine the reactivity and facial stereoselectivity of 5-substituted cyclopentadienes. **B.J. Levandowski**, L. Zou, K.N. Houk

**ORGN 199.** Calculated molar volume profiles. **D.B. Lawson**

**ORGN 200.** Density functional theory studies of transition-state topologies in the amide-acetal Claisen rearrangement. **R. Kretsch**, M. Hartley, G.W. Daub, R.J. Cave

**ORGN 201.** Kinetic studies on the isomerization of humulone. **S. Johnson**, M.D. Mosher

**ORGN 202.** Generating vinyl nitrene from aromatic azides. **A. Das**, K. McKissic, J. Mack, A.D. Gudmundsdottir

## Section G

San Diego Convention Center  
Hall D

### Total Synthesis of Complex Molecules

R. D. Broene, *Organizer*

8:00 - 10:00

**ORGN 203.** New methods toward the total synthesis of azaspirene: A potent angiogenesis inhibitor. **T. Montgomery**, M.J. Kelly, M.B. Bergdahl

**ORGN 204.** Progress toward the synthesis of the akummline alkaloid strictamine. **E. Andreatsky**, S. Blakey

**ORGN 205.** Nitrenium-ion-mediated oxamidation to synthesize the common diazatricyclic core of madangamine. **A. Bhattacharjee**, S. DeJong, M. Gerasimov, D.J. Wardrop

**ORGN 206.** First total-synthesis of macroline indole alkaloids macrocarpine A-G via an efficient, enolate-driven, copper-mediated cross-coupling process. **M. Rahman**, J.M. Cook, J. Deschamps

**ORGN 207.** Progress toward the asymmetric total synthesis of (+)-cycloclavine. **Y. Zhang**, I. McArdle, B. Söderberg

**ORGN 208.** Progress toward the total synthesis of parthenolide. **C.A. Roberts**, M.E. Jung

**ORGN 209.** Toward the total synthesis of oxazolomycin A. **Z. Anderson**, L. Marx, A.W. Logan, J. Burton

**ORGN 210.** Design and synthesis of 2,4-DiPAM sugar to combat organophosphorus compounds. **B. Lipinski**, J.T. Koh

**ORGN 211.** Towards the total synthesis of the *anti*-trypanosomal macrolide, actinoalloides: Construction of a key linear intermediate. **J. Oshita**, Y. Noguchi, A. Watanabe, G. Sennari, T. Hirose, D. Oikawa, Y. Inahashi, M. Iwatsuki, A. Ishiyama, S. Omura, T. Sunazuka

**ORGN 212.** Towards unified access to ansa-bridged prodiginines: Exploring whether tactics employed in a recent roseophilin synthesis are adaptable to spirocyclic pyrrolophanes marineosins A & B. **T.K. Allred**, H. Ding, J. Frederich, P.G. Harran

**ORGN 213.** Studies toward a streamlined total synthesis of eleutherobin and analogues. **L. Synttrivianis**, F. Del Campo, L. Wong, J. Robertson

**ORGN 214.** Synthesis of antifungal alabrone and trineurone polyketides. **K.P. Reber**, A.R. Lewis

**ORGN 215.** Progress toward the total synthesis of cryptocaryol A. **M.J. Mitton-Fry**, E. Boedicker, Z. Li

**ORGN 216.** Synthesis of poly-fused scaffolds of *Corynanthe* and *Aspidosperma* indole alkaloids. **J. Beecher**, M. Wickman, E.K. Leggans

**ORGN 217.** Expedient synthesis of cryptobellin/endiandric tetracycles. **S.P. Wetzler**, L. Kim, A.Y. Chang, A. Dea, E. Go, D.A. Vosburg

**ORGN 218.** Withdrawn.

**ORGN 219.** Synthesis of the natural  $\alpha$ -alkylidene lactones subamolide D and E. **K. Ng**, T.G. Minehan

**ORGN 220.** Synthetic studies of kapakahine **C**. **K.A. Leets**

**ORGN 221.** Unified synthetic strategy toward the tubingsen alkaloids. **M. Corsello**, J. Kim, N.K. Garg

**ORGN 222.** Total synthesis of micromide and stereochemical revision on solid support. **L. Wang**, B. Banaski, A.S. Kanner, M.B. Bergdahl

**ORGN 223.** Total syntheses of the akummline alkaloids (+)-strictamine, (-)-2(S)-cathafoline, and (-)-aspidophylline **A**. **J. Moreno**, E. Picazo, L. Morrill, J. Smith, N. Garg

**ORGN 224.** Progress towards the synthesis of anserinones A and B. **S. David**, J. Whisenant, D. Vincent

**ORGN 225.** Exploring hops chemistry: Towards efficient, asymmetric syntheses of humulones and lupulones. **L.R. Sass**, K.V. Waynant

**ORGN 226.** Stereospecific total synthesis of macroline-related oxindoles: Macrogentone and alstonoxine  
A. G.O. Fonseca, M. Ahmed Khan, J. Deschamps, J.M. Cook

**ORGN 227.** Synthesis of conformationally constrained diarylether paracyclophanes.  
H. Caldera, F. Drozda-Samuels, B. Lindquist-Kleissler, T. Ozvat, Z. Tregillus, K.A. Miller

**ORGN 228.** Alkylloxonium and alkoxide: Synthesis of oxatriquinanetriol to trialkyl-oxonium alkoxide zwitterion. S. Manabe, M. Mascal

**ORGN 229.** Progress towards the synthesis of eight-membered heterocyclic natural products. A. Golonka, C. Schindler

**ORGN 230.** Modular approach to the synthesis of riccardin C analogs. D.V. Kadnikov, T. Payne, J. Magnuson, J.L. McMinn

**ORGN 231.** Studies into the synthesis of cyclacenes. S. Wegwerth, C.J. Douglas

**ORGN 232.** Synthesis of both enantiomers of pilosinine via a stereodivergent conjugate addition strategy. E.A. Prebihal, C. Zaremba, R.J. Mullins

**ORGN 233.** Withdrawn.

**ORGN 234.** Synthesis of the potent anti-malarial, anti-cancer natural product, lagunamide A, via iterations of the vinylogous Mukaiyama aldol reaction. B. Banasik, L. Wang, A.S. Kanner, M.B. Bergdahl

**ORGN 235.** Phosphate tethered-mediated approach towards the total synthesis of (+)-cryptocaryol A. C.N. Ndi, P.R. Hanson

**ORGN 236.** Synthetic access toward the total synthesis of aflavinine. M. Jo, Y. Kwak

### My Comments to the President's Task Force on Employment

Sponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

### My Experience with & Advice for Improving Diversity in Chemistry

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### My Experiences in & Advice for Organic Chemistry Courses

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## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 6A

**Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in honor of Phil S. Baran**

C. A. Maryanoff, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 **ORGN 237.** Selective synthesis of unusual lipids. N.Z. Burns

9:15 **ORGN 238.** Chemical synthesis of secondary metabolites. R.A. Shenvi

9:55 **ORGN 239.** Synthesis of complex terpenes from simple precursors. T.J. Maimone

10:35 Introductory Remarks.

10:40 **ORGN 240. Award Address** (Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator sponsored by the Pfizer Endowment Fund). Studies in natural product synthesis. P.S. Baran

### Section B

San Diego Convention Center  
Room 6B

**ACS Award for Affordable Green Chemistry: Symposium in honor of Martin D. Johnson, Joseph R. Martinelli & Shannon S. Stahl**

E. M. Skoda, *Organizer*

C. A. Faler, *Presiding*

8:00 Introductory Remarks.

8:05 **ORGN 241.** Innovation imperative: Transforming chemical process R&D. B.E. Huff

8:35 **ORGN 242.** Affordable green chemistry for pharmaceutical process & analytical chemistry: Success through collaboration. C.J. Welch

9:05 **ORGN 243.** Fixed-bed catalysis with gas/liquid system. D.M. Pfisterer, J. Hawkins, E.M. Cordi, T.M. Makowski, I. Mustakis, H.W. Ward

9:35 Intermission.

9:50 **ORGN 244. Award Address** (ACS Award for Affordable Green Chemistry sponsored by the Dow Chemical Company and endowed by the Rohm and Haas Company). Aerobic oxidation reactions for organic chemical synthesis: From fundamentals to practical applications. S.S. Stahl

10:20 **ORGN 245.** Membrane flow reactors for catalytic aerobic partial oxidations in pharmaceuticals and specialty chemicals: Tools for kinetic study and scale-up. T.W. Root

10:50 **ORGN 246. Award Address** (ACS Award for Affordable Green Chemistry sponsored by the Dow Chemical Company and endowed by the Rohm and Haas Company). Continuous reactor design, development, and scale-up for high pressure gas/liquid reactions. M.D. Johnson, S.A. May

11:20 **ORGN 247. Award Address** (ACS Award for Affordable Green Chemistry sponsored by the Dow Chemical Company and endowed by the Rohm and Haas Company). Development of a continuous flow aerobic oxidation for the production of a strained ketone. J.R. Martinelli, E.W. Conder, N. Zaborenko, C.M. Stobba-Wiley, G. Lambertus, W. Sun, D.L. Varie, T. Kramer, M. Paul, M.D. Johnson, M. Laurila

11:50 Concluding Remarks.

### Section C

San Diego Convention Center  
Room 6C

**Biologically-Related Molecules & Processes**

M. C. McIntosh, *Organizer*

T. Lavergne, *Presiding*

9:00 **ORGN 248.** DNA photo-cleavage by symmetrical quinoline carbocyanine dyes irradiated with near-infrared light. K.B. Grant, T. Fatemipouya, C. Holder, M. Henary

9:20 **ORGN 249.** Chemical inhibitor of the Skp2/p300 interaction that promotes p53-mediated apoptosis. H. Lim

9:40 **ORGN 250.** Topologically controlled G-quadruplex nucleic acid structures: Synthesis and applications from biology to biotechnology. L. Bonnat, D. Jerome, E. Defranco, T. Lavergne

10:00 **ORGN 251.** Chemical mutagenesis of an emissive RNA alphabet. A.R. Rovira, A. Fin, Y. Tor

10:20 **ORGN 252.** On-target synthesis and selection of modular therapeutic agents for myotonic dystrophy. L. Liu

10:40 **ORGN 253.** Development of the synthesis and scale-up of an AMPK activator clinical candidate. A.C. Smith, T.A. Brandt, E.L. Conn, P. Dent, M. Dowling, D. Fernando, J. Panteleev, C.R. Rose, T. Ryder, A. Shavnya, B. Thuma, J. Xiao

11:00 **ORGN 254.** Synthesis of novel vitamin D conjugates. J. Grote

11:20 **ORGN 255.** Synthesis and evaluation of novel proteasome-inhibiting syrbactin derivatives. N.A. Bakas, M.C. Pirrung, A.S. Bachmann

### Section D

San Diego Convention Center  
Room 5B

**Asymmetric Reactions & Syntheses**

M. C. McIntosh, *Organizer*

N. Takenaka, *Presiding*

8:00 **ORGN 256.** Diversification reactions of  $\gamma$ -silyl allenyl esters: Selective conversion to  $\gamma$ -substituted allenes and all-carbon quaternary centers. S. Jana, A. Roy, S.D. Lepore

8:20 **ORGN 257.** Sequencing alkene hydroacylation and  $\alpha$ -arylation of indoles and pyrroles: Enantioselective synthesis of heterocyclic ketones with  $\alpha$ -chiral quaternary stereogenic centers. A. Ghosh, J.A. Walker Jr., A. Ellern, L.M. Stanley

8:40 **ORGN 258.** Withdrawn.

9:00 **ORGN 259.** Recent studies on Lewis base catalysis of organotrchlorosilanes. N. Takenaka, C. Reep, S. Sun

9:20 **ORGN 260.** N-heterocyclic carbene-catalyzed synthesis of lactones via homoenolate anions in green solvents. D.C. Kidd, J.J. Kiddle

9:40 **ORGN 261.** Carbonyl-directed catalytic asymmetric hydroboration of vinyl arenes. G. Hoang, T.N. Nguyen, S. Zhang, J.M. Takacs

10:00 **ORGN 262.** Crossed-benzoin condensations utilizing N-heterocyclic carbenes in green solvents. L.R. Barber, J.J. Kiddle

10:20 **ORGN 263.** Withdrawn.

10:40 **ORGN 264.** Withdrawn.

11:00 **ORGN 265.** Withdrawn.

### Section E

San Diego Convention Center  
Room 1A

**Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species**

M. C. McIntosh, *Organizer*

B. Gold, *Presiding*

8:00 **ORGN 266.** Experimental and theoretical analysis of relative activation energies of various ketal Claisen rearrangements. M. Hartley, R.J. Cave, G.W. Daub

8:20 **ORGN 267.** Decreasing distortion energies without strain: Optimizing 1,3-dipolar cycloadditions of diazoacetamides. B. Gold, M. Aronoff, R.T. Raines

8:40 **ORGN 268.** Alkali metal cation vs. proton and methyl cation affinities: Structure and bonding mechanism. Z. Boughlala, C. Fonseca Guerra, F. Bickelhaup

9:00 **ORGN 269.** Efficient aminocatalytic conjugate addition via mechanistic studies on the role of additives. J. Bures, X. Companyo

9:20 **ORGN 270.** Computational study of the edges of nitrogen-doped graphene using heterocyclic model compounds. H.D. Banks

9:40 **ORGN 271.** Withdrawn.

10:00 **ORGN 272.** Withdrawn.

10:20 **ORGN 273.** Simulation of the electronic spectra of LH2 complex of bacteria through a polarizable QM/MM approach. M. Campetella, S. Jurinovich, B. Mennucci

10:40 **ORGN 274.** QM/excitonic approach to the electronic circular dichroism of biopolymers. D. Padula, S. Jurinovich, B. Mennucci

11:00 **ORGN 275.** Mechanistic insights from the aryl-alkyne ring closure of 10b-aza-10c-borapyrene. J.A. Jaye, B.S. Gelinias, G.M. McCormick, E.H. Fort

11:20 **ORGN 276.** Aromaticity criteria based on electron delocalisation measures. J. Poater

### Section F

San Diego Convention Center  
Room 1B

**New Reactions & Methodology**

M. C. McIntosh, *Organizer*

J. A. Read, *Presiding*

8:00 **ORGN 277.** Recent advances in triphenylphosphine oxide-catalyzed reduction reactions. P.H. Toy

8:20 **ORGN 278.** Rh(II) catalyzed C(sp<sup>3</sup>)-H alkylation of enol ethers and enamides: Furnishing  $\beta,\gamma$ -unsaturated 1,3-dicarbonyls. B. McLarney, M.A. Cavitt, T. Donnell, J. Musaeov, S.A. France

8:40 **ORGN 279.** Palladium catalysis for  $\beta$ -C-H functionalization of aliphatic amines and ketones. Z. Huang, G. Dong

9:00 **ORGN 280.** Ruthenium-catalyzed urea synthesis using methanol as the C1 source. S. Hong, S. Kim

9:20 **ORGN 281.** Green protection of pyrazole, catalytic thermal isomerization of tetrahydropyranpyrazoles, and telescoping synthesis of 3-alkyl- and 3,5-dialkylpyrazoles. B.M. Ahmed, G. Mezei

9:40 **ORGN 282.**  $\alpha$ -Chelate diastereoselectivity without a kinetic preference for the  $\alpha$ -chelate: Reconciling the diffusion-controlled reactivity of allylmagnesium halides with  $\alpha$ -chelation control. J.A. Read, K.A. Woerpel

10:00 **ORGN 283.** Gold(I)-catalyzed anti-Markovnikov hydrofunctionalization reactions of alkylidenecyclopropanes. J. Timmerman, B.D. Robertson, S. Laulhe, R. Widenhoefer

10:20 **ORGN 284.** Functionalization of enamines via aza-allyl cations. M.A. Saputra, N.S. Dange, F. Fronczek, R. Kartika

10:40 **ORGN 285.** 1,4-Dicarbonyl synthesis using oxallyl cations. J.R. Stepherson, R. Kartika

11:00 **ORGN 286.** Phase-transfer-catalyzed oxidative esterification of primary alcohols by TEMPO. S. Hackbusch, A. Franz

**11:20 ORGN 287.** Divergent/convergent approach towards the synthesis of the propionate acid and alcohol moieties of (-)-dolabriferol and (-)-dolabriferol B from a common precursor. **K. Morales, J.A. Prieto**

**Is There a Crisis in Organic Chemistry Education?**

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**Start-up Businesses in Drug Discovery**

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**MONDAY AFTERNOON**

**Section A**

San Diego Convention Center  
Room 6A

**Ernest Guenther Award in the Chemistry of Natural Products: Symposium in honor of Eric Block**

F. A. Davis, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 288.** Selenium in biochemistry and biophysics: Novel functions of selenoproteins and new approaches for their characterization. **S. Rozovsky**

**1:50 ORGN 289.** Selenium: From poison to the 21st amino acid. **R.S. Glass**

**2:35 ORGN 290.** Stereocontrolled reactions for complex molecule synthesis. **A.J. Frontier**

**3:20 ORGN 291.** Catalytic, enantioselective synthesis of sulfur-containing compounds: An homage to Eric Block. **S.E. Denmark**

**4:05 ORGN 292. Award Address (Ernest Guenther Award in the Chemistry of Natural Products sponsored by Givaudan).** Fifty years of smelling sulfur: From the chemistry of garlic and onion to the molecular basis for olfaction. **E. Block**

**Section B**

San Diego Convention Center  
Room 6B

**Green Chemistry: Enhancing Organic Synthesis in Pharma**

S. G. Koenig, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 293.** Applications of CH activation reactions in drug discovery and synthesis. **J. Yu**

**1:40 ORGN 294.** C-H functionalization as an enabling technology for the synthesis of pharmaceutically relevant molecules. **H.A. Malik**

**2:15 ORGN 295.** Use of tools and metrics to drive culture change in R&D chemistry. **H. Sneddon**

**2:50** Intermission.

**3:10 ORGN 296.** Recent advances in non-precious metal catalysis. **N.K. Garg**

**3:45 ORGN 297.** Greening a medicinal chemistry organization. **M.C. Bryan**

**4:20 ORGN 298.** Integration of green chemistry: Enabling tools in the oncology portfolio. **D.T. Richter, P. Richardson**

**4:55** Concluding Remarks.

**Section C**

San Diego Convention Center  
Room 6C

**Frontiers in Molecular Recognition**

A. K. Mapp, *Organizer*

P. Arora, *Presiding*

**1:20** Introductory Remarks.

**1:25 ORGN 299.** Biological activity and potential for clinical application of pyrrole-imidazole polyamides. **N. Nickols, F. Yang, A. Kurmis, P.B. Dervan**

**1:55 ORGN 300.** Combining arrays and mass spectrometry for high-throughput discovery in chemistry and biology. **M. Mrksich**

**2:25 ORGN 301.** Recent developments in strategies and tactics towards complex secondary metabolites including human-derived natural products. **E.M. Carreira**

**2:55** Intermission.

**3:25 ORGN 302.** Mimicry of polypeptide recognition surfaces with foldamers. **S.H. Gellman**

**3:55 ORGN 303.** Chemical basis for allostery in the EGFR receptor tyrosine kinase. **A. Schepartz**

**4:25 ORGN 304.** Polymer probes of immunity and tolerance. **L.L. Kiessling**

**4:55** Concluding Remarks.

**Section D**

San Diego Convention Center  
Room 5B

**Molecular Recognition & Self-Assembly**

M. C. McIntosh, *Organizer*

A. R. Urbach, *Presiding*

**1:00 ORGN 305.** Photoinduced, highly selective dimerizations and polymerizations in the presence of two different self-assembled bis-urea confinements. **S. Salpage, L. Donevant, M.D. Smith, A. Bick, L.S. Shimizu**

**1:20 ORGN 306.** Near-IR-triggered, remote-controlled release of metal ions: A novel strategy for caged ions. **B. Uyar, A. Atilgan, R. Guliyev, E. Tanriverdi Eçik, S. Erbas-Cakmak, E.U. Akkaya**

**1:40 ORGN 307.** Phenylene vinylene macrocycles: Synthesis, aggregation study, and transmembrane channel activities. **C. Yu, C. Zhang, X. Hu, Z. Liu, W. Zhang**

**2:00 ORGN 308.** Self-assembly of complex molecular architectures based on dynamic hydrazone linkages in water. **H. Li**

**2:20 ORGN 309.** Supramolecular rotation: The fascinating motion of an Ir<sup>+</sup> complex within Rebek's self-folding octaamide cavitand. **S. Serapian, S. Korom, C. Bo, P. Ballester**

**2:40 ORGN 310.** Molecular recognition and sensing of peptides and proteins with cucurbit[n]uril synthetic receptors. **A.R. Urbach**

**3:00 ORGN 311.** Withdrawn.

**3:20 ORGN 312.** Development of sugar-containing & sugar-responsive supramolecular G-quadruplexes. **L.A. Prieto-Costas**

**3:40 ORGN 313.** Resorcinarenes as tetravalent halogen bond acceptors: Networks in solid state vs. dynamic assemblies in solution. **T. Tero, K. Salorinne, S. Malola, H. Hakkinen, M. Nissinen**

**Section E**

San Diego Convention Center  
Room 1A

**Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species**

M. C. McIntosh, *Organizer*

G. O. Jones, *Presiding*

**1:00 ORGN 314.** Role of computational chemistry in the development of new organocatalytic routes for poly(ether) synthesis. **G.O. Jones**

**1:20 ORGN 315.** Identifying a more specific photochemical property that is responsible for the sun sensitivity side effects observed in commonly prescribed antibiotics. **A. Bills, J. Andrews**

**1:40 ORGN 316.** Molecular acids as a proxy to study formaldehyde oligomerization at lower pH: A computational study. **J. Kua, K.R. Adwan**

**2:00 ORGN 317.** Rules for metal-promoted ring closure: Alkylmetalation reactions of group 10-12. **B. Fiser, J.M. Cuerva, E. Gomez-Bengoa**

**2:20 ORGN 318.** First-principles study on the microsolvation of melamine on graphene. **A. Rodriguez Garcia, A.B. Muñoz-García, O. Crescenzi, E. Vazquez, M. Pavone**

**2:40 ORGN 319.** Applications of recyclable phosphorus reagents: Mechanistic insights drive improvements towards greener methodologies. **J. Buonomo, C. Eiden, C.C. Aldrich**

**3:00 ORGN 320.** Theoretical insights into the mechanism and selectivity of the Diels-Alder/lactonization (DAL) organocascade catalyzed by a chiral isothiourea. **B. Hudson, M.E. Abbasov, D. Romo, D.J. Tantillo**

**3:20 ORGN 321.** Dynamics of 1,4-diazabicyclo[2.2.2]octane and dipolar ligands derived of fluoro-bicyclo[2.2.2]octane in paddle-wheel, metal-organic frameworks. **S. Perez Estrada, B.V. Rodriguez-Molina, H. Wang, S. Brown, M.A. Garcia-Garibay**

**3:40 ORGN 322.** Photorelease of biologically relevant molecules using near-IR light. **C.J. Regan, D.P. Walton, D.A. Dougherty**

**4:00 ORGN 323.** Photophysics of N-carbazoyl-benzoates: Push-pull chromophores with switchable emissive states. **L.M. Lifshits, J.K. Klosterman**

**Section F**

San Diego Convention Center  
Room 1B

**New Reactions & Methodology**

M. C. McIntosh, *Organizer*

J. Magolan, *Presiding*

**1:00 ORGN 324.** Introducing Fe-Non: A synthetic iron-rich nontronite clay for green oxidations. **J. Magolan, M. Karki, H.C. Araujo, S.D. Holmbo, J.J. Dalton, L. Baker**

**1:20 ORGN 325.** Use of alumina for Luche-selective reduction of ketones. **J. Magolan, E. Jones-Mensah, L.A. Nickerson, H.J. Knox**

**1:40 ORGN 326.** Proline sulfonamide-catalyzed process for asymmetric synthesis of amine- and alcohol-containing bicyclo[2.2.2]octanes. **M. El Mansy, J. Yong Kang, R. Lingampally, R.G. Carter**

**2:00 ORGN 327.** Ruthenium porphyrin-catalyzed, intramolecular alkylcarbene insertion to C-H bonds of alkyldiazomethanes generated *in situ* from N-tosylhydrazones. **C. Zhou**

**2:20 ORGN 328.** Highly selective *ortho* C-H nitration of nitrostilbenes and protected anilines with *t*-BuONO. **X. Peng**

**2:40 ORGN 329.** C-H amination of arenes and heteroarenes via hindered zinc-amide base mediated zincation and copper-catalyzed electrophilic amination. **C.E. Hendrick, K. Bitting, Q. Wang**

**3:00 ORGN 330.** 5-[1-Halo-2-(arylsulfonyl) vinyl]uracil nucleosides: New probes for cross-linking with amino acids. **Y. Liang, S. Suzoi, Z. Wen, A.G. Artiles, I. da Silva, M. Dinh, A. Akinniyi, S.F. Wnuk**

**3:20 ORGN 331.** New routes to *N,O*-heterocycles for alkaloid synthesis. **R. Bates, R.N. Khanizeman**

**3:40 ORGN 332.** Nickel-catalyzed activation of amides and simple esters. **L. Hie, N.F. Fine Nathel, X. Hong, T.K. Shah, E.L. Baker, Y. Yang, P. Liu, K.N. Houk, N.K. Garg**

**4:00 ORGN 333.** Catalytic C-H arylation of aliphatic amines via a four membered ring cyclopalladation pathway. **C. He, M. Gaunt**

**4:20 ORGN 334.** Copper-catalyzed coupling of thioamides and  $\alpha$ -diazocarbonyl compounds: Synthesis of enamines. **A. Pal, S.R. Hussaini**

**Diversity-Quantification-Success?**

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

**Computers in Chemistry: Bridging the Gap between Clients & Software**

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**LGBT Chemists' Symposium on Chemical Biology**

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**Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza**

Sponsored by INOR, Cosponsored by ENVF, ORGN and POLY

**MONDAY EVENING**

**Section A**

San Diego Convention Center  
Halls D/E

**Sci-Mix**

R. D. Broene, *Organizer*

**8:00 - 10:00**

123, 129, 139, 147, 172, 204, 217, 221, 231. See previous listings.

434, 445-446, 449, 457, 472, 482, 485-486, 515, 522, 525, 655, 703, 710, 735, 755, 766. See subsequent listings.

**TUESDAY MORNING**

**Section A**

San Diego Convention Center  
Room 6A

**Josef Michl ACS Award in Photochemistry: Symposium in honor of Frederick D. Lewis**

J. S. Siegel, *Organizer, Presiding*

M. Fox, *Presiding*

**8:20** Introductory Remarks.

**8:25 ORGN 335.** New structures for singlet fission. P. Dron, P. Del Rey, J. Kaleta, E. Buchanan, Z. Havlas, P. Felkel, J.C. Johnson, T. Magnera, J. Michl

**8:55 ORGN 336.** Light harvesting and photoinduced electron transfer in artificial photosynthetic constructs. A.L. Moore, T.A. Moore, J.D. Gust, M.E. Tejada-Ferrari, A. Teillant, S. Hammes-Schiffer, M.T. Huhnh

**9:25 ORGN 337.** Missing C<sub>1</sub>-C<sub>5</sub> cycloaromatization reaction: Self-terminating photo-release of formaldehyde for the synthesis of fulvenes from enynes. I. Alabugin, R. Mohamed, S. Mondal, T. Faria Delgado, V. Lobodin, K. Jorner, H. Ottosson

**9:55 ORGN 338.** Engineering reactions in crystalline solids: From molecular information to solid-state reactivity. M.A. Garcia-Garbay

**10:25 ORGN 339.** Materials for multicolor fluorescence drawings. J. Yang

**10:55** Introduction of Awardee.

**11:05 ORGN 340. Award Address** (Josef Michl ACS Award in Photochemistry sponsored by the Josef Michl Award Endowment). Tracking photoinduced charge separation in DNA: Charge injection, transport, and trapping. F.D. Lewis

## Section B

San Diego Convention Center  
Room 6B

### Chemical Methods to Investigate Protein Posttranslational Modifications

E. Weerapana, *Organizer*

E. E. Carlson, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 ORGN 341.** Affinity reagents for studying active signaling complexes. D.J. Maly

**8:40 ORGN 342.** Metabolic regulation of histone acetyltransferases by endogenous acyl-CoA cofactors. J.L. Meier

**9:15 ORGN 343.** Investigating the role of protein sumoylation in eukaryotic gene transcription by semisynthesis. C. Chatterjee

**9:50** Intermission.

**10:10 ORGN 344.** Chemoselective identification of protein glutathionylation in response to mitochondrial ROS. Y. Ahn, K.T. Samarasinghe, D.N. Munkanatta Godage, G.C. VanHecke

**10:45 ORGN 345.** Sirtuins and novel protein, posttranslational modifications. H. Lin

**11:20 ORGN 346.** Chemical-proteomic approaches to investigate cysteine post-translational modifications. E. Weerapana

**11:55** Concluding Remarks.

## Section C

San Diego Convention Center  
Room 6C

### ACS Award for Research at an Undergraduate Institution: Symposium in honor of Thomas E. Goodwin

J. Aube, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:10 ORGN 347.** New and efficient methods for the construction of bioactive pyrroles. J.T. Gupton

**9:00 ORGN 348.** Chemical and biological approaches for the treatment of protein misfolding and aggregation diseases. C.B. Cooley

**9:50** Intermission.

**10:00 ORGN 349.** New platforms for discovery of enzyme inhibitors. D.B. Lowe

**10:50** Introductory Remarks.

**11:00 ORGN 350. Award Address** (ACS Award for Research at an Undergraduate Institution sponsored by Research Corporation for Science Advancement). Adventures in research with undergraduates and other mammals. T.E. Goodwin

## Section D

San Diego Convention Center  
Room 5B

### Molecular Recognition & Self-Assembly

M. C. McIntosh, *Organizer*

M. Levine, *Presiding*

**8:00 ORGN 351.** Carbohydrate recognition by Ca<sup>2+</sup>-dependent dimeric synthetic receptors. Y. Zheng, B. Schmidt, A.B. Braunschweig

**8:20 ORGN 352.** Development of a multimodal smart probe for imaging enzyme activity in brain gliomas. J.L. Klockow, K.S. Hettie, T.E. Glass, F.T. Chin

**8:40 ORGN 353.** Unimolecular tubular artificial transmembrane channels. J. Hou

**9:00 ORGN 354.** Dynamic oligomers and stereoisomers controlled by cucurbiturils. E. Masson

**9:20 ORGN 355.** Cocrystallization technique for improved physicochemical properties of carvedilol, an antihypertensive drug. S. Bhandaru, R. Akkinapally

**9:40 ORGN 356.** Synthetic polymers and macrocycles for enhanced supramolecular complexation and detection. M. Levine, B. Radaram, I. Tamgho

**10:00 ORGN 357.** Hexagon-in-hexagon: Synthesis and self-assembly of discrete concentric hexagons. M. Wang, X. Li

**10:20 ORGN 358.** Design of a multimodal smart optical probe for the selective detection of astrocytic gliomas. K.S. Hettie, F.T. Chin

**10:40 ORGN 359.** Photophysical properties of hydrophilic dyes entrapped in interfacially crosslinked reverse micelles. P. Rathinam Arivalagan, Y. Zhao

**11:00 ORGN 360.** New redox-responsive ureidopyrimidone 4 H-bond array based on a pyridinium redox couple. D.K. Smith, B.T. Tamashiro, G. Darzi

**11:20 ORGN 361.** Cooperatively enhanced receptors for cation binding and  $\pi$ - $\pi$  interactions. X. Xing, Y. Zhao

**11:40 ORGN 362.** Halogen-bond templated [2+2] photodimerizations in the solid state. M. Sinnwell, L. MacGillivray

## Section E

San Diego Convention Center  
Room 1A

### Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

M. C. McIntosh, *Organizer*

B. Hudson, *Presiding*

**8:00 ORGN 363.** Computational elucidation of the role of abietadiene synthase in the production of abietadienyl cation. S.R. Hare, D.J. Tantillo

**8:20 ORGN 364.** Exploring the origins of organocatalysis using theoretical, active-site models. N. Celebi-Olcum

**8:40 ORGN 365.** Synthetically accessible virtual inventory (SAVI). Y. Pevzner, W. Ihlenfeldt, M.C. Nicklaus

**9:00 ORGN 366.** Double [6+4] cycloaddition of tropone to dimethylfulvene: A computational study. P. Yu, T.Q. Chen, Z. Yang, C.Q. He, A. Patel, C. Lam, K.N. Houk

**9:20 ORGN 367.** Discovery of UV-filter synergies via design of experiment and computational modeling. S.H. Chirch, A. Bernard, A. Shah, J. Simonnet, R. Weinkauff

**9:40 ORGN 368.** Systematic study and comparison of the photochemical properties of spiroopyrans and spirooxazines. E.I. Balmond, B. Tautges, A. Faulkner, V. Or, B. Hodur, A. Louie, J.T. Shaw

**10:00 ORGN 369.** What is special in aromatic/aromatic interactions? S. Zaric, D. Ninkovic, P. Petrovic, D. Vojislavjevic-Vasilev, V. Medakovic, E. Brothers, M.B. Hall

**10:20 ORGN 370.** Complete mechanism of aldol condensation. C. Perrin, K. Chang

## Section F

San Diego Convention Center  
Room 1B

### New Reactions & Methodology

M. C. McIntosh, *Organizer*

J. Griffin, *Presiding*

**8:00 ORGN 371.** Synthesis of 1,2,3,6-tetrahydropyridines via aminophosphate enabled anionic cascade and acid-catalyzed cyclization approaches. P. Das, J.T. Njardarson

**8:20 ORGN 372.** Application of the PCDFH technique in the synthesis of helicenes and discotic liquid crystal. Z. Li, R. Twieg

**8:40 ORGN 373.** Highly reactive and chemoselective manganese catalyst for intramolecular C(sp<sup>2</sup>)-H amination. J. Griffin, S.M. Paradine, J. Zhao, A.L. Petronico, S. Miller, M. White

**9:00 ORGN 374.** Cyclopropane synthesis via stereospecific intramolecular reductive cross-electrophile couplings. E. Tollefson, L.W. Erickson, E.R. Jarvo

**9:20 ORGN 375.** Multimetallic reductive cross-coupling of vinyl bromides with vinyl triflates: A facile route to 1,3-dienes. A.M. Olivares, D.J. Weix

**9:40 ORGN 376.** Catalytic enantioselective trioxegenation of enals. G.A. Abeykoon, J.S. Chen

**10:00 ORGN 377.** Dearomative functionalization with arenophiles. J. Pospech, E.H. Southgate, J. Fu, D. Sarlah

**10:20 ORGN 378.** Copper-catalyzed H-F insertions. E. Gray, K.A. Choquette, A.G. Doyle

**10:40 ORGN 379.** Short and flexible route to substituted tetrahydropyran-4-ones from 2-methyleneoxetanes. D. Caldwell

**11:00 ORGN 380.** Nickel-catalyzed reductive conjugate addition: New electrophiles and stereoselectivity. K.M. Huihui, D.J. Weix

**11:20 ORGN 381.** Regio- and stereoselective copper (I)-mediated allylic alkylations of  $\alpha,\beta$ -epoxy- $\gamma,\delta$ -unsaturated ketones. E. Amoah

### Cannabis: Exploring the Chemistry, History & Future

*Sponsored by SCHB, Cosponsored by AGFD, CHAS and ORGN*

### Driving Change: Impact of Funders on the Research Data & Publications Landscape

*Sponsored by CINF, Cosponsored by MEDI and ORGN*

### Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza

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### Supramolecular Chemistry: A Crown & Anchor Approach

*Sponsored by INOR, Cosponsored by ORGN*

## TUESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 6A

### Herbert C. Brown Award for Creative Research in Synthetic Methods: Symposium in honor of Alois Fürstner

O. Reiser, *Organizer, Presiding*

**1:20** Introductory Remarks.

**1:25 ORGN 382.** Metal-catalyzed cross-coupling reactions of alkyl electrophiles. G.C. Fu

**2:15 ORGN 383.** Pattern recognition in synthesis. D. Trauner

**3:05 ORGN 384.** Ni-catalyzed C-O bond-cleavage and reductive carboxylation techniques with carbon dioxide. R. Martin

**3:55 ORGN 385. Award Address** (Herbert C. Brown Award for Creative Research in Synthetic Methods sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment). From alkylidynes via alkynes to carbenes: Mechanistic and synthetic implications. A. Fürstner

**4:55** Concluding Remarks.

### Section B

San Diego Convention Center  
Room 6B

### Chemical Methods to Investigate Protein Posttranslational Modifications

E. E. Carlson, *Organizer*

E. Weerapana, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 386.** Decoy probes to measure kinase activity in live cells. L.L. Parker

**1:40 ORGN 387.** Chemical tools to decipher the bacterial glycodecode. D.H. Dube

**2:15 ORGN 388.** Mechanisms of deubiquitinases. E.R. Strieter

**2:50** Intermission.

**3:10 ORGN 389.** Multiscale chemical approaches to map oxidative stress. B. Martin

**3:45 ORGN 390.** Site-specific investigation of O-GlcNAc modifications using synthetic proteins. M. Pratt

**4:20 ORGN 391.** Chemical probes for histidine kinase protein profiling and inhibitor discovery. E.E. Carlson

**4:55** Concluding Remarks.

## Section C

San Diego Convention Center  
Room 6C

**James Bryant Conant Award in High School Chemistry Teaching: Symposium in honor of Julia Winter**

*Cosponsored by CHED*

R. D. Broene, *Organizer, Presiding*

**1:20** Introductory Remarks.

**1:25 ORGN 392.** Teaching moments in (and lessons learned from) the research laboratory. T.R. Hoye

**2:05 ORGN 393.** Clash of two stereochemical cultures: Stereoisomerism in Werner complexes from an organic perspective. J.A. Gladysz

**2:45 ORGN 394.** Computational exploration of guanine oxidation mechanisms. H.B. Schlegel

**3:25 ORGN 395.** Synthetic modifications of proteins to make new biomaterials. A.C. Obermeyer, M.B. Francis, J.B. Jarman

**4:05 ORGN 396. Award Address** (James Bryant Conant Award in High School Chemistry Teaching sponsored by Thermo Fisher Scientific). Building mobile games for organic chemistry. J. Winter

## Section D

San Diego Convention Center  
Room 5B

**Molecular Recognition & Self-Assembly**

M. C. McIntosh, *Organizer*

J. L. Fantini, *Presiding*

**1:00 ORGN 397.** Deep-cavity cavitands as protein inhibition agents. J.H. Jordan, B.C. Gibb

**1:20 ORGN 398.** Water-soluble, molecularly imprinted nanoparticles (MINPs) with internal hydrogen bonds. M. Arifuzzaman, Y. Zhao

**1:40 ORGN 399.** Linear free energy relationships of CH hydrogen bonds: Unusual anion and substituent effects. B.W. Tresca, R.J. Hansen, M.M. Haley, D.W. Johnson

**2:00 ORGN 400.** Trimeric porphyrin-based macrocycles: Synthesis, host-guest chemistry, and transmembrane channel activities. C. Yu, X. Hu, Z. Liu, W. Zhang

**2:20 ORGN 401.** Solid-state chemistry and reactivity of a common anti-cancer drug. A.J. Duncan, R.L. Dudovitz, S.J. Dudovitz, J. Stojakovic, L. MacGillivray

**2:40 ORGN 402.** Preparation and characterization of ammonium receptors that target bacterial membranes. M. Alsuri, D.H. Burns

**3:00 ORGN 403.** Structure modification strategies to control layer-by-layer self-assembly of polyelectrolytes. W. Wan, X. Yang, C. Conrad, M. Bedford, R. Smith

**3:20 ORGN 404.** Methylene-bridge-linked dicalixarene as component for supramolecular assemblies in aqueous media. J.L. Fantini, E.D. Cosco, R.S. Rabb, M.E. Lance

**3:40 ORGN 405.** Synthesis of small molecule/DNA hybrids and their application towards self-assembled plasmonic material. K.D. Okochi, W. Zhang

**4:00 ORGN 406.** Withdrawn.

**4:20 ORGN 407.** Computer-aided visualization of flexible and shape-persistent macrocycles. Y. Liu, A. Singharoy, B. Venkatakrishnan, C.G. Mayne, A. Zlotnick, K. Raghavachari, K. Schulten, A.H. Flood

## Section E

San Diego Convention Center  
Room 1A

**Total Synthesis of Complex Molecules**

M. C. McIntosh, *Organizer*

J. S. Chen, *Presiding*

**1:00 ORGN 408.** Total synthesis of (-)-stemaphylline using lithiation-borylation methodology. A. Varela, D. Leonori, V.K. Aggarwal

**1:20 ORGN 409.** Total synthesis of biologically active carbazole alkaloids. H. Knolker

**1:40 ORGN 410.** Progress towards the enantioselective total synthesis of batrachotoxin. J. DeForest, J.A. Hilf, S.D. Rychynovsky

**2:00 ORGN 411.** Synthetic chemistry and synthetic biology: The bottom-up approach to taxane synthesis. B. Marsh, C. Hayes

**2:20 ORGN 412.** Asymmetric total synthesis of kopsia alkaloids. S. Arai, M. Nakajima, A. Nishida

**2:40 ORGN 413.** Iterative Suzuki couplings and biomimetic Diels-Alder reactions to fused and bridged tetracycles: Synthetic and computational results. D.A. Vosburg, E. Go, S.P. Wetzler, K.J. Kron, R.J. Cave

**3:00 ORGN 414.** Synthetic efforts toward the ambiguous class of natural products. R.E. Johnson, S. Kulyk, R. Sarpong

**3:20 ORGN 415.** Total synthesis of fluorinated prostacyclin PGI<sub>2</sub>-F<sub>2</sub>. I. Perez-Powell, P.R. Moore, V.K. Aggarwal

**3:40 ORGN 416.** Biogenetically inspired total synthesis of lingzhiol. K. Sharmah Gautam, V. Birman

**4:00 ORGN 417.** Enantioselective C-H insertions for the synthesis of complex natural products. K.N. Lamb, N.P. Burlow, A.J. Kwong, J.T. Shaw

**4:20 ORGN 418.** Stereoselective synthesis of tetrahydropyranyl natural products by oxa-Michael addition. R. Bates, T. Lek, D. Csokas, K. Wang

**4:40 ORGN 419.** Benzyne-insertion route toward the synthesis of hetisine-type C<sub>20</sub>-diterpenoid alkaloids. J.J. Pflueger, J. Kiszunzu, T. Kiho, E.L. Fisher, K.B. Clagg, T. Lebold, L. Morrill, R. Sarpong

## Section F

San Diego Convention Center  
Room 1B

**New Reactions & Methodology**

M. C. McIntosh, *Organizer*

B. J. Stokes, *Presiding*

**1:00 ORGN 420.** Dehydro-Diels-Alder of putative allenylpyridines: A new isoquinoline synthesis. A. Morrison, G.B. Dudley

**1:20 ORGN 421.** Unique non-classical hydrogen bond interactions in 2-oxypentadienyl cations. C. Ayala, N.S. Dange, J.R. Stephenson, J. Henry, T. Tugwell, J. Hamideh, F. Fronczek, R. Kartika

**1:40 ORGN 422.** Use of ArcOPd species for arylation and esterification reactions under microwave irradiation. M. Al-Masum

**2:00 ORGN 423.** Direct radical functionalization of alcohols using cobalt photocatalysis. D.B. Martin, D.R. Chambers, R. Sullivan

**2:20 ORGN 424.** Novel directing group strategy for the  $\beta$ -amination of alcohols. K. Nakafuku, M. Bekkaye, D. Nagib

**2:40 ORGN 425.** Brønsted superacid-catalyzed cyclizations of 3-aryl-1-propenes for the preparation of highly substituted indanes. X. Cai, A. Keshavarz, J. Omaque, B.J. Stokes

**3:00 ORGN 426.** Catalytic synthesis of alpha-tetrasubstituted amines via tandem condensation-allylation. K.G. Nelson, C.H. Larsen

**3:20 ORGN 427.** Chemo- and regioselective cobalt-catalyzed reactions of 1,3- and 1,4-dienes with silyl hydrides. B. Raya, T. RajanBabu

**3:40 ORGN 428.** Synthesis of hindered amines: Copper-catalyzed radical addition with nitroso compounds. A. Samoshin, D. Fisher, G.L. Burnett, G. Hammersley, E. La, J. Read De Alaniz

**4:00 ORGN 429.** Research initiatives in the quest for an enantioselective, allenolate Claisen rearrangement. A.G. Wenzel

**4:20 ORGN 430.** Efficient aerobic linear allylic C-H amination: Overcoming benzoquinone inhibition. C.C. Pattillo, I.I. Strambeanu, P. Calleja, N.A. Vermeulen, T. Mizuno, M. White

**Driving Change: Impact of Funders on the Research Data & Publications Landscape**

*Sponsored by CINF, Cosponsored by MEDI and ORGN*

**Supramolecular Chemistry: A Crown & Anchor Approach**

*Sponsored by INOR, Cosponsored by ORGN*

## TUESDAY EVENING

## Section A

San Diego Convention Center  
Hall D

**Biologically-Related Molecules & Processes**

R. D. Broene, *Organizer*

**8:00 - 10:00**

**ORGN 431.** Base-modified 7-deazapurine nucleosides. R. Rayala, S. Kavoosi, B. Walsh, M. Barrios, S.F. Wnuk

**ORGN 432.** Photo-activation of immune system with caged agonists. K. Ryu, A.P. Esser-Kahn

**ORGN 433.** Synthesis of singly and triply bridged diporphyrin appended with six thioglucose units. S. Singh

**ORGN 434.** Development of reaction-based fluorescent probes for hydrogen sulfide. B. Peng, W. Chen, S. Xu, A. Pacheco, M. Xian

**ORGN 435.** Synthesis, characterization, anti-cancer and antibacterial study of Schiff bases derived from 6,6-dimethyl-2,2-bipyridyl. M.R. Karim, M. Razzak

**ORGN 436.** Investigations on rare rhenium complexes containing tridentate ligands. M. Ndinguri, C. Black, F. Fronczek

**ORGN 437.** Rational design of highly sensitive fluorescence probes for hydrogen polysulfides. W. Chen, J.J. Day, A. Pacheco, M. Xian

**ORGN 438.** Synthesis of dopaminergic compounds for analysis in SULT1A3. C. Cochrane, J.C. Rote, G.E. Bailey, D. Bigler, M.L. Cafiero, L.W. Peterson

**ORGN 439.** Effect of 8-hydroxy-7,8-dihydroguanosine on the structure and function of RNA hairpins and aptamers of preQ<sub>1</sub> and theophylline. K. Gibala, Y.J. Choi, K. Van Deventer, M.J. Resendiz

**ORGN 440.** Synthesis of novel fluorescent, universal DNA nucleosides. J. Izaguirre, T.J. Kaelin, L. Davis

**ORGN 441.** Synthesis and analysis of dopaminergic derivatives as inhibitors of catechol-O-methyltransferase. A.K. Hatstat, M. Morris, M.L. Cafiero, L.W. Peterson

**ORGN 442.** Redox chemistry of 9,10-diacetoxy-1,4-methano-1,4-dihydroanthracene derivatives. M.B. Wilson, Z.A. Lyons, K.M. McKenney, E. Tsogtbaatar, D.E. Lewis

**ORGN 443.** Free radical mechanism for the  $\gamma$ -glutamyl carboxylase reaction: A computational study. D.E. Lewis, Z.A. Lyons

**ORGN 444.** Design, synthesis, and zinc binding analysis of natural substrate analogues of LpxC. K. Wilson, G. Lamanila, S. Malkowski, M.L. Cafiero, L. Peterson

**ORGN 445.** Computational investigation of the P450-catalyzed oxidative cyclization step in the biosynthesis of griseofulvin. J.M. Grandner, R.A. Cacho, Y. Tang, K.N. Houk

**ORGN 446.** Reversibly photoswitchable fluorescent tag for no-wash live-cell imaging. W. Sheng, C. Vasileiou, J.H. Geiger, B. Borhan

**ORGN 447.** Polymyxin-based cell penetrating scaffolds. K. Hamill, L.C. McCoy, J. Esko, Y. Tor

**ORGN 448.** Synthesis and DNA binding profile of dimers of the azinomycin chromophore. H. Panesar, T.G. Minehan

**ORGN 449.** Sculpting the carbonyl skeleton: A synthetic strategy to access designed abscisic acid analogs. B.S. Wang

**ORGN 450.** Electron-induced site specific formation and reactions of the aminyl radical in 2'-azido-2'-deoxycytidine and its 4'-azidocytidine analogue. M. Mudgal, A. Adhikary, C.G. Hanson, A.O. Petrovici, M.D. Sevilla, S.F. Wnuk

**ORGN 451.** Design, synthesis and characterization of novel 5, 6-dimethoxy indanone molecules. V. Patil, S. Patil, S. Patil

**ORGN 452.** Novel peptidomimetic inhibitors for the West Nile virus NS2B-NS3 protease. J. Truong, B. Espinosa, N. Keppetipola, N.T. Salzameda

**ORGN 453.** Peptidomimetic sulfonyl amide inhibitors of the botulinum neurotoxin. T. Bingham, I. Vargas, B. Paterson, N.T. Salzameda

**ORGN 454.** Synthesis and structure-activity relationship study of PreQ<sub>1</sub>-thiazole orange fluorogenic probes for RNA-TAG. E.C. Zhou, S. Alexander, N.K. Devaraj

**ORGN 455.** Synthesis of fluorinated glucopyranosyl selenoureas as new generation of glucosidase inhibitors. Z.J. Witzczak, G. Mloston, M. Celeda

**ORGN 456.** Developing water-soluble, near-IR sensors for blood glucose monitoring. N.P. Cooley, H. Sepasizangabadi, T.E. Glass

**ORGN 457.** Against all odds: Prebiotic synthetic chemistry in surfactant assemblies leading to tetrapyrrole macrocycles. E.J. Alexy, C.W. Hintz, M. Taniguchi, J.S. Lindsey

**ORGN 458.** Directed immune responses via covalently-linked TLR agonist combinations. T.J. Albin, J. Tom, A. Esser-Kahn

**ORGN 459.** Specific, cell-permeable fluorescent probes in the imaging of enzymatic pathways in living cells. A.G. Reeves, A. Lippert

**ORGN 460.** Enhancing the cell permeability of ATP analogs for kinase-catalyzed labeling. A.E. Fouda, M.K. Pflum

**ORGN 461.** Antimicrobial activity of synthetic 5'-amino-ribonucleosides. R.P. Van Ostrand, A. Chavez, A.M. Awad

- ORGN 462.** Clickable and photocleavable lipid analog for cell membrane delivery and release. **S. Alam**, M.D. Best, A.M. Bayer
- ORGN 463.** Nitric oxide-releasing glucosamine as a therapeutic for cystic fibrosis. **P.R. de Jesus-Cruz**, M.H. Schoenfish, D. Suchyta
- ORGN 464.** Exploring the synthesis of C1-substituted carbapenems. **T.Q. Nguyen**, M. Alqurafi, J. Kim, P. Nguyen, S. Casco, M. Bennett, C. Edwards, C. Chiang, M. Lohry, E. Kim, D. Le, M. Cox, S. Smriti, P. Gupta, B. Meshram, M. Chepuru, R. Chepuru, P. Oelschlaeger, J.D. Buynak
- ORGN 465.** Development of clickable triazabutadienes as cleavable cross-linkers. **B.M. Cornali**, F. Kimani, J.C. Jewett
- ORGN 466.** Directed evolution of RebH for catalyst-controlled selective halogenation. **M. Andorfer**, J. Payne, C. Poor, J.C. Lewis
- ORGN 467.** Exploring the synthesis of C6-substituted carbapenems. **M. Alqurafi**, W. Chai, M. Lohry, T.Q. Nguyen, J. Kim, S. Casco, M. Chepuru, R. Chepuru, P. Oelschlaeger, J.D. Buynak
- ORGN 468.** Novel class of immune modulators: Covalent toll-like receptor-7 agonist. **A.C. Chon**, A. Esser-Kahn
- ORGN 469.** Phenol variation in the dual Ugi-Smiles Diels-Alder process. **M. Meyers**, A.M. Fox, S.B. Luesse
- ORGN 470.** Component variation in the Passerini-Smiles reaction. **C. Summers**
- ORGN 471.** Structural effects on catalysis with bifunctional, enzyme-like, helical peptide catalysts. **J. Duval**, M. Kinghorn, D. Michaelis
- ORGN 472.** Rational design of bifunctional helical peptide catalysts with enzyme-like activity. **M. Kinghorn**, D. Chantry, S. Draper, D. Michaelis
- ORGN 473.** Convenient synthesis of azido ribonucleosides as antimicrobial and antiviral agents. **G. Tolentino**, R. Trude, L. Utley, A. Kaplan-Hernandez, A.M. Awad
- ORGN 474.** BODIPY-functionalized hyaluronic acid as a photosensitizer for photodynamic therapy. **Y. Bae**, S. Thayumanavan
- ORGN 475.** Substituent effects on fluorescent cytidine analogues. **D.D. Burns**, R. Lee, B.W. Purse
- ORGN 476.** Small molecule synthesis of potential inhibitors of hepatitis C virus translation. **W.W. Frauman**
- ORGN 477.** Novel approaches to the chemical synthesis of ketosteroid and related compounds, inhibitors of sterol biosynthesis. **E.J. Parish**, H. Shyu, H. Honda, T. Wei
- ORGN 478.** Investigation on the utilization of collagen as a scaffold for multichromophore assembly. **R.M. Malamakal**, Y. Zhang, S.L. Meloni, J.M. Anna, D.M. Chenoweth

## Section B

San Diego Convention Center  
Hall D

### Metal-Mediated Reactions & Syntheses

R. D. Broene, *Organizer*

8:00 - 10:00

- ORGN 479.** Nickel-catalyzed regio- and stereoselective hydrocyanation of allene. **Y. Amako**, S. Arai, A. Nishida
- ORGN 480.** DFT studies of unique mechanistic differences in the Rh-catalyzed synthesis of  $\beta$ - and  $\gamma$ -lactones. **S.R. Hare**, D.J. Tantillo

- ORGN 481.** Novel application to allylic and benzylic oxidations of steroids with transition metal reagents. **E.J. Parish**, Y. Lo, H. Honda, T. Wei
- ORGN 482.** One-pot sequential synthesis of  $\alpha$ -alkylated ketones from easily accessible feedstocks. **F. Li**, J. Ma, R. Wang
- ORGN 483.** Synthesis and isolation of a dehydroindolizidine from 2-methylpyrrole using the electron-rich tungsten dearomatization agent (WTP(NO)(PMe<sub>3</sub>)). **B. Liebov**, D. Iovan, W.H. Myers, W.D. Harman
- ORGN 484.** Suzuki-Miyaura couplings with SuFEx-derived heteroaryl fluorosulfates. **E. Zhang**, J. Tang, S. Li, P. Wu, K.B. Sharpless
- ORGN 485.** Magnetic graphitic carbon nitride: Application in C-H activation and oxidative cyanation of amines. **S. Verma**, N.R. Baig, M. Nadagouda, R.S. Varma
- ORGN 486.** Copper-catalyzed divergent addition reactions of enoldiazoacetamides with nitrones. **Q. Cheng**, M.P. Doyle
- ORGN 487.** Investigating the use of copper photoredox catalysts in the  $\alpha$ -benzylation of aldehydes. **M.R. Jilek**, S.A. Sarah, K.H. Jensen
- ORGN 488.** Room temperature borylation of N-heterocycles using a Lewis acid effect. **R. Tobolowsky**, A. Green, C.A. Merlic
- ORGN 489.** Withdrawn.
- ORGN 490.** New diastereoselective synthesis of (Z)-trisubstituted alkenes containing a p-methoxyphenyl and trimethylsilyl moieties via organoboranes. **N.G. Bhat**
- ORGN 491.** Metal-catalyzed reactions towards novel pyridio[3,4-b]indoles. **S. Khanal**, J.G. Varelas, M. O'Donnell, S.P. Mulcahy
- ORGN 492.** Method development for copper-catalyzed synthesis and glycodiversification reactions of 2-amino sugar building blocks. **J. Lam**, M.A. Miller, A.A. Oviatt, A.M. Scharnow, R.L. Starr, C.M. Rojas
- ORGN 493.**  $\beta$ -Borylation and  $\beta$ -silylation of enals toward a method to access trisubstituted vinyl boronate esters and vinyl silanes. **T.A. Thane**, T.B. Clark
- ORGN 494.** Synthesis of biaryl ethers from benzylic amine boronate esters by the copper-catalyzed Chan-Evans-Lam etherification. **J.S. Marcum**, C.J. Ferber, K.A. McGarry, T.B. Clark
- ORGN 495.** Synthesis and structural revision of epoxydine A via palladium-catalyzed cyclitolization. **K. Francisco**, Y. Li, G.A. O'Doherty
- ORGN 496.** Withdrawn.
- ORGN 497.** C-H functionalization by dual metal cooperativity. **J. Gair**, J.C. Lewis
- ORGN 498.** Modification of Ugi-Smiles products via ring-opening reactions. **A. Harris**, S. Luesse
- ORGN 499.** Effect of electron-deficient, fluorinated phosphines on the catalytic properties of bifunctional catalysts. **F. Barmare**, E.R. Paulson, H.N. Tran, D.B. Grotzahn
- ORGN 500.** Oxidative Heck-type aminations with heterobimetallic Pd-Ti catalysts. **R. Stokes**, W. Walker, D. Michaelis
- ORGN 501.** Evaluation of copper photoredox catalysts in the synthesis of chiral molecules. **M.R. Hurst**, T.G. Trimble, K.H. Jensen
- ORGN 502.** Preparation of amino-epoxyisoindolines via chemoselective reduction. **M. Raeesi**, S.B. Luesse
- ORGN 503.** Employing alkene cross-metathesis reactions for the synthesis of organosilane-functionalized silica surfaces. **J. Ochoa**, B.J. Stokes

- ORGN 504.** Insight into crosslink DNA-adducts through monofunctional platinum complexes. **B.A. Freeman**, M. Ndinguri
- ORGN 505.** Facile microwave synthesis of iridium polypyridyl photosensitizers. **R. McAtee**, A. Sun, T. Monos, C. Stephenson
- ORGN 506.** Catalytic reductive coupling and deoxygenation of activated alcohols. **G.R. Kasner**, C. Boucher-Jacobs, K.M. Nicholas
- ORGN 507.** Novel approaches to the synthetic study and structural activity relationship of citronellol-type compounds and their derivatives. **Y. Lo**, H. Honda, T. Wei, H. Shyu
- ORGN 508.** Novel approaches to the chemical synthesis of haloindoles for the development of ergot alkaloids compounds for an alternative route to the lysergic acid. **Y. Lo**, W. Huang, H. Honda, T. Wei
- ORGN 509.** Substituted tricyclic structure synthesized through gold-catalyzed homopropargyl alcohol addition to alkyne followed by Diels-Alder reaction. **S. Hosseyini**
- ORGN 510.** Carbohydrate-porphyrin (CPCs) and carbohydrate-bacteriochlorin conjugates (CBCs) synthesized using Huisgen cycloaddition. **D. Dennis**, M. Burch, R. Dolewski, M. George, B. Doornbos, D. Enyart, B. Blough, D. Akrobetu, E. Xu, N.L. Snyder, J.V. Ruppel
- ORGN 511.** Co(II)-salen catalyzed carbon-carbon bond formation via C-H functionalization for the elaboration of heterocycles. **A. De Los Santos**, A. Schafer, S. Blakey
- ORGN 512.** Substitution at allylic stereogenic centers of a [13]-macrolactone: Effects on macrocyclization efficiency and topology. **K. Rutledge**, A.N. Magpusao, B.Q. Mercado, M. Peczu
- ORGN 513.** Selective photocatalytic C-C bond cleavage under ambient conditions with earth abundant vanadium complexes. **H. Soo**, S. Gazi, M. Dokić

## Section C

San Diego Convention Center  
Hall D

### Molecular Recognition & Self-Assembly

R. D. Broene, *Organizer*

8:00 - 10:00

- ORGN 514.** Synthesis, structure, and dynamics of orange-emitting squaraine rotaxane. **C. Collins**, A.M. Elifritz
- ORGN 515.** Supramolecular microenvironment strategy for the catalytic acceleration of a transition metal-mediated, cross-coupling reaction. **D. Kaphan**, M. Levin, R.G. Bergman, K.N. Raymond, D. Toste
- ORGN 516.** Syntheses and supramolecular chemistry of functionalized "Texas-sized" molecular boxes. **R. Wu**, J.L. Sessler
- ORGN 517.** Synthesis, guest binding, and metal coordination of functionalized self-folding deep cavitands. **M. Mettry**, R.J. Hooley
- ORGN 518.** Influence of dimensionality and size on anion binding in thiourea-based acyclic receptors. **M. Emami Khansari**, D.R. Powell, M. Hossain
- ORGN 519.** Click chemistry-derived aqueous supramolecular nanostructures based on amphiphilic molecules. **I. Kim**, Y. Jeong, S. Jo, E. Lee
- ORGN 520.** Synthesis of water-soluble cubic metallocomplexes. **A.R. Metell**, J.D. Thoburn

- ORGN 521.** Cooperatively enhanced synthetic receptors and lipid membrane sensors. **R.W. Gunasekara**, Y. Zhao
- ORGN 522.** Study of stacking interactions between benzene and cyclohexane. **S. Zanic**, D. Ninkovic, D. Vojislavjević-Vasilev, V. Medakovic, E. Brothers, M.B. Hall
- ORGN 523.** Threaded and non-threaded host-guest complexes based on bipyridinium and sulfonated crown ether species in aqueous solution. **R.A. Lunala-Ixmatalaha**, R. Cervantes, J. Tiburcio
- ORGN 524.** Synthesis of a functionalized metal-ligand-coordinated supramolecular capsule for appending into polymers. **S. Martin**, K. Teppang, S. Journey, S. Moss, B.W. Purse

## Section D

San Diego Convention Center  
Hall D

### Peptides, Proteins & Amino Acids

R. D. Broene, *Organizer*

8:00 - 10:00

- ORGN 525.** Regulation of emission via proton-host solvatochromic fluorophores. **E.M. Santos**, J.H. Geiger, B. Borhan
- ORGN 526.** Novel probes to map cell wall growth & division in *Staphylococcus aureus* at the nanoscale. **B.E. Cottrell**
- ORGN 527.** Concise synthesis of N-boc-2,3-methanoproline methyl ester. **M.J. Mitton-Fry**, A.D. Landgraf, J. Bellenger, B. Khunte
- ORGN 528.**  $\beta$ -hairpin peptide derived from transthyretin 106-121 that forms square hydrophobic channels. **S. Yoo**, N. Truex, A. Kreutzer, J.S. Nowick
- ORGN 529.** Mechanistic re-investigation on Strecker synthesis of aminonitrile. **R. Johnston**, W. Li, X. Song, I.J. Posey
- ORGN 530.** Effect of hydrophobicity and charge in the oligomerization of amyloidogenic peptides and the design of a pH-switchable oligomer. **Y. Wang**, N. Truex, H. Wali
- ORGN 531.** Simple sequencing strategy for bicyclic peptoids/peptides via one-pot ring-opening and cleavage reaction. **C. Seo**, H. Lim
- ORGN 532.** Converting one-face  $\alpha$ -helix mimetics into amphiphilic  $\alpha$ -helix mimetics as potent inhibitors of protein-protein interactions. **M. Shin**, H. Lim
- ORGN 533.** Stapled  $\alpha$ -helix mimetic small-molecules. **Y. Lee**, H. Lim
- ORGN 534.** Efforts toward the synthesis of new collision-induced dissociation cleavable protein cross-linkers. **S. Block**, E. Novitsky, C. Yu, L. Huang, S.D. Rychnovsky
- ORGN 535.** Solid-phase synthesis of heterodisulfide peptidomimetic CN2097. **S. Kotla**, K. Parang, R. Tiwari
- ORGN 536.** Development of phosphoprotein selective and aqua-soluble chemosensor. **H. Yeo**, Y. Kwak, S. Kim, B. Park

## WEDNESDAY MORNING

### Section A

San Diego Convention Center  
Room 6A

### Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of Donna G. Blackmond

*Cosponsored by CATL and WCC*

D. M. Huryn, *Organizer, Presiding*

8:00 Introductory Remarks.

**8:05 ORGN 537.** Development, mechanistic study, and applications of copper-catalyzed hydroamination processes. S.L. Buchwald

**8:40 ORGN 538.** Mechanisms in catalysis: Case studies of metal-mediated transformations in complex molecule synthesis. M.D. Eastgate

**9:15 ORGN 539.** Developing a stereomodel for enantioselective C-H activation reactions. J. Yu

**9:50 ORGN 540.** Seeing is believing: Direct observation of reaction progress in challenging systems. J. Hein

**10:25 ORGN 541.** Mechanistic analysis of anion-abstraction catalysis. E.N. Jacobsen

**11:00** Introductory Remarks.

**11:05 ORGN 542. Award Address** (Gabor A. Somorjai Award for Creative Research in Catalysis sponsored by the Gabor A. and Judith K. Somorjai Endowment Fund). New paradigm for stereocontrol in organocatalysis. D.G. Blackmond

## Section B

San Diego Convention Center  
Room 6B

### Supramolecular Chemistry

*Cosponsored by INOR*  
*Financially supported by Elsevier, Supramolecular Chemistry, Royal Society of Chemistry*

P. A. Gale, J. Jayawickramarajah, D. W. Johnson, D. J. Magda, *Organizers*

A. E. Gorden, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:10 ORGN 543.** Interlocked host molecules for anion recognition and sensing. P. Beer

**8:30 ORGN 544.** Anion-recognition/ion-pairing approaches to asymmetric catalysis. D. Seidel

**8:50 ORGN 545.** Supramolecular ion-pairing assemblies based on anion-responsive  $\pi$ -systems. H. Maeda

**9:10 ORGN 546.** Use of anion receptors to control cation selectivity in liquid-liquid systems. B.A. Moyer, N.J. Williams, V.S. Bryantsev, R. Custelcean

**9:30 ORGN 547.** Recognition and catalysis in deep cavitand. J. Rebek

**9:50** Intermission.

**10:10 ORGN 548.** Anion recognition and switching at interfaces. A.H. Flood

**10:30 ORGN 549.** Anions and hydrophobic cavities. B.C. Gibb

**10:50 ORGN 550.** Tethering BODIPY through boron. B. Liu, N. Novikova, M.C. Simpson, B.L. Stocker, T. Soehnel, M.S. Timmer, D.C. Ware, P. Brothers

**11:10 ORGN 551.** Recognition and sensing of creatinine using phosphonato aryl-extended calix[4]pyrroles. P. Ballester

**11:30 ORGN 552.** Meso-aryl calix[4]pyrroles bearing covalently linked fluorophore as a sensitive 'turn on' FDDA anion sensor. C. Lee

## Section C

San Diego Convention Center  
Room 6C

### Heterocycles & Aromatics

M. C. McIntosh, *Organizer*

I. Alabugin, *Presiding*

**8:00 ORGN 553.** Synthesis of azabicycles using intramolecular reductive amination. E. Lanier, A.L. Wolfe

**8:20 ORGN 554.** Synthesis, molecular modeling, and DNA-binding studies of atropisomeric  $\beta$ -carboline as novel molecular probes. M. Draeger, S.P. Mulcahy

**8:40 ORGN 555.** Synthesis of 4,4'-functionalized BODIPYs from F-BODIPYs and dipyrins. A.L. Nguyen, P.N. Bobadova-Parvanova, F. Fronczek, K.M. Smith, G. Vicente

**9:00 ORGN 556.** Cyclic ether synthesis via palladium-catalyzed, directed, dehydrogenative annulation at unactivated terminal positions. S.J. Thompson, G. Dong

**9:20 ORGN 557.** Design and synthesis of near-IR BODIPYs via cross-couplings and benzo-fusions. Q. Meng, F. Fronczek, G. Vicente

**9:40 ORGN 558.** Synthesis of tetrasubstituted furans from propargylic diols. J.T. Ippoliti, A.K. Peterson, M. Sirianni, T.S. Tuohy, A.T. Kuelbs, C.M. Pahl

**10:00 ORGN 559.** Regioselective reduction of 1*H*-1,2,3-triazoles diesters and triesters. C.R. Butler, A.M. Schoffstall

**10:20 ORGN 560.** Oxidative heterocyclizations with malonoyl peroxides. C. Alamillo Ferrer, N.C. Tomkinson

**10:40 ORGN 561.** Withdrawn.

**11:00 ORGN 562.** Stereoelectronic control of radical and metal-catalyzed cyclizations and fragmentations. I. Alabugin

**11:20 ORGN 563.** Withdrawn.

**11:40 ORGN 564.** Synthesis of a triple FRET probe through marriage of click chemistry and the sequential aminolysis reactivity of benzotriuranone (BTF). A.N. Bartley, M.B. Baker, R.K. Castellano

## Section D

San Diego Convention Center  
Room 5B

### Chemistry of Fullerenes, Carbon Nanotubes & Graphene

M. C. McIntosh, *Organizer*

R. Jordan, *Presiding*

**9:00 ORGN 565.** Catching the big fullerene: Selectivity of self-assembled molecular capsules towards C<sub>70</sub> and C<sub>84</sub>. S. Serapian, E. Huerta, E. Santos, C. Bo, J. de Mendoza

**9:20 ORGN 566.** Tailored carbon nanomaterials prepared from reactive molecular precursors at room temperature. H. Frauenrath, S. Schrettli, B. Schulte

**9:40 ORGN 567.** Nanoscale Raman characterization of carbon-based materials. A. Krayev, S. Bashkurov, D. Evplov, V. Gavriluyk, V. Zhizhimontov, M. Chaigneau, S. Saunin

**10:00 ORGN 568.** Bottom-up synthesis of graphene nanoribbons via the topochemical polymerization of polyacetylenes. R. Jordan, Y. Wang, S. Khan, R.B. Kaner, Y.F. Rubin

**10:20 ORGN 569.** Withdrawn.

**10:40 ORGN 570.** Lithium intercalation of graphene/hexagonal-boron nitride heterostructures. G. Elbaz, S. Zhao, D. Efetov, J. Ravichandran, L.E. Brus, X. Roy, P. Kim

## Section E

San Diego Convention Center  
Room 1A

### Total Synthesis of Complex Molecules

M. C. McIntosh, *Organizer*

R. E. Johnson, *Presiding*

**8:00 ORGN 571.** Total synthesis of the pentacyclic guanidinium core of apoptosis-inducing marine natural products. Y. Moazami, J. Pierce

**8:20 ORGN 572.** Exploiting cyclobutanol reactivity toward the total synthesis of (+)-phomactin A. P. Leger, S. Chang, D.J. Wang, R. Sarpong

**8:40 ORGN 573.** Breitfussins A and B: Total synthesis reveals a facile halide migration. A. Khan, J.S. Chen

**9:00 ORGN 574.** Progress towards the total synthesis of yaku'amide A. Y. Cai, S.L. Castle

**9:20 ORGN 575.** Expedient approach towards highly oxygenated furanyl diterpenes. S. Goswami, R.G. Carter

**9:40 ORGN 576.** Synthetic studies towards obtusanal. P.K. Waldenmaier, R.G. Carter

**10:00 ORGN 577.** Progress toward the synthesis of difluorinated anthocyanins. R. Hazlitt, D.A. Colby

**10:20 ORGN 578.** Approaches toward the total synthesis of amomaxin A and B. M. Jean, V. Albert, J. Boukouvalas

**10:40 ORGN 579.** Design and synthesis of a novel hyperpolarizable <sup>19</sup>N<sub>2</sub>-labeled diazine for magnetic resonance imaging. G. Ortiz, Q. Wang

**11:00 ORGN 580.** Withdrawn.

**11:20 ORGN 581.** Second-generation synthesis of palmerolide A. P. Batsomboon, G.B. Dudley

**11:40 ORGN 582.** Oxidative radical reactions for total synthesis. J. Burton

## Section F

San Diego Convention Center  
Room 1B

### New Reactions & Methodology

M. C. McIntosh, *Organizer*

J. A. Prieto, *Presiding*

**8:00 ORGN 583.** Preparation of functionalized alky- and alkenyltrifluoroborates compounds via hydroboration. T.E. Cole, D. Zillman, K. Alanqari, S. Singh, L. Daley, R. Newman, N. Felix

**8:20 ORGN 584.** Photothermal catalysis provides light-mediated access to thermally controlled transformations. R.C. Steinhart, A. Esser-Kahn

**8:40 ORGN 585.** Development of carbocation-trapping metathesis reaction. D.J. Nasrallah, J. Ludwig, J. Gianino, C. Schindler

**9:00 ORGN 586.** Epoxide-based methodology for the non-aldol construction of the mycalolide A and crocacin C polypropionate fragments. J.A. Prieto, A. Cruz-Montanez, J. Rentas-Torres

**9:20 ORGN 587.** Condensation vs. hydroamination for the direct, catalytic synthesis of alpha-tetrasubstituted amines. C. Pierce, M. Nguyen, Z.L. Palchak, D. Lussier, C.H. Larsen

**9:40 ORGN 588.** Non-metal promoted, intermolecular amination using an N-centered radical approach. A. Lamar

**10:00 ORGN 589.** C-H functionalization of phyllanthusmin natural products: Rapid generation of a library of anticancer agents. C.M. Hambira, S. Fosu, M. Bettinger, J.L. Woodard, J. Fuchs, D. Nagib

**10:20 ORGN 590.** Discovery and mechanistic study of triple aryne-tetrazine reaction enabling rapid access to a new class of polyaromatic heterocycles. S. Suh, D.M. Chenoweth, S. Barros

**10:40 ORGN 591.** Double Diels-Alder/Nazarov tandem cyclization of 1,4-dialkynylpentan-3-ones to generate [6-5-6] tricyclic products. R.A. Carmichael, W. Chailifoux

**11:00 ORGN 592.** Selective aziridination and derivatization of silyl-allenes. E. Burke

## Computational Materials & Nanoscience: Theory Meets Experiment

### Forum: Materials Genome & Materials Informatics

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

## WEDNESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 6A

### Ralph F. Hirschmann Award in Peptide Chemistry: Symposium in honor of Ronald T. Raines

L. A. Marcaurelle, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 593.** Exploring the dark matter of protein space through *de novo* peptide design. D.N. Woolfson

**2:00 ORGN 594.** Mimicry of protein surfaces with peptides and peptidomimetics. P. Arora

**2:55 ORGN 595.** Quantifying protein carbohydrate interactions. W. Chen, C. Hsu, A. Murray, J.L. Price, E.K. Culyba, S.R. Hanson, C. Wong, E.T. Powers, J.W. Kelly

**3:50** Ralph F. Hirschmann Award Presentation.

**4:00 ORGN 596. Award Address** (Ralph F. Hirschmann Award in Peptide Chemistry sponsored by Merck Research Laboratories). Unappreciated forces that stabilize peptides and proteins. R.T. Raines

**4:55** Concluding Remarks.

### Section B

San Diego Convention Center  
Room 6B

### Supramolecular Chemistry

*Cosponsored by INOR*  
*Financially supported by Elsevier, Supramolecular Chemistry, Royal Society of Chemistry*

P. A. Gale, A. E. Gorden, D. W. Johnson, D. J. Magda, *Organizers*

J. Jayawickramarajah, *Organizer, Presiding*

**1:00 ORGN 597.** Design of nano-mechanical DNA origami devices with dynamic characters. Y. Ohya, M. Kaino, M. Hashizume, A. Kuzuya

**1:20 ORGN 598.** Expansion of a novel RNA-binding scaffold to target HIV-1 TAR RNA. A.E. Hargrove

**1:40 ORGN 599.** Texas-sized molecular box: Building block of anion-induced self-assembly. H. Gong, Y. Yang, J. Shang

**2:00 ORGN 600.** Towards more sustainable (poly)condensation and oxidation reactions. **B. Andrioletti**

**2:20 ORGN 601.** Mild dehydrative aromatization protocol for accessing highly distorted *para*-phenylenes. **B.L. Merner**

**2:40** Intermission.

**3:00 ORGN 602.** Supramolecular methods to achieve input responsive protein-binders. **J. Jayawickramarajah, X. Su, C.H. Battle, G.H. Aryal**

**3:20 ORGN 603.** Nanostructures prepared from self-assembly of pillararene-based amphiphiles and supra-amphiphiles. **F. Huang, G. Yu, Y. Yao**

**3:40 ORGN 604.** Pi-radicals as building blocks for electron-responsive molecular materials and organized assemblies. **C. Bucher**

**4:00 ORGN 605.** Supramolecular properties of subphthalocyanines. **T. Torres-Cebada, G. Lavarda, J. Guilleme, D. González-Rodríguez, I. Sanchez-Molina, C. Claessens, D. Guzman, O. Trukhina, G. Zango, M. Martínez-Díaz**

**4:20 ORGN 606.** Pillar[n]arene-based supra-molecular assemblies for multi-layer films and carbon fibers with controlled pores at angstrom level. **T. Ogoshi**

**4:40** Concluding Remarks.

### Section C

San Diego Convention Center  
Room 6C

#### Heterocycles & Aromatics

M. C. McIntosh, *Organizer*

R. Baxter, *Presiding*

**1:00 ORGN 607.** Synthesis of benzo[b] thiophenes via iron(III) mediated 5-*endo*-dig electrophilic cyclization. **T. Kesharwani, C. Kornman, A. Tonnaer, A. Royappa**

**1:20 ORGN 608.** Syntheses, structures, and reactivity of fluorinated isoindenone dimers. **M. Etzkorn, J.L. Franklin, V.L. Wait**

**1:40 ORGN 609.** Bismethoxy-isoindenone dimers: A synthetic platform toward novel (heterocyclic) frameworks with laterally displaced arene units. **J.L. Franklin, V.L. Wait, C. Strickland, M. Etzkorn**

**2:00 ORGN 610.** Versatile, one-pot, two-step synthesis of oxazoles from epoxides. **D.L. Sellers, S. Punhani, E. Schoffers**

**2:20 ORGN 611.** Modular approach to crowded benzoquinolines. **D.J. Dibble, A. Mazaheripour, R. Lopez, D.E. Laidlaw, M.J. Umerani, Y.S. Park, A.A. Gorodetsky**

**2:40 ORGN 612.** Practical synthesis of disymmetric quinoxalines. **M.R. Angelastro, R.A. Farr, B. Gieske, J.T. Klein, T.R. Nieduzak, P. Shum, N.B. Sizemore, P.M. Weintraub**

**3:00 ORGN 613.** Various N-functionalized, nitrogen-rich azoles as high energy density materials. **P. Yin, J.M. Shreeve**

**3:20 ORGN 614.** Efficient synthesis of drug-like polycyclic compounds such as naphthyridines and aza-indoles. **C. Agrios**

**3:40 ORGN 615.** Inspired by chelation drugs, 1,2,3-triazole chemosensors: Synthesis and application. **K.S. Aiken, S.M. Landge, D. Ghosh**

**4:00 ORGN 616.** Synthesis of alpha-tetra-substituted triazoles by silyl deprotection in tandem with catalytic azide cycloaddition. **Z.L. Paichak, P.T. Nguyen, C.H. Larsen**

**4:20 ORGN 617.** One-step catalytic synthesis of alkyl- and pyridyl-quinolines. **M. Sterling, C.H. Larsen**

**4:40 ORGN 618.** New strategies for radical additions to aromatic heterocycles. **R. Baxter**

### Section D

San Diego Convention Center  
Room 5B

#### Flow Chemistry & Continuous Processes

M. C. McIntosh, *Organizer*

M. G. Organ, *Presiding*

**2:00 ORGN 619.** Putting spin on flow chemistry. **J. Britton, C.L. Raston, G.A. Weiss**

**2:20 ORGN 620.** Self-optimizing flow reactors in pharmaceutical development for rapid process optimization. **N. Holmes, R.A. Bourne, J. Blacker, R.E. Meadows, R.L. Woodward**

**2:40 ORGN 621.** Combined chemo- and bio-catalysis for the dynamic kinetic resolution of chiral amines in continuous flow. **L.A. Thompson, J. Blacker, R.A. Bourne, N. Turner, W.R. Goundry**

**3:00 ORGN 622.** Flow chemistry: Reactor design, in-line analytics, and feedback control. **D. Mallik, M. Tilley, G. Li, P. Zhang, A.Q. Rutter, M.A. McGuire, M.G. Organ**

**3:20 ORGN 623.** Flow chemistry at Merck. **R. Ruck**

**3:40 ORGN 624.** Prebiotic flow synthesis of bioactive nucleoside precursors. **A.C. Evans, J. Kading**

**4:00 ORGN 625.** Bench-top resistively heated reactor for flow chemistry. **J. Rydfjord, J. Savmarker, M. Fagrell, M. Lahed**

### Section E

San Diego Convention Center  
Room 1A

#### Total Synthesis of Complex Molecules

M. C. McIntosh, *Organizer*

K. M. Maloney, *Presiding*

**1:00 ORGN 626.** Total synthesis of  $\gamma$ -hydroxybutenolide-containing acetogenins. **R. Muddala, R.P. Loach, J. Boukouvalas**

**1:20 ORGN 627.** Synthesis and biological evaluation of pharbinilic acid and derivatives as inhibitors of the NF- $\kappa$ B pathway. **J. Annand, P. Bruno, A.K. Mapp, C. Schindler**

**1:40 ORGN 628.** Withdrawn.

**2:00 ORGN 629.** Toward the total synthesis of the arcutine family of diterpenoid alkaloids. **K. Owens, M. Weber, R. Sarpong**

**2:20 ORGN 630.** New anhydride Mannich reaction: The total synthesis of bisavenanthramide B. **M.J. Di Maso, G. Nepomuceno, M.A. St. Peter, H. Gitre, N.P. Burlow, K. Martin, J.T. Shaw**

**2:40 ORGN 631.** Total synthesis of (-)-isolybin A. **B. McDonald, A.E. Nibbs, K. Scheidt**

**3:00 ORGN 632.** Phosphate tether-mediated, one-pot, sequential protocols for the synthesis of Sch725674, 13-desmethyl-lyngbouillose and corresponding simplified analogs. **S. Javed, M. Bodugam, A. Ganguly, J. Torres, R. Chegondi, P.R. Hanson**

**3:20 ORGN 633.** Synthetic studies towards spiroleucettadine. **R. Lamb, B. Hawkins**

**3:40 ORGN 634.** Development of a commercial manufacturing process for ceftiozane, the cephalosporin antibiotic found in Zerbaxa. **K.M. Maloney, G.R. Humphrey, M. McLaughlin, H. Ren**

### Section F

San Diego Convention Center  
Room 1B

#### Materials, Devices & Switches

M. C. McIntosh, *Organizer*

J. J. Reczek, *Presiding*

**1:00 ORGN 635.** Doubly N-confused hexaphyrin bis-metal complexes for near-IR optical materials. **M. Ishida, K. Ogasahara, H. Furuta**

**1:20 ORGN 636.** Withdrawn.

**1:40 ORGN 637.** Contractile polymers from the integrated motions of molecular machines and motors. **E. Moulin, G. Fuks, N. Giuseppone**

**2:00 ORGN 638.** Drug-based lipidic ionic liquids: A new class of biomaterials. **A. Mirjafari, R.A. O'Brien, R. Sykora, M. Sanchez Zayas, Y. Sheng**

**2:20 ORGN 639.** Dynamic and topological properties of dibrigehead diphosphines and their oxides. **S. Kharel, J. Bluemel, J.A. Gladysz**

**2:40 ORGN 640.** Rotational dynamics of a bulky triptycene rotator in organic solids and metal-organic frameworks (MOFs). **X. Jiang, H. Duan, M.A. Garcia-Garibay**

**3:00 ORGN 641.** Modular synthesis of luminescent and benchtop-stable, boron-containing PAHs. **V. Hertz, M. Wagner**

**3:20 ORGN 642.** Development of small molecule reagents for down-selection in point-of-need assays. **A.D. Brooks, S.T. Phillips**

**3:40 ORGN 643.** Design and synthesis strategies for small molecule and polymer amplification reagents. **T.J. Cordes, S.T. Phillips**

**4:00 ORGN 644.** Revisiting the potential for quinone-based diarylethene photochromes: A theoretical and experimental study on naphthoquinone diarylethenes for advanced organic materials. **D.G. Patel**

**4:20 ORGN 645.** Light powered ratchet. **L. Zhu, F. Tong, C. Salinas, M.K. Al-Muhanna, F. Tham, D.J. Kisailus, R.O. Al-Kaysi, C.J. Bardeen**

**4:40 ORGN 646.** Structural control of molecular aromatic charge-transfer liquid crystals leads to strongly dichroic organic films. **J.J. Reczek**

#### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Powering the Future: Novel Materials for Solar Cell Technologies

Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY

## WEDNESDAY EVENING

### Section A

San Diego Convention Center  
Hall F

#### Heterocycles & Aromatics

R. D. Broene, *Organizer*

**7:00 - 9:00**

**ORGN 647.** Cooking up a STORM: Synthesis and analysis of dyes for stochastic, optical reconstruction microscopy (STORM). **D. Jenkinson, S. Jones, A. Cadby**

**ORGN 648.** Comparing Dowex to sulfuric acid as catalysts for the synthesis of benzyl acetate. **L.J. Brissette, D. Baker**

**ORGN 649.** Heterobiaryl as winding-vine shaped molecular asymmetry. **A. Mori, Y. Okayama, Y. Toyomori, K. Maruhashi, D. Matsuoka**

**ORGN 650.** Expedient synthesis of 1,3-oxazinones. **B. Hawkins**

**ORGN 651.** 7-Hydroxy-8-(2-hydroxynaphthalen-1-yl)quinoline: A new member of the azaBINOL family with superior configurational stability and solubility to 7,7'-dihydroxy-8,8'-biquinoyl. **S. Banerjee, P.R. Blakemore**

**ORGN 652.** Diastereoselective one-pot synthesis of endoperoxide containing 1,2,4-dioxazinanes. **M. Abdel, R. Marfatia, H. Sharma, D.M. Rubush**

**ORGN 653.** Regioselective lithiation of various substituted pyridines. **M.B. Alshammari**

**ORGN 654.** Triple benzannulation of naphthalene via a 1,3,6-naphthotriyne synthetic equivalent: Synthesis of dibenz[a,c]anthracene. **E.O. Onyango, P.Z. Mannes, E.E. Kim, G.W. Gribble**

**ORGN 655.** Novel oxygen transfer chemistry to "impossible" sites using HOF/CH<sub>3</sub>CN. **S. Rozen**

**ORGN 656.** Synthesis of 1,2,3-triazole-based bent core nematic liquid crystals via microwave mediated "click reaction". **K. Wang, R. Twieg, A. Jakli, J.T. Gleeson, S. Sprunt**

**ORGN 657.** Highly regioselective nitration of toluene over reusable zeolite H $\beta$ . **M.H. Alotaibi, K. Smith, G.A. El-Hiti**

**ORGN 658.** Synthesis of piperazine-containing systems via a two-step amidation-intramolecular alkylation with N-substituted-2-chloro-ethan-1-amine. **T.P. Tran, C. Wright**

**ORGN 659.** Green synthesis of 5,5-phenylhydantoin. **V. Sublett, D.J. Swartling**

**ORGN 660.** Synthesis and photochemical characterization of water-soluble pegylated hydroporphyrins. **M. Liu, N. Zhang, J. Jiang, C. Chen, A. Mandal, D. Holten, D.F. Bocian, J.S. Lindsey**

**ORGN 661.** Effect of  $\sigma$ - $\pi$  conjugation between Si-Si bond and pyridine ring in tris(trimethylsilyl)pyridine on its spectroscopic property and SN<sub>2</sub> reaction with methyl iodide. **W. Ichinose, H. Abe, S. Shuto**

**ORGN 662.** Recyclable triethylamine and organophosphane: Synthesis of highly functionalized furan derivatives via catalytic Wittig reaction. **C. Lee**

**ORGN 663.** Synthesis of catechol analogs. **C.L. Echevarria Maldonado, A. Batista Parra**

**ORGN 664.** Benzo[4,5]imidazo[2,1-b]quinazolin-12-ones and benzo[4,5]imidazo[1,2-a]pyrido[2,3-d]-pyrimidine-5-ones by a sequential N-acylation-S<sub>N</sub>Ar reaction. **K. Gnanasekaran, N. Muddala, R.A. Bunce**

**ORGN 665.** Studies on the vinylogous SNAr reaction. **R.A. Bunce, K. Gnanasekaran, J. Yoon**

**ORGN 666.** Synthesis of a PAH-porphyrin hybrid. **R. Gao, T.D. Lash**

**ORGN 667.** Synthesis of 3-hydroxybenzoxazoles via Mitsunobu-triggered, chromatography-free heterocyclizations of salicylhydroxamic acids. **D. Van Eker, J. Chauhan, L. Chen, S. Fletcher**

**ORGN 668.** Towards covalent organic cages derived from expanded porphyrins. **T. Sarma, H. Zhang, A.D. Lammer, J.L. Sessler**

**ORGN 669.** Effect of cyclopentadienyl ligands on alkene isomerization catalysts. **P.J. Brklycica, E.R. Paulson, D.B. Grotjahn**



- ORGN 670.** Heterocycle synthesis via oxidative cyclization reactions of nucleophile-containing oxime derivatives. **J. Dang**, A.S. Alshreimi, P. De Lijser
- ORGN 671.** Short, green synthesis of proton pump inhibitors. **I. Larraza, E.D. Clutter**
- ORGN 672.** Towards the biological enhancement of ferrocenyl derivatives: An improvement with heterocyclic moieties. **J.C. Aponte-Santini**, I. Montes, J. Dávila-Calderón, D.J. Sanabria Rios, A. Molina-Villarino, A.R. Guadalupe Quinones, E. Colón-Lorenzo, A. Serrano, F.T. Halaweish, V. Washington
- ORGN 673.** Ferrocenyl chalcones salts derivatives as potential antimalarial agents. **S.M. Delgado-Rivera**, G.E. Pérez-Ortiz, I. Montes-González, A.R. Guadalupe-Quinones, E. Colón-Lorenzo, A. Serrano
- ORGN 674.**  $\beta$ -Lactams as anticancer agent: Design, synthesis, and biological evaluation. **D. Bandyopadhyay**, J.M. Rock, O. Espino, V.M. Cano, M.F. Subedar, J. Galindo, B. Serrata, M. Tupper, R. Nandipaty, F.A. Padilla
- ORGN 675.** Microwave-assisted, new green route toward chromeno[4,3-b]chromen-6(7H)-one. **D. Bandyopadhyay**, V.M. Cano, I.M. Chapa, A. Velasco, J.M. Rock
- ORGN 676.** Stereo-, regio-, and site-selective 1,3-dipolar cycloaddition of conjugated dienes. **J. Clark**, S.T. Diver
- ORGN 677.** Aminoalcohols derived from phenanthroline and phenanthrene epoxides as potential sensors for nerve agents. **D.L. Sellers**, N. Kapolka, L. Kohler, E. Schoffers, H. Marshall
- ORGN 678.** Withdrawn.
- ORGN 679.** Azulene-modified polysiloxane for use as a gas chromatography stationary phase. **M. Jackson**, J. Schaffer, C.M. Garner
- ORGN 680.** Concise synthesis of structurally diverse, *P*-stereogenic bicyclic phosphoramidates by ring-closing metathesis. **J. Torres**, S. Javed, P.R. Hanson
- ORGN 681.** One-pot, sequential enyne ring-closing metathesis/Diels-Alder protocol for the synthesis of bi- and tricyclic phosphorus heterocyclic compounds. **A. Ganguly**, S. Javed, J. Torres, M. Bodugam, M.A. Khan, P.R. Hanson
- ORGN 682.** Electrophilic sultams: Synthesis and reactivity. **M.A. Khan**, Q. Zang, E. Gao, J. Loh, N. Asad, P.R. Hanson
- ORGN 683.** Study on synthesis of thiadiazolic derivatives. **J. Jenis**, L. Zhaimuhambetova, M. Dyusebaeva
- ORGN 684.** Development of water-soluble and highly photosensitive 8-azacoumarin-4-ylmethyl-type photolabile-protecting groups for dynamic analysis of bioactive molecules. **H. Takano**, T. Narumi, W. Nomura, T. Furuta, H. Tamamura
- ORGN 685.** Cyclic alkynes as useful synthetic building blocks. **J. Medina**, T. McMahon, B. Simmons, N.K. Garg
- ORGN 687.** Sulfonimidation via ring-opening of 2-oxazolines with acidic sulfonimide nucleophiles. **D. Gutierrez**, D.R. Dean, C.M. Laxamana, M. Migliozzi-Smith, **C.J. O'Brien**, C.L. O'Neill, J. Li
- ORGN 688.** Study on ring-opening addition reaction of an epoxide intermediate in efinaconazole (KP-103) manufacturing. **M. Watanabe**, T. Yamada, M. Mimura
- ORGN 689.** Withdrawn.
- ORGN 690.** Suzuki coupling of diaryl tellurides for the synthesis of unsymmetrical biaryl compounds. **J. Jin**, M. Lolla, S. Zhang, C. Yen, D. Whipple
- ORGN 691.** Palladium-catalyzed Sonogashira reactions of diaryltellurides. **S. Zhang**, C.K. Aileni, P. Siraswal, J. Jin
- ORGN 692.** Visible-light-mediated oxidation of hydroxylamines: A new pathway to indole synthesis. **L. Baldwin**, N. Zheng
- ORGN 693.** Redox behavior of  $\alpha$ -amino allenylphosphonates: From  $\alpha$ -amino vinylphosphonates to spirodienone lactams. **P. Adler**, A. Fadel, **N. Rabasso**
- ORGN 694.** Palladium-catalyzed decarboxylative vinyltrifluoromethylation of aryl halides. **K. Suppan**
- ORGN 695.** Synthesis and biological activity of beta-substituted tryptamines. **K.M. Maiden**, J. Kidd, J.B. Morgan
- ORGN 696.** Novel approaches to the chemical syntheses of new functionalized tetracyanoquinodimethanes and precursors. **E.J. Parish**, M. Hsiao, **H. Honda**, T. Wei
- ORGN 697.** Efficient synthesis of *N*-arylamino benzamide as a MEK inhibitor. **T. Ikeda**, M. Murakata
- ORGN 698.** [3+2] [3+2] Cycloaddition/rearrangement of electron-poor alkenes with activated and unactivated alkynes/cycloaddition/rearrangement of electron-poor alkenes with activated and unactivated alkynes. **E. Donckele**, F.N. Diederich
- ORGN 699.** Selective cyclization of ambident nitronate anions: C- vs. O-alkylation. **V. Perez**, **N. Rabasso**, A. Fadel
- ORGN 700.** Cyclization studies of intermediates derived from aromatic silyl ketones. **E.D. Li**, L.M. Bradley
- ORGN 701.** Preparation of *t*-butyldimethylphosphine borane and *t*-butyldiethylphosphine borane by selective Grignard reagent substitution of phosphorus trichloride. **A.G. Butterfield**, M.B. Prater, **N.S. Werner**
- ORGN 702.** Palladium catalyzed cyclopropanation reactions of ketone enolates. **D. Sun**, T. Dwight, M.E. Jung
- ORGN 703.** Using ring strain to control 4 $\pi$  electrocyclic reactions: Torquoselectivity in ring closing of medium ring dienes and ring opening of bicyclic cyclobutenes. **B.A. Boon**, A. Green, P. Liu, K.N. Houk, C.A. Merlic
- ORGN 704.** Withdrawn.
- ORGN 705.** Reactions of alkynyl- and 1,1'-dialkylferrocenes with tetracyanoethylene (TCNE): Unanticipated TCNE addition at the less electron-rich of two triple bonds. **H. Butenschoen**, N. Krausse, M. Kielmann, J. Ma
- ORGN 706.** Synthesis of enantioenriched  $\beta$ -substituted tryptamine derivatives. **K. Van Hecke**, H. Rubin, J. Mills, J. Cockrell, J.B. Morgan
- ORGN 707.** Lignin depolymerization strategy using visible-light photoredox catalysis. **G. Magallanes**, M.D. Kaerkaes, B. Matsuura, C. Stephenson
- ORGN 708.** Novel method for the synthesis of highly substituted hydroxylamines. **S. Dhanju**, D. Crich
- ORGN 709.** Withdrawn.
- ORGN 710.** Bio-inspired, catalytic *E* $\rightarrow$ Z isomerization and photo-cascade cyclization of activated olefins: A facile route to functionalized coumarins. **J.B. Metternich**, R. Gilmour
- ORGN 711.** Preparation of  $\alpha$ -hydroxy esters, propargylic, and allylic cyanohydrins for ISNC reactions. **J. Stevens**, J.L. Duffy-Matzner
- ORGN 712.** Cyclopropanol rearrangements in diastereoselective syntheses of novel peptide isosteres. **C.K. Zercher**, D. Bhogadhi, R. Chhetri, K. Bala
- ORGN 713.** Intramolecular [4+2]-cycloaddition between a 1,3-diene and a diazo ester. **H. Qiu**, M. Doyle
- ORGN 714.** Oxidative esterification via photocatalytic C-H activation using oxo-vanadium VO@o-C<sub>3</sub>N<sub>4</sub> catalyst. **S. Verma**, N.R. Baig, M. Nadagouda, R.S. Varma
- ORGN 715.** Nickel-catalyzed Suzuki-Miyaura coupling of amides. **N.A. Weires**, E.L. Baker, N.K. Garg
- ORGN 716.** Carbon-carbon bond formation between cyclobutylalanines and tetrahydrofuran using a titanium based photocatalyst. **M.G. Calaway**, N. Zheng
- ORGN 717.** Diamidation of unsaturated  $\alpha$ -alkyl hydroxamates: A versatile approach to intra/intermolecular alkene diamination. **D.J. Wardrop**, A. Sinha, D. Dickson, M. Gerasimov, A. Sussman
- ORGN 718.** Lewis-base catalyzed regioselective chlorination of activated aromatic compounds. **S.M. Maddox**, J. Gustafson
- ORGN 719.** Novel syntheses of (Z)- $\beta$ -amino  $\alpha$ -substituted- $\alpha,\beta$ -unsaturated amides and via rearrangement or replacement reaction. **X. Liu**, H. Cao, W. Yi
- ORGN 720.** Redox-triggered  $\alpha$ -C-H functionalization of pyrrolidines: Synthesis of unsymmetrically 2,5-disubstituted pyrrolidines. **Y. Cheng**, Q. Jin
- ORGN 721.** 1,N-rearrangement of allylic alcohols promoted by hot water: Application to the synthesis of navenone B, a polyene natural product. **L. Peifang**
- ORGN 722.** New mode of chiral recognition for the chiral resolution of lactols. **X. Company**, J. Bures
- ORGN 723.** Alkene *anti*-dihydroxylation with malonyl peroxides. **C. Alamillo Ferrer**, N.C. Tomkinson
- ORGN 724.** New synthetic methods for the rapid synthesis of biologically active biaryl scaffolds. **R. Watson**
- ORGN 725.** Synthesis and evaluation of unsymmetrical single-isomer rhodamine dyes for use in immunoassays and super-resolution imaging. **R.A. Haack**, S. Gayda, Q. Ruan, K.M. Swift, J.P. Skinner, P.J. Macdonald, R. Himmelsbach, S. Tetin
- ORGN 726.** Chemo- and site-selective azide reductions with heterogeneous nanoparticle catalysts. **H. Nazari**, V.R. Udumula, D. Michaelis
- ORGN 727.** Intramolecular carbonyl-ene reactions catalyzed by a triflylphosphoramidate. **L. Davis**, M. Santos, H. Dahlmann, A. McKinney
- ORGN 728.** Synthesis of substituted 1,4-cyclohexadienes via a regioselective Diels-Alder reaction of conjugated 2,4-dienones. **K. Hamal**
- ORGN 729.** Synthesis of highly functionalized chromones by tandem Friedal-Crafts acylation/oxo-Michael addition/elimination process. **R. Bam**
- ORGN 730.** Preparation and reactivity of activated IBA-OTf reagent. **A. Yoshimura**, K.C. Nguyen, S. Klasen, A. Saito, V. Nemykin, V.V. Zhdankin
- ORGN 731.** Synthesis of acerogenin C, acerogenin L and galeon derivatives of for the development of anticancer therapeutics. **A.M. Rahman**, Y. Lu, W. Yin, Y. Jahng
- ORGN 732.** Electrophilic amidation using novel saccharin-based  $\mu$ -oxo imidoiodane. **J. Fuchs**, S.R. Koski, A. Yoshimura, A. Saito, V. Nemykin, V.V. Zhdankin
- ORGN 733.** Use of silane protecting groups for intramolecular hydride transfer and use in stereoselective syntheses. **N.S. Jackson**, Z.E. Nichols, C. Nicholson
- ORGN 734.** Withdrawn.
- ORGN 735.** Direct N-formylation of amines with N,N-dimethylformamide facilitated by water and oxygen. **C.M. DeAngelo**, **N.A. Petasis**
- ORGN 736.** Bridged polycyclic silanes: Structure-reactivity studies for the development of synthetic applications. **C.M. Poteat**, C.L. Brantley, T.C. Coombs
- ORGN 737.** Use of 2-bromocyclohexenone as an intermediate toward the preparation of a dual Michael acceptor. **A. Glass**, D.A. Hunt
- ORGN 738.** Preparation and utility of highly functionalized 2-aminobenzophenones. **A. Grossman**, D.A. Hunt
- ORGN 739.** Reactions of HPPH<sub>2</sub> with cyclopalladated complexes resulting in ligand phosphination. **J. Kukowski**, I.P. Smoliakova, V.A. Stepanova
- ORGN 740.** Rapid versification of the chlorodifluoromethyl group on arenes and heteroarenes. **R. McAtee**, J. Beatty, C. Stephenson
- ORGN 741.** Withdrawn.
- ORGN 742.** Novel reaction of ArCOPdCl species and tertiary alcohols for highly substituted esters. **M. Al-Masum**, **C. Snagg**, S.L. Chrisman
- ORGN 743.** Ru-catalyzed C2-H silylation of gramines, tryptamines and related (hetero) arenes. **K. Devaraj**, C. Sollert, C. Judds, P.G. Gates, L.T. Pilarski
- ORGN 744.** Development of an indium-mediated radical addition to heteroarenes. **J. Starr**, M. Glucini, J. Chen, D.P. Uccello
- ORGN 745.** Lewis acid-catalyzed formation of functionalized cyclopentadienes. **C. McAtee**, J. Ludwig, C. Schindler
- ORGN 746.** One-pot, four-component green synthesis of medicinally privileged pyranopyrazoles. **D. Bandyopadhyay**, S.S. Huerta, A. Pardo, O. Espino
- ORGN 747.** Synthesis of spiro indole-3,1'-naphthalene tetracyclic system: A green approach. **D. Bandyopadhyay**, J.C. Salinas, O. Espino
- ORGN 748.** Uncatalyzed synthesis of N-carboxyanhydrides with diphosgene at room temperature. **J.E. Semple**, B. Sullivan
- ORGN 749.** Synthesis and design of organoferrous compounds as anti-tumor agents. **C. Hoong**, J.M. O Connor, M. Aubrey, N.C. Gianneschi, M.T. Proetto
- ORGN 750.** Mild organocatalytic sulfenylation of electron-rich heterocycles. **C.J. Nalbandian**, E. Miller, J. Gustafson
- ORGN 751.** New developments of the asymmetric vinyllogous Mukaiyama aldol reactions. **A.S. Kanner**, N. Kohnen, J. Garcia, B. Banasik, L. Wang, M.B. Bergdahl
- ORGN 752.** Synthesis of potassium trifluoroalkylphosphonates via hydroboration of vinylphosphonates. **L. Daley**, **K. Alanqari**, B. Manookian, T.E. Cole

Section B

San Diego Convention Center  
Hall D

New Reactions & Methodology

R. D. Broene, *Organizer*

7:00 - 9:00

**ORGN 686.** Sulfate radical anion (SO<sub>4</sub><sup>-</sup>) mediated C(sp<sub>3</sub>)-H nitrogenation/oxygenation in N-aryl benzylic amines. **K. Tummalapalli**

- ORGN **753.** Alkylation of acids, alcohols, and phenols using N-1-adamantyl-O-isopropyl-4-nitrobenzenesulfonimide. **H. Nguyen, T.J. Maricich, F.S. Hussain, L. Digal**
- ORGN **754.** Synthesis of amino alkyltrifluoroborate compounds via hydroboration. **S. Singh, R. Newman, N. Felix, T.E. Cole**
- ORGN **755.** Enantioselective silver-catalyzed propargylation reactions of *N*-sulfonyl ketimines. **T. Endean, C. Osborne, E.R. Jarvo**
- ORGN **756.** Synthesis of fused benzo[4,5]imidazo[1,2-*a*]pyrimidin-2-yl)methanone derivatives using copper-catalyzed aerobic oxidation via tandem approach. **S.R. Kotla, K. Parang, R.K. Tiwari**
- ORGN **757.** Toward a method for synthesis of allylic tosylates. **C. Paquin, D.W. Boerth**
- ORGN **758.** Bulky silane, tri-*tert*-butoxychlorosilane, for the protection and alkylation of primary amines. **M.T. Wentzel, K. Fuetmann, L.J. Moloney, T. Hoye**
- ORGN **759.** Redox-neutral decarboxylative halogenation of carboxylic acids via photoredox catalysis. **A. Sun, J.W. Beatty, M. Frias Rodriguez, C. Stephenson**
- ORGN **760.** Catalytic methods for rapid access to alpha-tetrasubstituted amines. **K.G. Nelson, Z.L. Palchak, C.H. Larsen**
- ORGN **761.** Novel synthesis of lanost-8-en-3 $\beta$ -ol-7,11-dione, an inhibitor of cholesterol biosynthesis. **E.J. Parish, Y. Lo, H. Honda, T. Wei**
- ORGN **762.** Novel approaches to the chemical synthesis of methylhydrazineacetic acid for inhibitory activity against bacteria. **E.J. Parish, H. Honda, T. Wei, H. Shyu**
- ORGN **763.** Novel approaches to the chemical synthesis of  $\beta$ -lactam azetidionones from amino acids by intramolecular condensation using a condensing reagent. **E.J. Parish, J. Wu, H. Honda, T. Wei**
- ORGN **764.** Flipped etherification method: Reactions between enolates and peroxides. **M. Locklear, P. Dussault**
- ORGN **765.** Total solar synthesis of ibuprofen. **D.J. Swartling, B. Agee, G.A. Mullins**
- ORGN **766.** Synthesis of oxacycles via reaction of stabilized carbanions with peroxides. **A. Horn, P.H. Dussault**
- ORGN **767.** Withdrawn.
- ORGN **768.** Amidation of aminoisobutyric acid using oxazolone as a synthetic tool. **M. Jo, H. Choi, Y. Kwak**
- ORGN **769.** One-pot, sequential ring opening and  $S_NAr$ : From aziridine to 10- and 11-membered benzo-fused sultams. **J. Jun**
- ORGN **770.** Oxidative addition of low-valent transition metals to *meso*-aziridines. **E. Timpy, J.B. Morgan**

THURSDAY MORNING

Computational Materials & Nanoscience: Theory Meets Experiment

Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY

PHYS

Division of Physical Chemistry

G. Engel, Program Chair

OTHER SYMPOSIA OF INTEREST:

Chemical Imaging: Applications, Advances, & Challenges (see ANYL, Wed, Thu)

Time-Dependent Dynamics & Electronic Excited States (see COMP, Wed, Thu)

Directed Polymer Assembly (see PMSE, Sun, Mon)

Catalytic Processes at Interfaces: Fundamentals & Applications (see CATL, Wed, Thu)

Catalysis at the Sub-Nanometer Scale (see CATL, Sun, Mon)

Nanomaterials for Energy Conversion & Storage (see ENFL, Mon, Tue, Wed)

SUNDAY MORNING

Section A

San Diego Convention Center Room 29A

Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events

R. Elber, R. M. Levy, C. F. Wong, D. M. Zuckerman, Organizers  
L. T. Chong, Presiding

8:00 **PHYS 1.** Recent techniques for acceleration and interpretation of molecular dynamics simulations. **E. Vanden-Eijnden**

8:30 **PHYS 2.** Markov models at multiple thermodynamic states with applications to protein-ligand complexes. **F. Noe**

9:00 **PHYS 3.** Markovian MD simulations for computing on- and off-rates. **T. Yu, A. Bucci, E. Vanden-Eijnden, C.F. Abrams**

9:30 Intermission.

9:45 **PHYS 4.** Advancements in milestone: Computational speedup by re-weighting artificially accelerated trajectories and venturing into the non-equilibrium with coarse-grained random walks in milestone space. **G. Grazioli, I. Andricioaei**

10:15 **PHYS 5.** Improved estimation of long-time kinetics using non-Markovian analysis of trajectory segments: Application to protein folding and unfolding. **E. Suarez, D.M. Zuckerman**

10:45 Intermission.

11:00 **PHYS 6.** Multiscale estimation of binding kinetics using molecular dynamics, Brownian dynamics, and milestone. **R.E. Amaro, L. Votapka**

11:30 **PHYS 7.** Exact milestone. **J.M. Bello-Rivas, R. Elber**

Section B

San Diego Convention Center Room 28C

Decoding the Spectroscopic Signatures of Large Amplitude Motions: Challenges & Opportunities for Theory & Experiment

Z. Bacic, Organizer  
M. A. Johnson, Organizer, Presiding

8:00 **PHYS 8.** Using diffusion Monte Carlo to decode spectral signatures of large amplitude motions in molecules and ions. **A.B. McCoy, A.S. Petit, Z. Lin, J. Ford, M. Marlett**

8:40 **PHYS 9.** Case studies of spectral consequences of delocalized zero-point motion. **J.M. Bowman**

9:20 **PHYS 10.** Withdrawn.

10:00 Intermission.

10:20 **PHYS 11.** First-principles anharmonic computational spectroscopy of peptides: Determination of the 3D structures of conformers. **R.B. Gerber, T. Roy**

10:40 **PHYS 12.** Assessing internal energy in gas-phase cluster ions: Measurement, modeling and structural effects. **J.M. Lisy**

11:00 **PHYS 13.** Imaging bond breaking and vibrational energy transfer in hydrogen-bonded clusters. **A.K. Samanta, K. Zuraski, D. Kwasniewski, H. Reiser**

11:40 **PHYS 14.** Dissociative photodetachment dynamics of cold negative ions. **R.E. Continetti**

Section C

San Diego Convention Center Room 28D

Electrochemistry at Solid/Liquid Interfaces

Y. Qi, Organizer  
O. Borodin, Organizer, Presiding

8:00 Introductory Remarks.

8:05 **PHYS 15.** Considering the electrochemical environment in the first-principles modeling of electrocatalytic processes. **A. Gross, S. Sakong, F. Gossenberger, T. Roman**

8:45 **PHYS 16.** Modelling heterogeneous electrocatalysis under realistic conditions. **S.N. Steinmann, C. Michel, P. Sautet**

9:05 **PHYS 17.** Model free method to measure the surface potential of colloidal particles in aqueous solution. **C. Luetgebaucks, G. Gonella, S. Roke**

9:45 **PHYS 18.** Microscopic dynamics of charge separation at the aqueous electrochemical double layer. **A. Willard, J.A. Kattirtzi, D. Limmer**

10:05 Intermission.

10:20 **PHYS 19.** Electrochemical reduction, ionization, and solvation of Brønsted acids in ionic liquid solutions. **L. Yu**

10:40 **PHYS 20.** Ultrafast spectroelectrochemistry. **S. Toyouchi, Y. Sun, D.D. Dlott, N. Garcia Rey**

11:00 **PHYS 21.** Potential dependent IR/visible double resonance sum frequency generation spectroscopy to probe electronic structure at electrochemical interfaces. **K. Uosaki, H. Noguchi, S. Yang**

11:20 **PHYS 22.** Nanoscale Li-S battery interfaces investigated with in-situ electrochemical transmission electron microscopy. **K. Jungjohann, K.L. Harrison, A. Leenheer, N. Hahn, K.R. Zavadil**

Section D

San Diego Convention Center Room 28E

Frontiers in Solar Light Harvesting Processes

T. Krauss, A. Mohite, O. V. Prezhdo, S. Tretiak, Organizers

V. D. Kleiman, Presiding

8:00 Introductory Remarks.

8:05 **PHYS 23.** Can we really be inspired by natural light-harvesting systems to convert solar energy? Some answers from multiscale models based on quantum chemistry. **B. Mennucci**

8:45 **PHYS 24.** Molecular level design principles for efficient and robust light harvesting in LH2 of purple bacteria. **S. Jang**

9:25 **PHYS 25.** Importance of excitation and trapping conditions in photosynthetic energy transport. **R. Leon-Montiel, I. Kassal, J.P. Torres**

9:45 Intermission.

10:10 **PHYS 26.** Correlating the photophysics of organic-inorganic perovskites with local chemistry. **S.D. Stranks**

10:50 **PHYS 27.** The effects of electronic impurities and electron-hole recombination dynamics on large grain organic-inorganic perovskite photovoltaic efficiencies. **J. Blaccon, W. Nie, A.J. Neukirch, G. Gupta, S. Tretiak, L. Cognet, A. Mohite, J. Crochet**

11:30 **PHYS 28.** Dye-sensitized bipolar ion-exchange membranes as artificial light-driven ions pumps for use in solar fuels devices. **R.S. Reiter, W. White, C.D. Sanborn, S. Ardo**

Section E

San Diego Convention Center Room 29B

Physical Chemistry of Complex Environmental Interfaces

Cosponsored by COLL

V. H. Grassian, Organizer

G. M. Nathanson, Organizer, Presiding

8:00 **PHYS 29.** Fundamental studies of sea spray aerosol composition and climate properties using an ocean-in-the-laboratory approach. **K.A. Prather**

8:40 **PHYS 30.** Selectivity in the enrichment of organic molecules in sea spray aerosol. **R. Cochran, T. Jayarathne, H. Morris, A.V. Tivanski, E.A. Stone, V.H. Grassian**

9:00 **PHYS 31.** Aerosol emissions at the ocean-atmosphere interface: The PlanetSolar Deep Water Expedition. **M. Beniston, N. Berti, V. Djambazova, E. Gascon-Diaz, C. Hassler, R. Houlman, B. Ibelings, J. Kasparian, D. Kiselev, A. Le, T. Magouroux, M. Moret, T. Neri, D. Palomino, S. Pfander, G. Sousa, D. Stadler, F. Tettamanti, J. Wolf**

9:40 Intermission.

10:00 **PHYS 32.** Exploring the nature of indoor oxidative multiphase chemistry. **J.P. Abbatt**

10:40 **PHYS 33.** Influence of organic matter and biological activity on the surface chemical composition and physical properties of sea spray aerosols. **C. Sultana, C. Lee, D.B. Collins, K.A. Prather**

11:00 **PHYS 34.** Recent multiphase aerosol chemistry studies: Laboratory and model developments. **H. Herrmann, T. Schaefer, T. Otto, L. Schöne, H. LePhuoc, X. Li, J. Schindelka, A. Tilgner, E. Hoffmann**

**11:40 PHYS 35.** Complex mineral-organic-water interface and environmental fate of arsenicals. **H.A. Al-Abadleh**, A. Situm, S.R. Goldberg, N. Allen, N. Kabengi

## Section F

San Diego Convention Center  
Room 29C

### Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory

#### Active Sites

*Cosponsored by BIOL*

H. S. Shafaat, *Organizer*

S. Stoll, *Organizer, Presiding*

K. M. Lancaster, *Presiding*

**8:30 PHYS 36.** Many-electron quantum chemistry in enzymes. **G.K. Chan**

**9:05 PHYS 37.** Engineering nickel-substituted azurin for energy conversion reactions. **A. Manesis**, M. O'Connor, H.S. Shafaat

**9:25 PHYS 38.** DFT and molecular dynamics for oxygen activation and proton pumping in the catalytic cycle of cytochrome c oxidase. **L. Noodleman**, W. Han Du, L. Yang, A. Skjævik, A.W. Goetz, R.C. Walker

**9:45 PHYS 39.** Paramagnetic resonance methods and enzymatic [e<sup>-</sup>H<sup>+</sup>]/[H] addition & extraction. **B.M. Hoffman**

**10:20** Intermission.

**10:40 PHYS 40.** Enzymatic chemistry with radicals and cyanide and carbon monoxide, be careful there! **R.D. Britt**

**11:15 PHYS 41.** Theoretical study of dynamics at intersystem crossings in the active sites of metal-sulfur proteins. **S.A. Varganov**, D. Kaliakin, A.O. Lykhin, G.E. dePolo

**11:35 PHYS 42.** Origins of stereoselectivity in evolved ketoreductases. **E.L. Noey**, N. Tibrewal, G. Jimenez-Oses, S. Osuna, J. Park, C. Bond, D. Cascio, J. Liang, X. Zhang, G.W. Huisman, K.N. Houk

## Section G

San Diego Convention Center  
Room 29D

### Towards Predictive Calculations in Strongly Correlated Molecules & Materials

T. C. Berkelbach, E. Neuscamman, *Organizers*

G. E. Scuseria, *Presiding*

**8:00 PHYS 43.** Applications of density matrix renormalization group algorithm-based multireference correlation theories. **Y. Kurashige**

**8:45 PHYS 44.** Low-rank tensor approximations for many-electron wavefunctions in Hilbert space. **Z. Li**, G.K. Chan

**9:10 PHYS 45.** Active space decomposition for excited states and strongly correlated electronic structure. **T. Shiozaki**

**9:55** Intermission.

**10:15 PHYS 46.** Ab initio quantum chemistry for multiradical molecules: A spin-flip approach. **N. Mayhall**, M.P. Head-Gordon

**11:00 PHYS 47.** PySCF: A novel open-source computational tool for the electronic structure problem. **Q. Sun**

### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

#### Protein-Ligand Binding & Dynamics

*Sponsored by COMP, Cosponsored by PHYS*

## Multiscales Chemistry

### Energy

*Sponsored by MPPG, Cosponsored by ANYL, BIOL, COMP and PHYS*

### Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications

*Sponsored by COMP, Cosponsored by CATL and PHYS*

## SUNDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 29A

### Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events

R. M. Levy, C. F. Wong, D. M. Zuckerman, *Organizers*

R. Elber, *Organizer, Presiding*

**1:30 PHYS 48.** Increasing the power of accelerated molecular dynamics methods. **A.F. Voter**

**2:00 PHYS 49.** Exploring rare events in proteins with adaptive molecular dynamics. **C. Clementi**

**2:30 PHYS 50.** Characterization of the GroEL – GroES interface and the mechanism of reversible chaperonin association. **P.J. Rossky**

**3:00** Intermission.

**3:15 PHYS 51.** WESTPA: An interoperable, highly scalable software package for weighted ensemble simulation and analysis. **L.T. Chong**

**3:45 PHYS 52.** Insight into folding, binding, and peptidomimetic design from molecular simulations and kinetic network models. **V.A. Voelz**, A. Razavi, S. Mukherjee, G.A. Pantelopulos, G. Zhou

**4:15** Intermission.

**4:30 PHYS 53.** Modeling density fluctuations and thermodynamics of membranes with milestone. **A.E. Cardenas**, R. Elber

**5:00 PHYS 54.** Large scale studies of molecular binding processes on computational grids and heterogeneous hardware resources. **E. Gallicchio**, B. Zhang, D. Kilburg, R. Kumar Pal, H. Tancredi, J. Xia, . Flynn, A. Montes, N. Deng, R.M. Levy

### Section B

San Diego Convention Center  
Room 28C

### Decoding the Spectroscopic Signatures of Large Amplitude Motions: Challenges & Opportunities for Theory & Experiment

M. A. Johnson, *Organizer*

Z. Bacic, *Organizer, Presiding*

**1:30 PHYS 55.** Vibrational spectral signatures of an excess proton in water clusters. **K.D. Jordan**, T. Odbadrakh, C. Wolke, J. Fournier, M.A. Johnson

**2:10 PHYS 56.** Dissecting the vibrational spectra of water from the gas to the condensed phase through many-body molecular dynamics simulations. **F. Paesani**

**2:50 PHYS 57.** Ion microsolution probed by cryogenic ion trap vibrational spectroscopy. **K.R. Asmis**

**3:30** Intermission.

**3:50 PHYS 58.** Attaching water clusters to aromatic solutes: Spectroscopic signatures of large-amplitude motions and Fermi resonance in the OH stretch region. **D.P. Tabor**, R. Kusaka, P.S. Walsh, E.L. Sibert, T.S. Zwier

**4:30 PHYS 59.** Using vibrational spectra to probe structure and local environment. **E.L. Sibert**, D.P. Tabor, J. Korn, D.M. Hewett, T.S. Zwier

**5:10 PHYS 60.** Withdrawn.

## Section C

San Diego Convention Center  
Room 28D

### Electrochemistry at Solid/Liquid Interfaces

O. Borodin, Y. Qi, *Organizers, Presiding*

**1:30 PHYS 61.** Carbon-electrolyte interfaces and their effect on capacitive energy storage. **B. Dyatkin**, K. Van Aken, E. Mamontov, N. Osti, H. Wang, J. Black, G. Feng, Y. Zhang, M.K. Thompson, P.T. Cummings, D. Wesolowski, **Y. Gogotsi**

**2:10 PHYS 62.** *Ab initio* simulations of charged interface effects in graphene-based supercapacitors. **B. Wood**

**2:50 PHYS 63.** Dynamic charge storage in nanopores filled with ionic liquids. **R. Qiao**, Y. He, A.A. Kornyshev, J. Huang, B. Sumpter

**3:30** Intermission.

**3:40 PHYS 64.** Capacitance of graphene-based electrodes from combined first principles and classical simulations. **C. Zhan**, J. Neal, Y. Zhang, J. Wu, P.T. Cummings, D. Jiang

**4:00 PHYS 65.** In-situ study of electric double layers and ionic transport across the solid/liquid interface using scanning probe microscopy. **J. Come**, J. Black, N. Balke

**4:20 PHYS 66.** Modeling charge transfer and dielectric response of atomistic and continuous media. **M.H. Muser**

**5:00 PHYS 67.** Ionic liquids at charged interfaces: Static and dynamic properties from atomistic simulations. **J. Vatamanu**, D. Bedrov

## Section D

San Diego Convention Center  
Room 28E

### Frontiers in Solar Light Harvesting Processes

T. Krauss, O. V. Prezhdo, S. Tretiak, *Organizers*

A. Mohite, *Organizer, Presiding*

**1:30 PHYS 68.** Chemistry of making and breaking of perovskites. **P.V. Kamat**

**2:10 PHYS 69.** Hysteresis-free large-area crystalline perovskite solar cells via temperature controlled doctor blading in ambient conditions. **G. Gupta**, A. Mallajosyula, S. Bhatt, W. Nie, A. Mohite

**2:50 PHYS 70.** Layered perovskite solar cells with 11.2 % efficiency, superior crystallinity and environmental stability. **H. Tsai**, W. Nie, J. Blancon, C. Stoumpos, R. Verduzco, B. Harutyunyan, S. Tretiak, G. Gupta, M.A. Alam, J. Even, M.J. Bedzyk, J. Lou, P. Ajayan, M.G. Kanatzidis, A. Mohite

**3:10** Intermission.

**3:35 PHYS 71.** Optoelectronic properties and molecular disorder in the plastic crystal phase of hybrid perovskites. **J. Even**

**4:15 PHYS 72.** Optoelectronic properties of large grain hybrid perovskites solar cells and device photo-stability. **W. Nie**

**4:55 PHYS 73.** Hot phonon-bottleneck in lead halide perovskite films. **Y. Yang**, M.C. Beard, J. van de Lagemaat

## Section E

San Diego Convention Center  
Room 29B

### Physical Chemistry of Complex Environmental Interfaces

*Cosponsored by COLL*

G. M. Nathanson, *Organizer*

V. H. Grassian, *Organizer, Presiding*

**1:30 PHYS 74.** Withdrawn.

**1:50 PHYS 75.** Reactions of nitrogen oxides at atmospheric interfaces: A unique probe for interfacial halide concentration. **T.H. Bertram**, O.S. Ryder, S. Staudt

**2:30 PHYS 76.** Insights into the heterogeneous reactivity of biologically derived components of sea spray aerosols. **J. Trueblood**, A.D. Estillore, C. Lee, J. Dowling, K.A. Prather, V.H. Grassian

**2:50 PHYS 77.** Atmospheric chemistry at the ocean surface: Using novel detectors to probe air-sea exchange. **L.J. Carpenter**, A.C. Lewis, X. Pang, A. Saint, M. Shaw

**3:30** Intermission.

**3:50 PHYS 78.** Photochemical effects of halides at liquid and frozen aqueous surfaces. **D. Donaldson**

**4:30 PHYS 79.** Microscopic structure and uptake kinetics at aqueous solution surfaces. **A. Morita**, T. Ishiyama

**5:10 PHYS 80.** Reactive collisions of N<sub>2</sub>O<sub>3</sub> with salty water: Formation of interfacial halogen species. **M.A. Shaloski**, T.H. Bertram, G.M. Nathanson

## Section F

San Diego Convention Center  
Room 29C

### Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory

#### Conformations & Dynamics

*Cosponsored by BIOL*

H. S. Shafaat, *Organizer*

S. Stoll, *Organizer, Presiding*

A. Kohen, *Presiding*

**1:00 PHYS 81.** Changing paradigms in enzyme catalysis. **J. Klinman**

**1:35 PHYS 82.** Proton-coupled electron transfer in soybean lipoxygenase: Hydrogen tunneling and conformational motions. **S. Hammes-Schiffer**

**1:55 PHYS 83.** Protein dynamics role in catalyzing two different chemical steps along thymidylate synthase catalysis. **V. Moliner**, A. Kohen

**2:15** Intermission.

**2:30 PHYS 84.** Direct probing of GroEL unfoldase/foldase activity by relaxation-based NMR measurements. **G.M. Clore**, D. Libich, V. Tugarinov

**3:05 PHYS 85.** What can we learn from <sup>13</sup>C NMR studies of C<sub>60</sub> substituted dipeptides: A computational study. **B.S. Hudson**, O. Melton, E. Kleist

**3:25 PHYS 86.** Protein dynamics and enzymatic catalysis. **S.D. Schwartz**

**3:45** Intermission.

**4:00 PHYS 87.** Conformational sampling scheme as a mechanism for drug-resistance evolution in HIV-1 protease. Z. Liu, J.T. Norell, X. Huang, I.S. de Vera, L. Hu, T. Tran, K.M. Poole, B. Mahon, K. Li, N.E. Goldfarb, R. McKenna, B.M. Dunn, G.E. Fanucci

**4:35 PHYS 88.** Enzymatic mechanisms of membrane-bound proteins viewed with pulse dipolar ESR. E.R. Georgieva, P.P. Borbat, B.J. Orlando, M. Malkowski, O. Boudker, J.H. Freed

**4:55 PHYS 89.** Effects of deuteration on the formation and vibrational structure of a neutral tryptophan W48 radical in azurin. J. Liang, J. Rivera, J.E. Kim

## Section G

San Diego Convention Center  
Room 29D

### Towards Predictive Calculations in Strongly Correlated Molecules & Materials

T. C. Berkelbach, E. Neuscamman, *Organizers*  
T. Shiozaki, *Presiding*

**1:30 PHYS 90.** Renormalization group approaches for strongly correlated electrons. F.A. Evangelista

**2:15 PHYS 91.** Combining density matrix renormalization group and n-electron valence perturbation theory. S. Guo, G.K. Chan

**2:40 PHYS 92.** Efficient multireference dynamic correlation from time-dependent perturbation theory. A. Sokolov, G. Chan

**3:25** Intermission.

**3:45 PHYS 93.** Solving a challenge posed by experiment: Characterizing the ground and excited states of nickel silicide. G. Schoendorff, A. Morris, E. Hu, A.K. Wilson

**4:10 PHYS 94.** Recent progress in multi-reference dynamic correlation methods based on density matrix renormalization group. T. Yanai, M. Saitow, Y. Kurashige

**4:55 PHYS 95.** Non-perturbative diagrammatic calculation of ionization potential using R12-correlator operator. M. Bayne, A. Chakraborty

## Multiscales Chemistry

### Mini-Platform

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

### Discussions with the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

‡Cooperative Cosponsorship

## From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

### Protein Folding, Surfaces & Membranes

*Sponsored by COMP, Cosponsored by PHYS*

### Global Initiatives in Research Data Management & Discovery

#### Global Landscape

*Sponsored by CINF, Cosponsored by ANYL, COMP, MEDI and PHYS*

### E. Bright Wilson Award in Spectroscopy: Symposium in honor of Robert G. Griffin

*Sponsored by BIOL, Cosponsored by PHYS*

### Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications

*Sponsored by COMP, Cosponsored by CATL and PHYS*

## SUNDAY EVENING

### My Comments to the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

### My Experience with & Advice for Improving Diversity in Chemistry

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 29A

### Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events

R. Elber, R. M. Levy, C. F. Wong, D. M. Zuckerman, *Organizers*

R. D. Coalson, *Presiding*

**8:00 PHYS 96.** Long-time and large-scale conformational kinetics in biomolecular systems. I. Andricioaei

**8:30 PHYS 97.** Replica exchange transition interface sampling: The latest method developments and applications using *ab initio* molecular dynamics. T. van Erp

**9:00 PHYS 98.** Describe protein dynamics using diffusion maps with an improved Gaussian kernel. S. Huo

**9:30** Intermission.

**9:45 PHYS 99.** Large-scale conformational transitions in the transport cycle of the ATP-driven calcium pump. B. Roux, A. Das

**10:15 PHYS 100.** Temperature-accelerated and multi-scale simulation algorithms for exploration and generation of free energy landscapes of molecular crystals and oligopeptides. M.E. Tuckerman

**10:45** Intermission.

**11:00 PHYS 101.** Quantitative comparison of macromolecular pathways. O. Beckstein, S. Seyler, A. Kumar, M.F. Thorpe

**11:30 PHYS 102.** Time-dependent effects of DNA replication on mRNA noise. J.R. Peterson, J. Cole, J. Fei, T. Ha, Z. Luthey-Schulten

## Section B

San Diego Convention Center  
Room 28C

### Decoding the Spectroscopic Signatures of Large Amplitude Motions: Challenges & Opportunities for Theory & Experiment

Z. Bacic, M. A. Johnson, *Organizers*

H. Reisler, *Presiding*

**8:00 PHYS 103.** Slow electron velocity-map imaging of cryogenically cooled anions. D.M. Neumark

**8:40 PHYS 104.** Vibrational spectroscopy on partial peptides SIVSF of adrenaline receptor. M. Fujii

**9:20 PHYS 105.** Spectroscopy and dynamics of the nitrate cation NO<sub>3</sub><sup>-</sup>. K. Takematsu, J. Stanton, G.A. Garcia, L. Nahon, M. Okumura

**10:00** Intermission.

**10:20 PHYS 106.** High amplitude vibrational overtone transitions: Sunlight driven atmospheric reactions. V. Vaida

**10:40 PHYS 107.** Transient THz spectroscopy probes large amplitude motions of proteins and collective low frequency protein/hydration modes. M. Havenith

**11:20 PHYS 108.** Monitoring the excited state relaxation of complex systems by multi-state non-adiabatic dynamics. A. Ponzi, M. Sapunar, P. Decleva, N. Doslic

## Section C

San Diego Convention Center  
Room 28D

### Electrochemistry at Solid/Liquid Interfaces

O. Borodin, *Organizer*

Y. Qi, *Organizer, Presiding*

**8:00 PHYS 109.** How SEI forms in aqueous electrolytes. L. Suo, C. Wang, O. Borodin, K. Xu

**8:40 PHYS 110.** Mechanism of Li<sub>x</sub>Ni<sub>0.5</sub>Mn<sub>1.2</sub>O<sub>4.5</sub> dissolution in organic carbonate electrolytes. A. Jarry, R. Kostecki

**9:20 PHYS 111.** *Ab initio* molecular dynamics simulations of Mn(II) dissolution from Li(x)Mn(2)O(4) surfaces. K. Leung

**10:00** Intermission.

**10:10 PHYS 112.** Modeling of oxidation decomposition reactions and transition metal dissolution at the electrolyte/cathode interface for the spinel-structured LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> high-voltage cathode. M. Olguin, O. Borodin

**10:30 PHYS 113.** Transport mechanisms in ionic liquid-based electrolytes for magnesium batteries. G.A. Giffin, S. Passerini

**11:10 PHYS 114.** Roles of solid electrolyte interphases in rechargeable lithium, sulfur and lithium, metal fluoride batteries. G. Yushin

## Section D

San Diego Convention Center  
Room 28E

### Frontiers in Solar Light Harvesting Processes

A. Mohite, O. V. Prezhdo, S. Tretiak, *Organizers*

T. Krauss, *Organizer, Presiding*

**8:00 PHYS 115.** Colloidal quantum dots in extreme electromagnetic environments. D.J. Norris

**8:40 PHYS 116.** Hole transfer dynamics from QDs to tethered ferrocene derivatives. P. Alivisatos

**9:20 PHYS 117.** Bridging the gap between group IV and binary semiconducting nanocrystals: The X,L,Z motif. N.C. Anderson, L. Wheeler, N.R. Neale, J.S. Owen

**9:40** Intermission.

**10:05 PHYS 118.** Early time carrier dynamics in quantum dot solids studied by ultrafast photocurrent spectroscopy. V.I. Klimov

**10:45 PHYS 119.** Role of surface ligands in formation of PbSe Nanoplates and their photophysics. S.W. Kilina

**11:25 PHYS 120.** Probing single-molecule interfacial electron transfer dynamics in solar energy systems. H. Lu

## Section E

San Diego Convention Center  
Room 29B

### Physical Chemistry of Complex Environmental Interfaces

*Cosponsored by COLL*

V. H. Grassian, G. M. Nathanson, *Organizers*

T. H. Bertram, *Presiding*

**8:00 PHYS 121.** Viscosity of secondary organic materials and atmospheric implications. M. Song, J. Grayson, P. Liu, Y. Zhang, S.T. Martin, A.K. Bertram

**8:40 PHYS 122.** Heterogeneous efflorescence of atmospherically relevant salts by mineral dust particles. S. Ushijima, R. Davis, S. Lance, J. Gordon, M. Tolbert

**9:00 PHYS 123.** Organic material at the gas-aerosol interface: Old dog, new tricks. V.F. McNeill, Y. Wu, W. Li, Y. Rao, H. Dai

**9:40** Intermission.

**10:00 PHYS 124.** Ultraviscous organic aerosol: Phase behaviour, gas-particle partitioning of volatiles and oxidation. J. Reid, A. Haddrell, F. Marshall, R.E. Miles, A. Rickards, Y. Song

**10:40 PHYS 125.** Exploring the interactions between room temperature ionic liquids and biological membranes. G.E. Lindberg, J.L. Baker

**11:00 PHYS 126.** Airborne soil organic particles. A. Laskin

**11:40 PHYS 127.** Quantifying the role of interfacial chemistry in perturbing the physical state of atmospheric aerosol. J. Davies, K.R. Wilson

## Section F

San Diego Convention Center  
Room 29C

### Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory

#### Active Sites

*Cosponsored by BIOL*

H. S. Shafaat, *Organizer*

S. Stoll, *Organizer, Presiding*

R. D. Britt, *Presiding*

**8:30** *PHYS* **128**. Systems for natural and artificial photosynthesis. V.S. Batista

**9:05** *PHYS* **129**. Spectroscopic studies of proton coupled electron transfer in photosynthetic oxygen evolution. B.A. Barry, U. Brahmachari, Z. Guo

**9:25** *PHYS* **130**. Intersystem crossings in the active site of rubredoxin. D.S. Kaliakin, G.E. dePolo, S.A. Varganov

**9:45** *PHYS* **131**. X-ray crystallography and spectroscopy for studying metalloenzymes using XFELs. J. Kern, R. Alonso-Mori, R. Chatterjee, F. Fuller, S. Gul, N. Sauter, U. Bergmann, V.K. Yachandra, J. Yano

**10:20** Intermission.

**10:40** *PHYS* **132**. Probing small molecule activation via high-resolution inelastic x-ray scattering. K.M. Lancaster, K. Silberstein, R.C. Walroth

**11:15** *PHYS* **133**. Molecular mechanism of hydrogen peroxide decomposition by monofunctional catalases and peroxidases. M. Alfonso-Prieto, P. Campomanes, P. Vidossich, X. Biarnés, U. Roethlisberger, C. Rovira

**11:35** *PHYS* **134**. Design of protein-based hybrid catalysts for light-driven CO<sub>2</sub> reduction. D. Sommer, M.Z. Ertem, G. Manbeck, A. Roy, J.T. Muckerman, E. Fujita, G. Ghirlanda

## Section G

San Diego Convention Center  
Room 29D

### Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials

A. P. Willard, *Organizer*

D. Eisele, *Organizer, Presiding*

**8:00** *PHYS* **135**. Elucidation of the molecular machinery in photosynthetic light harvesting. G. Schlau-Cohen

**8:30** *PHYS* **136**. Many-body dispersion and its effect in the interactions of organic chromophores and two-dimensional materials. A. Aspuru-Guzik

**9:00** *PHYS* **137**. Engineering nanometer-scale coherence in soft matter. C. Liu, Y. Zhang, P. Zhang, D.N. Beratan

**9:20** Intermission.

**9:40** *PHYS* **138**. Balance of order and disorder as the key to tailor various properties of soft materials. H. Frauenrath

**10:10** *PHYS* **139**. Photophysics of self-assembled carotenoid aggregates. M.J. Tauber, S. Doyle, C. Wang

## Section H

San Diego Convention Center  
Room 30A

### Towards Predictive Calculations in Strongly Correlated Molecules & Materials

T. C. Berkelbach, E. Neuscamman, *Organizers*

F. A. Evangelista, *Presiding*

**8:00** *PHYS* **140**. Stochastic and deterministic solutions of multireference linearized coupled cluster equations. S. Sharma

**8:45** *PHYS* **141**. Efficient modelling of transition metal systems using approximate projection: development and applications. L.M. Thompson, H.P. Hratchian

**9:10** *PHYS* **142**. Novel wavefunction approaches for strongly correlated electrons. G.E. Scuseria

**9:55** Intermission.

**10:15** *PHYS* **143**. Density functional model for nondynamic and strong correlation. J. Kong, E. Proynov

**10:40** *PHYS* **144**. Two-electron reduced density matrix methods for strongly correlated quantum systems. D.A. Mazziotti

**11:25** *PHYS* **145**. Photoionization and photodetachment spectra from equation-of-motion coupled-cluster Dyson orbitals. S. Gozem, A. Gunina, A. Krylov

### Global Initiatives in Research Data Management & Discovery

#### Role of Community & Standards

*Sponsored by CINF, Cosponsored by ANYL, COMP, MEDI and PHYS*

#### Protein Structure & Folding: From Solution to the Gas Phase

*Sponsored by ANYL, Cosponsored by PHYS*

#### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

#### Pushing the Envelope, Polarizability & Quantum Effects

*Sponsored by COMP, Cosponsored by PHYS*

#### Multiscales Chemistry Bio

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

#### Preparing for the Real World: Challenges Faced by Young Investigators

#### Choosing Grad Research Advisors & a Career in Academia or Industry

*Sponsored by MPPG, Cosponsored by CHED, CINF, COMP, PHYS and YCC*

#### Advances in Chemical Imaging: Ultra-Resolution to Single Molecules

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#### Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications

*Sponsored by COMP, Cosponsored by CATL and PHYS*

#### Computational Design of Advanced Materials

*Sponsored by COMSCI, Cosponsored by COMP and PHYS*

## MONDAY AFTERNOON

## Section A

San Diego Convention Center  
Room 29A

### Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events

R. Elber, R. M. Levy, C. F. Wong, D. M. Zuckerman, *Organizers*

C. F. Abrams, *Presiding*

**1:30** *PHYS* **146**. Proton transport in biomolecular systems: A remarkably complex and collective phenomenon. G.A. Voth

**2:00** *PHYS* **147**. How structure-directing agents control nanocrystal shape: Simulation of the PVP-mediated growth of Ag nanocubes from first principles. K.A. Fichthorn, X. Qi, T. Balankura

**2:30** *PHYS* **148**. Protein allostery and conformation dynamics. H. Zhou

**3:00** Intermission.

**3:15** *PHYS* **149**. Simple polymer brush model of the nuclear pore complex. R.D. Coalson

**3:45** *PHYS* **150**. Complex transitions in large protein-nucleic complexes from computer simulations. M. Feig

**4:15** Intermission.

**4:30** *PHYS* **151**. Over a decade of folding@home: How citizen science has led to key new advances in biophysics and fighting disease. V.S. Pande

**5:00** *PHYS* **152**. Statistical mechanics of protein-protein association. D. Kozakov, S.E. Mottarella, S. Vajda

## Section B

San Diego Convention Center  
Room 28C

### Frontiers in Solar Light Harvesting Processes

T. Krauss, A. Mohite, O. V. Prezhdo, S. Tretiak, *Organizers*

J. K. McCusker, *Presiding*

**1:30** *PHYS* **153**. Artificial photosynthesis: Progress, science prospects and technology outlook. H. Atwater

**2:10** *PHYS* **154**. Materials for solar energy conversion and storage. G.A. Galli

**2:50** *PHYS* **155**. Spin resolved electron dynamics of vanadium (IV) doped anatase. S.J. Jensen, T.M. Inerbaev, D. Kilin

**3:10** Intermission.

**3:30** *PHYS* **156**. Ultrafast charge transfer-state dynamics in first-row transition metal-based complexes: Making earth-abundant chromophores viable for light harvesting applications. J.K. McCusker

**4:10** *PHYS* **157**. Relationships between excited state dynamics and photochemistry of nanocrystal-catalyst complexes. G. Dukovic

**4:50** *PHYS* **158**. Photocatalytic conversion of nitrobenzene to aniline through sequential proton-coupled one-electron transfers from a cadmium sulfide quantum dot. S. Jensen, S. Homan, E. Weiss

## Section C

San Diego Convention Center  
Room 28D

### Electrochemistry at Solid/Liquid Interfaces

O. Borodin, *Organizer*

Y. Qi, *Organizer, Presiding*

**1:30** *PHYS* **159**. Electrochemical stability of solid electrolytes. C. Wang, F. Han

**2:10** *PHYS* **160**. Electrochemical stiffness in lithium ion battery anodes and cathodes. A.A. Gewirth

**2:50** *PHYS* **161**. Li-doped ionic liquid electrolytes: From bulk phase to interfacial behavior. J. Haskins, J. Lawson

**3:30** Intermission.

**3:40** *PHYS* **162**. Development of AMOEBA for ionic liquids and applications for Li<sup>+</sup> transport. H. Torabifard, Y. Tu, O.N. Starovoytov, R.E. Duke, G.A. Cisneros

**4:00** *PHYS* **163**. Electrochemical lithiation process into Si substrate. N. Aoki, A. Omachi, T. Kondo, K. Uosaki

**4:20** *PHYS* **164**. Using quartz crystal microbalance with dissipation (QCM-D) measurements to characterize *in situ* Li-ion battery solid-electrolyte interphases. M.C. Dixon, Z. Yang, L. Trahey

**4:40** *PHYS* **165**. Density functional theory screening of gas-treatment strategies for stabilization of high energy-density lithium metal anodes. S. Koch, A. Etxebarria, B. Morgan, O. Bondarchuk, M.A. Muñoz-Márquez, S. Passerini, G. Teobaldi

## Section D

San Diego Convention Center  
Room 28E

### Physical Chemistry of Complex Environmental Interfaces

*Cosponsored by COLL*

V. H. Grassian, G. M. Nathanson, *Organizers*

D. Donaldson, *Presiding*

**1:30** *PHYS* **166**. Observations of ice nucleation of monolayers and crystals of long-chain acids with relevance to atmospheric ice formation. P.J. DeMott, R.H. Mason, C. McCluskey, T.C. Hill, O. Laskina, C. Sultana, C. Lee, G.C. Cornwall, H. Al-Mashat, K. Moore, V.H. Grassian, D. Pham, R.C. Moffet, A.K. Bertram, K.A. Prather

**1:50** *PHYS* **167**. Effect of pH on the phase separation of organic aerosol. M. Freedman

**2:30** *PHYS* **168**. Macromolecular crowding effects on both translational and rotational diffusion of molecular probes. A.A. Heikal, M. Currie, B. Berry, T. Ward, E.D. Sheets

**2:50** *PHYS* **169**. Interfacial chemistry of organic aerosols. K.R. Wilson

**3:30** Intermission.

**3:50** *PHYS* **170**. Many faces of heterogeneous ice nucleation: Interplay between surface morphology and hydrophobicity. A. Michaelides

**4:30** *PHYS* **171**. Stacking disorder in ice grown from liquid but not from vapor: Polymorph selection by interfaces. A. Hudait, V. Molinero

**5:10** *PHYS* **172**. Origin of sea spray aerosol mixing state. X. Wang, K. Moore, C. Sultana, D.B. Collins, K.A. Prather

## Section E

San Diego Convention Center  
Room 29B

**Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory**

**Beyond the Active Site**

*Cosponsored by BIOL*

S. Stoll, *Organizer*

H. S. Shafaat, *Organizer, Presiding*

G. E. Fanucci, *Presiding*

**1:00 PHYS 173.** Membrane embedded enzymes survive in the gas phase enabling new mechanistic insight. C.V. Robinson

**1:35 PHYS 174.** Characterizing DHFR dynamics with NMR and x-ray crystallography. R. Fenwick, D. Oyen, P.E. Wright

**1:55 PHYS 175.** Some surprises in the biophysics of protein dynamics: Change of kinases and GPCRs. V.S. Pande

**2:15** Intermission.

**2:30 PHYS 176.** One is the loneliest number: Modeling multiple conformations using room temperature x-ray crystallography. E. Poss

**3:05 PHYS 177.** Physicochemical properties for functional genomics: Predicting enzyme function for structural genomics proteins. M.J. Ondrechen, C.L. Mills, P.J. Beuning

**3:25 PHYS 178.** Impact of directed evolution on flexible binding domains explained by molecular dynamics. G. Jimenez-Oses, E.L. Noey, S. Osuna, J. Park, K.N. Houk

**3:45** Intermission.

**4:00 PHYS 179.** Watching a signaling protein function with time-resolved x-ray crystallography and time-resolved x-ray scattering. P.A. Anfirud, F. Schotte, H. Cho

**4:35 PHYS 180.** Towards developing a quantum mechanical/molecular mechanical model for the ping-pong enzyme kinetics in quinone reductase. S. Bhattacharyay

## Section F

San Diego Convention Center  
Room 29C

**Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials**

D. Eisele, A. P. Willard, *Organizers*

S. Jang, *Presiding*

**1:30 PHYS 181.** Chiral porphyrin aggregates. T.S. Balaban

**2:00 PHYS 182.** Energy transport in nanotubular supramolecular cyanine aggregate systems. D. Vanden Bout, E.L. Kreuger

**2:20 PHYS 183.** Mobility of excitons in perylene bisimide aggregates. F. Fennel, S. Wolter, S. Lochbrunner, F. Wuertner

**2:40 PHYS 184.** Infrared invisibility stickers inspired by cephalopods. L. Phan, D.D. Ordinario, E. Karshalev, W. Walkup IV, M. Shenk, A.A. Gorodetsky

**3:00** Intermission.

**3:10 PHYS 185.** Molecular simulations of  $\pi$ - $\pi$  stacking mediated self-assembly in supramolecular filaments. M. Kang, P. Zhang, H. Cui, S. Loverde

**3:40 PHYS 186.** Understanding and designing self-assembled molecular J-aggregates for long-range coherent energy transport. J. Caram, D.M. Eisele, S. Doria, S. Lloyd, M.G. Bawendi

**4:00 PHYS 187.** Interchain charge-transfer states facilitate triplet formation in polymer aggregate nanofibers. A. Thomas, J. Garcia-Galvez, H.A. Brown, J.K. Grey

## Section G

San Diego Convention Center  
Room 29D

**Towards Predictive Calculations in Strongly Correlated Molecules & Materials**

T. C. Berkelbach, *Organizer*

E. Neuscamman, *Organizer, Presiding*

**1:30 PHYS 188.** Highly accurate fragment molecular orbital/quantum Monte Carlo method for large molecular systems. S.R. Pruitt, A. Benali, D. Fedorov

**1:55 PHYS 189.** Stochastic quantum chemistry for strong correlation. G. Booth, R. Thomas, N. Blunt, R. Anderson, Q. Sun, T. Shiozaki, A. Alavi

**2:40 PHYS 190.** Exchange-correlation energy of the warm dense electron gas. F.D. Malone, N. Blunt, J.J. Shepherd, D.K. Lee, J.S. Spencer, W.M. Foulkes

**3:25** Intermission.

**3:45 PHYS 191.** Obtaining trial wavefunctions on the cheap: A stochastic approach to multideterminant wavefunctions in auxiliary field quantum Monte Carlo.

B.M. Rubenstein, M. Morales-Silva, C. Chang, E. Landinez-Borda

**4:30 PHYS 192.** Electron correlation in an atomic chain of gold atoms. J. Greer, T. Kelly

## Section H

San Diego Convention Center  
Room 30A

**Physical Principles in Functional Nanoscience: Symposium in honor of Mostafa A. El-Sayed**

P. K. Jain, C. F. Landes, *Organizers*

S. Link, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35 PHYS 193.** Gold nanocrystals: Past, present and future. C.J. Murphy

**2:10 PHYS 194.** DNA-directed synthesis of silver clusters. J.T. Petty, M. Ganguly

**2:30 PHYS 195.** Sustainable plasmonics and plasmonics for sustainability. N.J. Halas

**3:05 PHYS 196.** Time-resolved and steady-state spectroscopies of single plasmonic nanoparticles and their assemblies. W. Chang

**3:25** Intermission.

**3:40 PHYS 197.** Magnetic-plasmonic core-shell nanoparticles: Shape-controlled synthesis, properties and applications in cancer detection. X. Huang

**4:15 PHYS 198.** Tale of two particles: Polymer nanotechnologies for rational combination therapies against metastatic tumors. E.C. Dreaden, Y. Kong, M.B. Yaffe, P.T. Hammond

**4:35 PHYS 199.** Nanoparticles and the protein corona: Relating protein composition and structure to cellular outcomes. C.K. Payne

**5:10 PHYS 200.** Circular differential scattering of single chiral self-assembled gold nanorod dimers. K.W. Smith, L. Wang, S. Dominguez, J. Olson, H. Zhang, W. Chang, N. Kotov, S. Link

## Multiscales Chemistry

## Mini-Platform

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

## Diversity-Quantification-Success?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

**From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules**

**Evolution, Extremes & Mechanisms**

*Sponsored by COMP, Cosponsored by PHYS*

**Protein Structure & Folding: From Solution to the Gas Phase**

*Sponsored by ANYL, Cosponsored by PHYS*

**Global Initiatives in Research Data Management & Discovery**

**Technical Infrastructures: Enabling Cultural Shifts**

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**Preparing for the Real World: Challenges Faced by Young Investigators**

**Research at PUI's**

*Sponsored by MPPG, Cosponsored by CHED, CINF, COMP, PHYS and YCC*

**Nonlinear Spectroscopy & Modeling**

*Sponsored by ANYL, Cosponsored by MPPG and PHYS*

**Elucidation of Mechanisms & Kinetics on Surfaces**

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

**Structure, Dynamics & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications**

*Sponsored by COMP, Cosponsored by CATL and PHYS*

## MONDAY EVENING

## Section A

San Diego Convention Center  
Halls D/E

## Sci-Mix

G. S. Engel, *Organizer*

**8:00 - 10:00**

367-369, 371, 373, 375-379, 381, 385, 388, 391, 398, 405-406, 414, 416, 419-420, 422, 424, 427, 431, 435-437, 441-442, 444, 451, 458-459, 467-468, 470, 472, 474, 476, 481, 483, 486-488, 501, 503-506, 510-511, 515, 518-519, 525-526, 531, 534, 539, 544, 547-548, 551, 559-561, 565-566, 571. See subsequent listings.

## TUESDAY MORNING

## Section A

San Diego Convention Center  
Room 29A

**Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events**

R. Elber, R. M. Levy, C. F. Wong, D. M. Zuckerman, *Organizers*

M. Feig, *Presiding*

**8:00 PHYS 201.** Ensemble refinement methods using molecular dynamics simulations and their relation to free energy calculations and long-time sampling. G. Hummer, J. Koefinger

**8:30 PHYS 202.** New biological problems enabled by multi-dimensional replica exchange molecular dynamics simulations. D.M. York

**9:00 PHYS 203.** Variational approach to enhanced sampling and free energy calculations. M. Parrinello

**9:30** Intermission.

**9:45 PHYS 204.** Calculation of protein-ligand binding affinities via free energy perturbation methods. R.A. Friesner

**10:15 PHYS 205.** Constant pH simulations in biomolecular systems. A.E. Roitberg

**10:45** Intermission.

**11:00 PHYS 206.** Orthogonal sampling of slow responses to enable efficient biomolecular simulations. W. Yang

**11:30 PHYS 207.** Integrated computational-experimental-Bayesian approach to quantify conformation ensembles of unstructured peptides. Y. Zhang

## Section B

San Diego Convention Center  
Room 28C

**Electrochemistry at Solid/Liquid Interfaces**

O. Borodin, Y. Qi, *Organizers*

J. Haskins, *Presiding*

**8:00 PHYS 208.** Improved methods for the *ab Initio* simulation of electrochemical systems. T.A. Barnes, D. Prendergast, P. Kent, J. Deslippe, O. Borodin, T.F. Miller

**8:40 PHYS 209.** Understanding the solid electrolyte-electrode interfaces in all-solid-state Li-ion batteries: First-principles computation on thermodynamics and kinetics. Y. Mo

**9:20 PHYS 210.** Structures of THF-solvated sodium ions attracted to a charged molecular surface. Q. Wu

**9:40 PHYS 211.** Ultrafast photo-induced electric field at the surfaces of p-GaN/P2 electrode. Y. Yang, M.C. Beard

**10:00 PHYS 212.** Electrochemical characterization of DNA-inspired organic nanowires. A.G. Wardrip, A. Mazaheripour, J. Jocsan, A. Bartlett, N. Huesken, A. Burke, M.N. Dickson, A.A. Gorodetsky

**10:20 PHYS 213.** Unprecedented efficiency to control orbital energies and vibrational properties of single molecules embedded in electrochemical STM junctions. I. Baldea

**10:40** Intermission.

**10:50 PHYS 214.** Studies of self-exchange electron transfer and charge accumulation at sensitized TiO<sub>2</sub> for multiple-electron-transfer chemistry using a series of amine-functionalized porphyrins. **J. Glancy-Logan**, H. Chen, J.M. Cardon, J. Angsono, S. Ardo

**11:10 PHYS 215.** Light-induced proton conductivity in a photo-acid doped polymer. **S. Haghigat**, S. Ostresh, J. Dawlaty

**11:30 PHYS 216.** Roles of self-exchange electron transfer between anchored metal-poly(pyridyl) dyes to mesoporous metal-oxide thin films. **J. Angsono**, J. Glancy-Logan, H. Chen, S. Ardo

## Section C

San Diego Convention Center  
Room 28D

### Frontiers in Solar Light Harvesting Processes

T. Krauss, A. Mohite, S. Tretiak, *Organizers*

O. V. Prezhdo, *Organizer, Presiding*

**8:00 PHYS 217.** Charge separation and recombination at single-walled carbon nanotube photovoltaic interfaces.

**J. Blackburn**, A. Ferguson, O. Reid, R. Ihly, A. Dowgiallo, S.L. Guillot, P. Schulz, M. Yang, K. Zhu, J. Berry, K. Mistry, N. Kopidakis, G. Rumbles

**8:40 PHYS 218.** Exciton transport in thin films of semiconducting carbon nanotubes using 2D white-light spectroscopy. **M.T. Zanni**, M. Arnold

**9:20 PHYS 219.** Design of better photovoltaic materials with cheminformatics approaches. **O. Isayev**

**9:40** Intermission.

**10:05 PHYS 220.** Insight into carbon nanotube surface structures for photovoltaics applications. **S.K. Doorn**, N. Hartmann, N. Subbailyan, R. Pramanik, A. Mallajosyula, A. Mohite, J. Blackburn

**10:45 PHYS 221.** Interplay between singlet fission and triplet transport in organic semiconductors revealed by ultrafast microscopy. T. Zhu, Y. Wan, Z. Guo, J.C. Johnson, **L. Huang**

**11:25 PHYS 222.** Self-assembled molecular p/n junctions for application in dye-sensitized solar energy conversion. **B.H. Farnum**, K. Wee, T.J. Meyer

## Section D

San Diego Convention Center  
Room 28E

### Physical Chemistry of Complex Environmental Interfaces

*Cosponsored by COLL*

V. H. Grassian, G. M. Nathanson, *Organizers*

K. R. Wilson, *Presiding*

**8:00 PHYS 223.** Chemistry and photochemistry of surface-bound neonicotinoids. **B.J. Finlayson Pitts**, K. Aregahegn, D. Shemesh, R.B. Gerber

**8:40 PHYS 224.** Ultrafast photolysis of iron(III) aqua ions studied by UV/UV femtosecond pump-probe spectroscopy. R.A. Danforth, **B. Kohler**

**9:00 PHYS 225.** Shine light on oceans and ...change air-sea interactions. **C. George**, P. Alpert, L. Tinell, S. Rossignol, F. Bernard, R. Ciuraru

**9:40** Intermission.

**10:00 PHYS 226.** Building molecular complexity with sunlight at aqueous interfaces. **V. Vaidya**, R. Perkins, A. Reed Harris, R. Rapt

**10:40 PHYS 227.** Formation of environmentally persistent free radicals from the heterogeneous reaction of ozone and common carbonaceous particles. **C. Borrowman**, J.P. Abbott, S. Zhou, T.E. Burrow

**11:00 PHYS 228.** Condensed-phase photochemical reactions in atmospheric organic aerosol. **S.A. Nizkorodov**

**11:40 PHYS 229.** Probing the phase state and formation and growth mechanisms of secondary organic aerosol from  $\alpha$ -cedrene ozonolysis. **Y. Zhao**, L.M. Wingen, V. Perraud, B.J. Finlayson Pitts

## Section E

San Diego Convention Center  
Room 29B

### Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials

D. Eisele, A. P. Willard, *Organizers*

S. Loverde, *Presiding*

**8:00 PHYS 230.** Dynamic peptide libraries for materials discovery. **R. Uljin**

**8:30 PHYS 231.** Generalized master equation approach for coarse grained excitation dynamics in supramolecular systems. **S. Jang**

**9:00 PHYS 232.** DFT-NEGF study of conducting protein filaments for solar energy harvesting. **H.P. Hendrickson**, N.S. Malvankar, V.S. Batista

**9:20 PHYS 233.** Correlating spectral shifts, polarization, and molecular orientation in conjugated organic thin films and microstructures. **J.M. Szarko**, A. Austin, X. Zhu

**9:40** Intermission.

**9:50 PHYS 234.** Bio-inspired supramolecular materials. **S.I. Stupp**

**10:20 PHYS 235.** Photophysical and electrochemical properties of perylene bisimide homo- and heterodimers. **A. Nowak-Król**, B. Fimmel, M. Son, D. Kim, F. Wuertner

**10:40 PHYS 236.** *In situ* liquid cell TEM observations of the size evolution pathways of amphiphilic polymer micelle nanoparticles. **L.R. Parent**, J.K. Kammeyer, J.P. Patterson, E. Bakalis, F. Zerbetto, C. Park, N.C. Gianneschi

**11:00 PHYS 237.** Excitonic structure and environment effects in porphyrin aggregates probed with low-temperature fluorescence. **C.W. Leishman**, J. McHale

## Section F

San Diego Convention Center  
Room 29C

### Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory

#### Photons, Protons, Electrons

*Cosponsored by BIOL*

S. Stoll, *Organizer*

H. S. Shafaat, *Organizer, Presiding*

T. Markland, *Presiding*

**8:30 PHYS 238.** Transcription repression, activation, and deactivation mechanisms by a metal-sensing regulator. **P. Chen**

**9:05 PHYS 239.** Electrochemical determination of the reactivity of the bifurcating enzyme NADH-dependent reduced ferredoxin:NADP<sup>+</sup> oxidoreductase. **D.P. Jennings**, G.J. Schut, M.W. Adams, A.K. Jones

**9:25 PHYS 240.** Probing single-molecule enzyme active-site conformational dynamics. **H. Lu**

**9:45 PHYS 241.** Picosecond hydrogen bond dynamics in proteins examined with femtosecond spectroscopy and molecular dynamics simulations. **P. Konold**, E. Yoon, J. Lee, P. Chapagain, B. Gerstman, C. Regmi, K. Piatkevich, V. Verkusha, T. Joo, **R. Jimenez**

**10:20** Intermission.

**10:40 PHYS 242.** Structural dynamics and tryptophan-mediated electron transfer in hemoproteins. **M. Chergui**

**11:15 PHYS 243.** Concerted multiple-site proton-coupled electron transfer (MS-PCET): Separating the proton and electron. **J.M. Mayer**, M.A. Bowring, W.D. Morris, J. Darcy, T.F. Markle, J.J. Warren, L.R. Bradshaw, D.R. Gamelin

**11:35 PHYS 244.** Direct simulation of charge-transfer dynamics in enzymatic systems. **J. Kretchmer**, T.F. Miller

## Section G

San Diego Convention Center  
Room 29D

### Towards Predictive Calculations in Strongly Correlated Molecules & Materials

E. Neuscamman, *Organizer*

T. C. Berkelbach, *Organizer, Presiding*

**8:00 PHYS 245.** Density matrix embedding theory: Accurate reaction paths and a second-quantized formulation for the local density of states. **S. Wouters**, G.K. Chan

**8:45 PHYS 246.** Two-dimensional embedded cluster method for accurate modeling of reactivity at oxide interfaces. **A.B. Muñoz-García**, J. Pascual Robledo, M. Pavone

**9:10 PHYS 247.** Bootstrap embedding. **T.A. Van Voorhis**, M. Welborn, T. Tsuchimochi, N. Ricke

**9:55** Intermission.

**10:15 PHYS 248.** Non-equilibrium electron dynamics from a real-time extension of density matrix embedding theory. **J. Kretchmer**, G. Chan

**10:40 PHYS 249.** Density functional embedding theory within the projector-augmented-wave formalism. **K. Yu**, E.A. Carter

**11:25 PHYS 250.** Prediction of pKa via a QM/QM approach. **P. Patel**, J. Wang, A.K. Wilson

## Section H

San Diego Convention Center  
Room 30A

### Physical Principles in Functional Nanoscience: Symposium in honor of Mostafa A. El-Sayed

P. K. Jain, C. F. Landes, S. Link, *Organizers*

C. D. Heyes, *Presiding*

**8:00 PHYS 251.** Nanocombinatorix via scanning probe block copolymer lithography. **C.A. Mirkin**

**8:35 PHYS 252.** Nanogap enhancement in Raman scattering. **Y. Suh**

**8:55 PHYS 253.** Nano-supra crystal: A new challenge. **M. Pileni**

**9:30 PHYS 254.** Highly luminescent nanoplates of perovskite cesium lead halide in stacked and oriented attachment assemblies. **Y. Bekenstein**, B.A. Koscher, P. Alivisatos

**9:50** Intermission.

**10:10 PHYS 255.** Using nanostructured assemblies to control fundamental physical processes: From energy harvesting and storage to nanomedicines. **S.H. Tolbert**

**10:45 PHYS 256.** Dimensionality effects at the single nanocrystal level: FRET between semiconductor nanorods and multiple dye acceptors. **I. Hadar**, S. Halivni, N. Even-Dar, A. Faust, U. Banin

**11:05 PHYS 257.** Gold nanoparticles as novel toolsets for directed-assembly of structures with sub-lithographic dimensions. **B. Nikoobakht**

**11:40 PHYS 258.** Energy transfer in self-assembled conjugates of PbS quantum dots and cyanine dye J-aggregates. **C. Wang**, E. Weiss

### Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Symposium in honor of Albert J. R. Heck

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## Multiscales Chemistry

### Soft Matter

*Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS*

### Computer-Aided Drug Design

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

### Quantum Mechanics

*Sponsored by COMP, Cosponsored by PHYS*

## TUESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 29A/B

### PHYS Division National Awards Symposium

G. S. Engel, *Organizer, Presiding*

**1:30 PHYS 259. Award Address** (Peter Debye Award in Physical Chemistry sponsored by E. I. du Pont de Nemours and Co.). By indirection find direction out: Modeling materials with essentially no usual ordering. **M.A. Ratner**

**2:05 PHYS 260. Award Address** (ACS Award in Theoretical Chemistry sponsored by the American Chemical Society). Water: A case study in ab-initio simulations. **R. Car**

**2:40 PHYS 261. Award Address** (ACS Award in the Chemistry of Materials sponsored by E.I. du Pont de Nemours and Co.). Power of Pi: A computational chemistry journey into pi-conjugated materials. **J.E. Bredas**

**3:15 PHYS 262. Award Address** (Irving Langmuir Award in Chemical Physics sponsored by GE Global Research and the American Chemical Society Division of Physical Chemistry). New perspectives in plasmonics. **G.C. Schatz**

**3:50** Intermission.

**4:15 PHYS 263. Award Address** (Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids sponsored by ExxonMobil Research and Engineering Company). Collective elasticity mediated activated relaxation in supercooled molecular liquids and thin films. K.S. Schweizer

**4:50 PHYS 264. Award Address** (Ahmed Zewail Award in Ultrafast Science and Technology sponsored by the Ahmed Zewail Endowment Fund established by the Newport Corporation (Newport)). Dynamics of protons in liquid water viewed through ultrafast IR spectroscopy. A. Tokmakoff

**5:25 PHYS 265. Award Address** (E. Bright Wilson Award in Spectroscopy sponsored by the ACS Division of Physical Chemistry). High frequency dynamic nuclear polarization. R.G. Griffin

## Multiscales Chemistry

### Liquids

Sponsored by MPPG, Cosponsored by BIOL, COMP and PHYS

### Computer-Aided Drug Design

Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDJ and PHYS

### Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

### Quantum Mechanics

Sponsored by COMP, Cosponsored by PHYS

## WEDNESDAY MORNING

### Section A

San Diego Convention Center  
Room 29A

#### Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events

R. Elber, R. M. Levy, C. F. Wong, D. M. Zuckerman, *Organizers*

A. E. Roitberg, *Presiding*

**8:00 PHYS 266.** Exploring energy and fitness landscapes of proteins for binding and allostery. R.M. Levy

**8:30 PHYS 267.** Computational thermodynamics of noncovalent binding. M.K. Gilson, A. Fenley, K. Gao, N.M. Henriksen, T.P. Kurtzman, H. Muddana, C.N. Nguyen, J. Yin

**9:00 PHYS 268.** Multi-resolution modeling of protein folding and function of a pH-dependent chaperone. C.L. Brooks

**9:30** Intermission.

**9:45 PHYS 269.** Computer-aided drug discovery: Dealing with flexibility and protonation. J.A. McCammon, Y. Miao

**10:15 PHYS 270.** Computer simulation of solution-phase thermodynamics: Free energies of hydration, volumes of solution, heats of vaporization, and liquid densities. J. Vilseck, J. Tirado-Rives, W.L. Jorgensen

**10:45** Intermission.

**11:00 PHYS 271.** Relative binding energies by the direct method. C.B. Post

**11:30 PHYS 272.** Mechanisms of membrane interaction and dimer formation of K-Ras4B. H. Jang, R. Nussinov

### Section B

San Diego Convention Center  
Room 28C

#### Decoding the Spectroscopic Signatures of Large Amplitude Motions: Challenges & Opportunities for Theory & Experiment

Z. Bacic, M. A. Johnson, *Organizers*

F. S. Menges, *Presiding*

**8:00 PHYS 273.** Nonadiabatic dynamics of photoinduced proton-coupled electron transfer processes. S. Hammes-Schiffer

**8:40 PHYS 274.** Insights into the structural motifs of aqueous clusters from the modeling of their infrared spectra. S.S. Xantheas

**9:20 PHYS 275.** Atomistic simulations for spectroscopic applications. M. Meuwly

**10:00** Intermission.

**10:20 PHYS 276.** Single molecule STM imaging and spectroscopic studies of the hydrogen-atom transfer reaction in porphyrane adsorbed to the Cu(110) surface. D.A. Baugh, T. Kumagai, S. Gawinkowski, J. Waluk, S. Levchenko, S. Liu, Z. Zhao

**10:40 PHYS 277.** Controlled formation and vibrational characterization of large solvated ionic clusters. E. Garand

**11:20 PHYS 278.** Vibrational motion of Zundel form of proton. J. Kuo

### Section C

San Diego Convention Center  
Room 28D

#### Electronic Structure & Dynamics of Metastable States

K. B. Bravaya, *Organizer*

K. D. Jordan, *Organizer, Presiding*

**8:00 PHYS 279.** Complex-variable approaches for metastable electronic states. A. Krylov

**8:40 PHYS 280.** Two-dimensional electron impact spectra, electrons and ionic liquids and electronic excitation of pyrimidine. M. Allan

**9:20 PHYS 281.** Equation-of-motion coupled-cluster method with complex absorbing potential for metastable electronic states. M. Schneider, A. Krylov

**9:40** Intermission.

**10:00 PHYS 282.** Algebraic diagrammatic construction scheme: A versatile approach to decaying electronic states. A. Dreuw

**10:40 PHYS 283.** Studies of medium-size temporary anions with complex absorbing potentials and the SAC-CI method. T. Sommerfeld, M. Ehara

**11:20 PHYS 284.** Complex absorbing potential extended multiconfigurational quasidegenerate perturbation theory. A. Kunita, A. Granovsky, K.B. Bravaya

### Section D

San Diego Convention Center  
Room 28E

#### Frontiers in Solar Light Harvesting Processes

T. Krauss, A. Mohite, O. V. Prezhdo, *Organizers*

S. Tretiak, *Organizer, Presiding*

**8:00 PHYS 285.** Effects of charge delocalization on long-lived charge carriers in low dielectric media. G. Rumbles

**8:40 PHYS 286.** Effect of intra- and interchain interaction on energy transfer in single conjugated polymers and aggregates. D. Vanden Bout, Z. Hu

**9:20 PHYS 287.** Evolutionary design of emitters for organic light-emitting diodes. Y. Shu, B.G. Levine

**9:40** Intermission.

**10:05 PHYS 288.** On the role of intermixed phases in organic photovoltaic blends. N. Stingelin

**10:45 PHYS 289.** Entropy and disorder enable charge separation in organic solar cells. S. Hood, I. Kassal

**11:25 PHYS 290.** Bias and energy dependent coupling between molecular states and metallic states in molecular junctions. Z. Liu, J. Neaton

### Section E

San Diego Convention Center  
Room 29B

#### Structure & Dynamics in Enzymatic Catalysis across Multiple Timescales: Experiment & Theory

##### The World of Vibrations

Cosponsored by BIOL

S. Stoll, *Organizer*

H. S. Shafaat, *Organizer, Presiding*

C. H. Londergan, *Presiding*

**8:30 PHYS 291.** Probing low frequency vibrational excitations and their effect on electron, proton, and group transport in proteins. P.M. Champion

**9:05 PHYS 292.** Protein dynamic fluctuations probed by QM/MM FTIR simulations. J. Gao

**9:25 PHYS 293.** Vibrational probe groups in enzymes: The importance of functional group diversity. C.H. Londergan

**9:45** Intermission.

**10:00 PHYS 294.** Coupling of vibrations to charge transfer processes in photochemical reactions relevant to enzyme catalysis. M.H. Khalil

**10:35 PHYS 295.** Using resonance Raman spectroscopy to probe cofactor assembly in R2lox, a novel heterobimetallic oxidase. P. Mauger, N. Trivelas, E.K. Miller, H.S. Shafaat

**10:55 PHYS 296.** Oxygenic ligands in the catalysis by iron enzymes.

D.A. Proshlyakov, Y.D. Proshlyakov, C. John, R. Banerjee, M. Farrugia, B. Zhang, M. Pantelias, C. Krebs, J.M. Bollinger, J.D. Lipscomb, R.P. Hausinger

**11:15** Intermission.

**11:30 PHYS 297.** Vibrational stark effects, solvatochromism and electric fields at the active sites of enzymes. S.G. Boxer, Y. Wu, S. Schneider

**12:05 PHYS 298.** Nuclear and electronic delocalization in enzyme hydrogen bond networks. L. Wang, S.D. Fried, S.G. Boxer, T. Markland

**12:25 PHYS 299.** Vibrational and electronic Stark effects in green fluorescent protein. J.D. Slocum, L.J. Webb

### Section F

San Diego Convention Center  
Room 29C

#### Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials

D. Eisele, *Organizer*

A. P. Willard, *Organizer, Presiding*

**8:00 PHYS 300.** Self-assembly and mechanical properties of a physically associating gel. S. Kundu, S. Hashemnejad, M. Zabet, S. Mishra

**8:30 PHYS 301.** Controlling interchromophore coupling in symmetric dimers: The role of bridge's electronic structure. C. Cruz, P. Christensen, E.L. Chronister, D. Casanova, M.O. Wolf, C.J. Bardeen

**8:50 PHYS 302.** Exploring the relationship between cage forming ligands and the network structure of their gels. E. Alt, A.P. Willard

**9:10** Intermission.

**9:20 PHYS 303.** Self-assembled nanocontainers assembled via the hydrophobic effect. B.C. Gibb

**9:50 PHYS 304.** Revealing relationships between conformation and photophysics in single conjugated polymers and aggregates. D.T. Hoang, J. Yang, H. Park, L. Kaufman

**10:10 PHYS 305.** Molecular dynamics study of self-assembly of low molecular mass organic gelators. M. Huda, N. Rai

### Section G

San Diego Convention Center  
Room 29D

#### Towards Predictive Calculations in Strongly Correlated Molecules & Materials

T. C. Berkelbach, E. Neuscamman, *Organizers*

T. A. Van Voorhis, *Presiding*

**8:00 PHYS 306.** Systematically improvable Green's function embedding methods for molecules and solids. D. Zgid

**8:45 PHYS 307.** Large scale Stochastic GF2 calculations. D. Neuhauser, R. Baer, E. Rabani, D. Zgid

**9:10 PHYS 308.** Hubbard operator density functional theory for Fermionic lattice models. Z. Cheng, C. Marianetti

**9:55** Intermission.

**10:15 PHYS 309.** Understanding correlated electron materials: The insight from the functional dynamical mean field approach. K. Haule

**11:00 PHYS 310.** Taming the dynamical sign problem in the real time evolution of quantum impurity problems. D.R. Reichman

### Section H

San Diego Convention Center  
Room 30A

#### Physical Principles in Functional Nanoscience: Symposium in honor of Mostafa A. El-Sayed

C. F. Landes, S. Link, *Organizers*

P. K. Jain, *Organizer, Presiding*

**8:00 PHYS 311.** 4D electron microscopy: A century of developments. A.H. Zewail

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)



**8:35 PHYS 312.** Super-resolution algorithm for 3D single-molecule microscopy imaging. **B. Shuang**, W. Wang, H. Shen, L.J. Tauzin, C. Flatebo, C.F. Landes

**8:55 PHYS 313.** Hydration structure of aqueous carbonic acid and carbon dioxide from x-ray absorption spectroscopy. **R.J. Saykally**

**9:30 PHYS 314.** Tuning the acoustic frequency of a gold nanodisk through its adhesion layer. **M. Su**, W. Chang, F. Wen, D. Chakraborty, Y. Zhang, B. Shuang, P.J. Nordlander, J.E. Sader, N.J. Halas, S. Link

**9:50** Intermission.

**10:10 PHYS 315.** Single nanoparticle SERS and TERS studies of plasmonic photochemistry. **R.P. Van Duyne**

**10:45 PHYS 316.** Carrier dynamics in cerium oxide nanoparticles observed by femto-second transient absorption spectroscopy. **N.W. Pettinger**, **B. Kohler**

**11:05 PHYS 317.** Laser trapping assembling and crystallization of nanoparticles at solution surface. **H. Masuhara**, K. Yuyama, M. Muramatsu, T. Sugiyama

**11:40 PHYS 318.** Laser-induced currents along nanoscale junctions. **L. Chen**, **I. Franco**

### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

#### Landscapes, Disorder & Enhanced Sampling

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#### The History of Chemistry & Computing

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#### Computer-Aided Drug Design

#### Real World Dynamics

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#### Elucidation of Mechanisms & Kinetics on Surfaces

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#### Quantum Mechanics

Sponsored by COMP, Cosponsored by PHYS

## WEDNESDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 29A

#### Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events

R. Elber, R. M. Levy, C. F. Wong, D. M. Zuckerman, *Organizers*

E. Gallicchio, *Presiding*

**1:30 PHYS 319.** Umbrella sampling folding of intrinsically disordered proteins. **A. Dinner**

**2:00 PHYS 320.** Exploring channel permeation with enhanced sampling. **M. Grabe**

**2:30 PHYS 321.** Complex role of solvation in micelle and reverse micelle environments. **J.E. Straub**, R. Urano

**3:00** Intermission.

**3:15 PHYS 322.** Modeling ligand-protein binding kinetics: the continuous and dynamical processes in ligand association/dissociation. **C. Chang**, W. You, M. Raymundo, Z. Tang

**3:45 PHYS 323.** Enhanced sampling and its applications in high-accuracy refinement of protein low-resolution models. **T. Zang**, J. Ma

**4:15** Intermission.

**4:30 PHYS 324.** Dependence of internal friction on local and global barrier height. **W. Zheng**, D. De Sancho, R.B. Best

**5:00 PHYS 325.** Molecular origins of friction in unfolded proteins. **D.E. Makarov**, S. Avdoshenko, A. Das

### Section B

San Diego Convention Center  
Room 28C

#### Decoding the Spectroscopic Signatures of Large Amplitude Motions: Challenges & Opportunities for Theory & Experiment

Z. Bacic, M. A. Johnson, *Organizers*

T. Markland, *Presiding*

**1:30 PHYS 326.** H<sub>2</sub>, D<sub>2</sub>, and HD inside C<sub>60</sub>: The coupled translation-rotation quantum dynamics and the selection rules in the inelastic neutron scattering spectroscopy. **M. Xu**, S. Ye, Z. Bacic

**2:10 PHYS 327.** Translational/rotational dynamics of multiple confined species. **P.M. Felker**

**2:50 PHYS 328.** Quantum translator-rotator dynamics of small molecule endofullerenes: Neutron scattering investigations of the nuclear spin-isomers of H<sub>2</sub> and H<sub>2</sub>O. **A.J. Horsewill**, M. Jimenez Ruiz, M. Johnson, M. Levitt, S. Mamone, J. Ollivier, S. Rols

**3:30** Intermission.

**3:50 PHYS 329.** Structure, dynamics and rotational tunneling of methane in metal-organic frameworks. **T. Yildirim**, W. Zhou

**4:30 PHYS 330.** Site selective spectroscopy: Interactions of adsorbed hydrogen in metal-organic frameworks. **S. Fitzgerald**, C. Eckdahl, K. Shinbrough, C. McDonald, H. Lai, J. Nelson

### Section C

San Diego Convention Center  
Room 28D

#### Electronic Structure & Dynamics of Metastable States

K. D. Jordan, *Organizer*

K. B. Bravaya, *Organizer, Presiding*

**1:30 PHYS 331.** Dynamics of anionic resonances probed by frequency, angle- and time-resolved photoelectron imaging. **J.R. Verlet**

**2:10 PHYS 332.** Role of metastable electronic states in the light-induced electron emission properties of biochromophore anions. **A.V. Bochenkova**

**2:50 PHYS 333.** Photoelectron wave function in photoionization: Plane wave or coulomb wave? **S. Gozem**, D.L. Osborn, J. Stanton, A. Krylov

**3:10** Intermission.

**3:30 PHYS 334.** Using chemistry to control electron emission from the photoactive yellow protein chromophore. **M. Parkes**, C. Phillips, M.J. Porter, **H. Fielding**

**4:10 PHYS 335.** Novel relaxation pathways in liquid phase: Concerted electronic and nuclear motion. **P. Slavicek**

**4:50 PHYS 336.** Reexamining the hydrated electron's first excited state lifetime through temperature-dependent femto-second transient absorption. **E.P. Farr**, C. Zhou, B.J. Schwartz

### Section D

San Diego Convention Center  
Room 28E

#### Frontiers in Solar Light Harvesting Processes

T. Krauss, A. Mohite, O. V. Prezhdo, S. Tretiak, *Organizers*

N. Stingelin, *Presiding*

**1:30 PHYS 337.** Regioregular narrow bandgap conjugated polymers for the fabrication of high performance solution deposited organic solar cells. **G.C. Bazan**

**2:10 PHYS 338.** Soft supra-molecular nanotubes for robust light harvesting. **D.M. Eisele**

**2:50 PHYS 339.** Size of triplet excitons in polythiophene: Evidence from resonance Raman spectra of oligomers. **M.J. Tauber**

**3:10** Intermission.

**3:30 PHYS 340.** Electronic processes in low bandgap polymers for OPV and photocatalytic applications. **L.X. Chen**

**4:10 PHYS 341.** New ways to activate organic triplet states for photon upconversion in the visible and near-infrared. **C.J. Bardeen**, Z. Huang, X. Li, M. Makhboub, K.M. Hanson, V. Nichols, C.D. Cruz, H. Le, M.L. Tang, E.L. Chronister

**4:50 PHYS 342.** Harvesting solar energy from singlet fission materials. **A.K. Le**, J. Bender, R. Pandey, A.P. Moon, **S.T. Roberts**

**5:10 PHYS 343.** Directional charge separation in isolated 7,8,15,16-tetraazaterrylene (TAT) crystalline nanowires. **M. Barnes**, J. Labastide, H.B. Thompson, S.R. Marques, A.L. Briseno

### Section E

San Diego Convention Center  
Room 29B

#### Physical Chemistry of Complex Environmental Interfaces

Cosponsored by COLL

V. H. Grassian, G. M. Nathanson, *Organizers*

V. Vaida, *Presiding*

**1:30 PHYS 344.** Direct views of aerosol particle surfaces. **F. Geiger**

**2:10 PHYS 345.** Water uptake and surface tension of individual submicron size sea spray aerosol particles studied with atomic force microscopy. **H. Morris**, V.H. Grassian, A.V. Tivanski

**2:30 PHYS 346.** Molecular level explanation of emulsion stability: it is not what you think. **E. Zdrali**, Y. Chen, **S. Roke**

**3:10** Intermission.

**3:30 PHYS 347.** Mechanisms and dynamics of atmospherically-relevant molecular reactions at liquid water surfaces. **R.B. Gerber**

**4:10 PHYS 348.** Toward understanding interfacial behavior of multi-component environmental systems. **L. McWilliams**, N.A. Valley, G.L. Richmond

**4:30 PHYS 349.** Modeling interfacial chemistry from many-body molecular dynamics simulations. **F. Paesani**

**5:10 PHYS 350.** Surface potential of DPPC monolayers on concentrated aqueous salt solutions as a model of marine aerosols. **D. Verreault**, E. Adams, C.B. Casper, H.C. Allen

### Section F

San Diego Convention Center  
Room 29C

#### Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials

D. Eisele, A. P. Willard, *Organizers*

R. Ulijn, *Presiding*

**1:30 PHYS 351.** Photophysical properties of multichromophoric architectures of perylene bisimide dyes. **F. Wuerthner**

**2:00 PHYS 352.** Three dimensional self-assembled monolayers around nanodroplets for lipid studies. **Y. Chen**, C. Luetgebaucks, H. Okur, **S. Roke**

**2:20 PHYS 353.** Discerning the effect of counter ions on supramolecular self-assembly. **S.J. Belh**, K. Ng, G. Huffman, A. Chowdhury, N. Yehya, D.M. Eisele

**2:40 PHYS 354.** Huddling together when something is missing: Supramolecular aggregation in monolacunary Keggin anions. **S. Serapian**, A. Neyman, C. Bo, I.A. Weinstock

**3:00** Intermission.

**3:10 PHYS 355.** Supramolecular self-assembly of amphiphilic synthetic redox proteins. **B.A. Fry**, G. Goparaju, C.C. Moser, P. Dutton, **B.M. Discher**

**3:40 PHYS 356.** Phase behavior of complex lipid mixtures: Signatures of spatial organization. **S. He**, K. Sapp, **L. Maibaum**

**4:00 PHYS 357.** Role of environmental conditions on the photochemical synthesis and self-assembly of amphiphiles in aqueous solution. **R. Rapf**, R. Perkins, V. Vaida

**4:20 PHYS 358.** Designing multiscale models for self-assembling peptides. **M. McCullagh**, P. Lake

### Section G

San Diego Convention Center  
Room 29D

#### Physical Principles in Functional Nanoscience: Symposium in honor of Mostafa A. El-Sayed

P. K. Jain, C. F. Landes, S. Link, *Organizers*

X. Huang, *Presiding*

**1:30 PHYS 359.** Symmetry breaking during the nucleation and growth of colloidal metal nanocrystals. **Y. Xia**

**2:05 PHYS 360.** Nanostructured stress transduction device: Combining piezoelectric and piezoresistive functional materials to drive metal insulator transitions for fast, low power electronics. **G.J. Martyna**

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- 2:25 PHYS 361.** Design principles for sustainable catalysis from fundamental surface chemistry. **C.M. Friend**, S.G. Karakalos, F. Hiebel, Y. Xu, W. Chen, F. Kabeer, M. Montemore, B. Zucig, J. Biener, A. Tkatchenko, E. Kaxiras, R.J. Madix
- 3:00 PHYS 362.** Imaging intermolecular energy transfer between single quantum dots and carbon nanotubes. **D. Nguyen**, J. Lyding, M. Gruebele
- 3:20 Intermission.**
- 3:40 PHYS 363.** Looking beyond plasmonics: Synergetic effects in silver nanoparticles coupled with thiolated gold clusters. **P.V. Kamat**, K. Stamplecoskie
- 4:15 PHYS 364.** Cation exchange at the single nanocrystal level: Mechanistic and kinetic insights. **A.L. Routzahn**, P.K. Jain
- 4:35 PHYS 365.** Plasmonic nanostructures as nanoscale electrodes. **K.A. Willets**
- 5:10 PHYS 366.** Withdrawn.

### From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules

#### Interactions at Small & Large Scales

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## WEDNESDAY EVENING

### Section A

San Diego Convention Center  
Hall D

#### Poster Session

G. S. Engel, *Organizer*

#### 7:00 - 9:00

- PHYS 367.** Relaxation mechanisms of model sea spray aerosols. **B.A. Wellen**, A.S. Vidalis, E.A. Lach, H.C. Allen
- PHYS 368.** Interactions of aromatic amino acids with phospholipid monolayers and bilayers. **R. Perkins**, V. Vaida
- PHYS 369.** Effect of cation enrichment on the organization of a DPPC monolayer at the air-aqueous interface. **E. Adams**

### Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

- PHYS 370.** Multiphase photochemistry of pyruvic acid and surface active products. **A. Reed Harris**, V. Vaida, R. Rapf, A. Monod, J. Doussin, A. Gratien, M. Cazaunau
- PHYS 371.** Determination of orientation of bipyridine Re(I) fac-tricarbonyl electrocatalysts on Au and on TiO<sub>2</sub> surfaces through computational SFG spectroscopy. **B. Rudshteyn**, A. Ge, M.L. Clark, B. Psciuk, C.P. Kubiak, T. Lian, V.S. Batista
- PHYS 372.** Role of aerosol water in secondary organic aerosol formation from volatile organic compounds. **J. Faust**, J. Wong, A. Lee, J.P. Abbatt
- PHYS 373.** Rapid autoxidation of squalene particles forms multifunctional hydroxyperoxides. **N. Heine**, K.R. Wilson
- PHYS 374.** Characteristics of ice nucleating particles in seawater and sea spray aerosol produced during laboratory phytoplankton blooms. **T.C. Hill**, C. McCluskey, J. Michaud, M.V. Santander, G.C. Cornwall, C. Sultana, C. Lee, H. Al-Mashat, O. Laskina, J. Trueblood, V.H. Grassian, C. Beall, K. Moore, K.A. Prather, S. Kreidenweis, P.J. DeMott
- PHYS 375.** Studies of the transfer of humic substances (HULIS) across the air-sea interface. **M.V. Santander**, C. Lee, J. Axson, M.J. Tauter, G. Deane, K.A. Prather
- PHYS 376.** Vacuum ultraviolet ionization studies of complexes and clusters in a molecular beam. **B. Bandyopadhyay**, Y. Fang, O. Kostko, M. Ahmed, A. White, M.P. Head-Gordon
- PHYS 377.** Impact of enzymatic activity on sea-spray aerosol climate properties. **O.S. Ryder**, J. Michaud, C. Lee, V.H. Grassian, C. Pohlker, M.O. Andreae, R.C. Moffet, K.A. Prather
- PHYS 378.** Assessment of saccharide enrichment in different compartments of the ocean using anion-exchange chromatography. **T. Jayarathne**, E.A. Stone
- PHYS 379.** Methodology improvements for calculation of vibrational sum-frequency spectra of aqueous organic interfaces. **B. Gordon**, G.L. Richmond, N.A. Valley
- PHYS 380.** Chemical adsorption kinetics of model trace organics at marine bubble interfaces. **J.L. Cox**, D. Stokes, G. Deane, G.M. Nathanson, T.H. Bertram
- PHYS 381.** Effect of biological processes on sea spray aerosol composition and the impact on nitric acid heterogeneous reactivity. **C. Lee**, O.S. Ryder, J. Michaud, J. Trueblood, A. Estillore, V.H. Grassian, K.A. Prather
- PHYS 382.** Secondary organic aerosol (SOA): Analyzing degree of internal complexity and effect of changing relative humidity (RH). **S. Niles**, A. Bondy, P.K. Peterson, R.C. Moffet, R. O'Brien, B. Wang, A. Laskina, M.V. Nhliziyo, S.B. Bertman, P.B. Shepson, K.A. Pratt, A.P. Ault
- PHYS 383.** Single particle studies of growth and phase changes in model sea-spray aerosols. **K.A. Nadler**, M. Miller, R.E. Continetti
- PHYS 384.** Development of new instrumental approaches to characterize the fundamental chemistry of the sea surface microlayer. **J. DePalma**, M.A. Johnson
- PHYS 385.** Withdrawn.
- PHYS 386.** Photolysis of atmospherically relevant carbonyl compounds in different phases. **S.H. Kim**, C.R. Engelmann, L.T. Fleming, K. Malecha, S.A. Nizkorodov
- PHYS 387.** Characterization of gaseous flow-fields using the stereo-VENOM technique. **M.H. McIlvoy**, F. Pan, R. Sanchez-Gonzalez, S.W. North, R.D. Bowersox
- PHYS 388.** Measuring uptake coefficients for amines on dicarboxylic acids as models for secondary organic aerosol growth. **M.C. Fairhurst**, M.J. Ezell, C. Kidd, B.J. Finlayson Pitts
- PHYS 389.** Ultraviolet absorption of the propargyl radical around 240 nm. **R. Li**, M.R. Hoffmann
- PHYS 390.** Investigating particle phase and growth mechanisms: Studying organic nitrate uptake into secondary organic aerosol. **A.C. Vander Wall**, V. Perraud, B.J. Finlayson Pitts
- PHYS 391.** Integrating composition and health effects of ambient ultrafine particles. **L.M. Wingen**, A. Keebaugh, D. Herman, S. Renush, M.T. Kleinman, B.J. Finlayson Pitts
- PHYS 392.** Importance of proton transfer in CO<sub>2</sub> capture and reduction. **J. Patrow**, J. Dawlaty
- PHYS 393.** Atmospheric microbiome: Implications for sea spray aerosol properties. **J. Michaud**, C. Lee, C. Sultana, A. Rabines, F. Malfatti, F. Azam, A. Allen, R. Knight, K.A. Prather, M.D. Burkart
- PHYS 394.** Crystal density of natural and artificial gas hydrates including hydrocarbons. **M. Kida**, M. Watanabe, Y. Konno, J. Yoneda, Y. Jin, J. Nagao
- PHYS 395.** Charge detection mass spectrometry and the aerosol impact spectrometer. **M.E. Miller**, B. Adamson, R. Otto, R.E. Continetti
- PHYS 396.** Design and implementation of a new sea surface microlayer sampler. **J. Sauer**, K.A. Prather, J. Mayer
- PHYS 397.** Exploring the effect of organics on new particle formation and growth from methanesulfonic acid, amines, and water. **K.D. Arquero**, J. Xu, M.J. Ezell, R.B. Gerber, B.J. Finlayson Pitts
- PHYS 398.** Furfural: Unimolecular photodissociation reactions of the simplest furanic aldehyde. **M. Winfough**, A. Bodi, G. Muller, G. Laguisma, G. Meloni
- PHYS 399.** Investigation of the anomalous spectroscopic signatures of the water dimer cation. **J. Talbot**, X. Cheng, J. Herr, R. Steele
- PHYS 400.** Characterization of gas selectivity of the ionic clathrate hydrate formed with tetra-*n*-butylammonium bromide. **S. Muromachi**, S. Takeya, Y. Yamamoto
- PHYS 401.** Thermodynamic inhibition of CO<sub>2</sub> hydrate in the presence of morpholinium and piperidinium ionic liquids. **C. Ha**, Y. Lee, S. Hyeon, **J. Kang**, **K. Kim**
- PHYS 402.** Decay kinetics of photosensitizer triplet states in model organic aerosol particles. **E. Woods**, Y. Jiang, A. Ofosuhenue, U. Ghani
- PHYS 403.** Novel evaluation of defoamer performance in brown stock washing. **C. Kirwan**
- PHYS 404.** Advances in computational modeling of the atmospheric chemistry of the Criegee intermediate. **K.T. Kuwata**
- PHYS 405.** Determination of the activation energy of the rate-limiting step of the Fenton reaction. **L. Ligon**, P. Tumlin, T. Cohen, T. Spence
- PHYS 406.** Dye-protein investigation with circularly polarized light. **A. Braimah**, W. Newhart, C.K. Johnson
- PHYS 407.** Spectroscopic study of energy transfer processes in the R<sub>2</sub>(C<sub>3</sub>H<sub>10</sub>O<sub>2</sub>)<sub>2</sub> coordination polymers. **Y. Lin**, S. Wen, K. Li, **B. Chang**
- PHYS 408.** Ion-radical pair characteristics in oxidized water clusters, (H<sub>2</sub>O)<sub>n=1-21</sub>. **J. Herr**

- PHYS 409.** Electronic sum-frequency generation (ESFG) spectroscopy: Theoretical formulation of resonances with symmetry-allowed and symmetry-forbidden excited states. **C. Lin**, Y. Yeh, S. Lin
- PHYS 410.** Interaction of water vapor with sugars and biological components of sea spray aerosol and mixtures of sea-salt with biologically derived compounds. **A.D. Estillore**, Z. Qin, A.V. Tivanski, V.H. Grassian
- PHYS 411.** Studies of kinetics and energy barriers to the oxidation of indigotetrasulfonate in a unique polyelectrolyte ink system. **B. Hoene**, D. Rivera
- PHYS 412.** Unimolecular rate constant determination for 1,1-DCI and 1,2-HCl elimination reactions from CD<sub>2</sub>CD<sub>2</sub>CHCl<sub>2</sub>. **A. Larkin**, G.L. Heard, B.E. Holmes
- PHYS 413.** Materials characterization and photobleaching utilizing Raman spectroscopy. **S. Lambeth**, A. Lipshaw, M.D. Sonntag
- PHYS 414.** Co-operative motion of multiple benzoquinone disks at the air-water interface. **J. Satterwhite**, D.K. Kondepudi, J.A. Dixon, J.F. Rusling
- PHYS 415.** Experimental unimolecular rate constants for the 2,1-DX, 1,1-HX (X = F, Cl) and 1,2-HCl elimination reactions for CD<sub>2</sub>ClCHCl<sub>2</sub>. **T.M. Brown**, M.J. Nestler, G.L. Heard, B.E. Holmes
- PHYS 416.** Probing band gaps of organic semiconductors at buried interfaces by electronic sum frequency generation spectroscopy. **Y. Li**, J. Wang, W. Xiong
- PHYS 417.** Application of the DSRG-MRPT2 in singlet-triplet gaps in organic diradicals and transition complexes. **K.P. Hannon**, C. Li, F.A. Evangelista
- PHYS 418.** Computational tools for the simulation of vibronic spectra of flexible systems. **A. Baiardi**, J. Bloino
- PHYS 419.** Phonon spectra from molecular dynamics. **I.B. Magdud**, G. Ackland
- PHYS 420.** Ultrafast proton transfer dynamics of a 5-substituted quinoline photobase series in aqueous solution. **E. Driscoll**, J. Dawlaty
- PHYS 421.** Investigation of charge transfer from a film of Zinc phthalocyanine to single- and double-layer graphene. **A. Biancardi**, C. Caraianni, M. Caricato
- PHYS 422.** Efforts towards prediction of NH(D) and CH(D) isotopic exchange effects on <sup>13</sup>C NMR spectra of small, rigid peptides via computational quantum chemistry. **E. Kleist**, B.S. Hudson
- PHYS 423.** Cluster model study of the structures and interactions in the formation of atmospheric aerosol nucleation embryos. **G. Hou**, M. Valiev, X. Wang
- PHYS 424.** Other conformations of caprylolactam: A computational study. **B.S. Hudson**, O. Melton, E. Kleist
- PHYS 425.** Thermodynamic properties and crystal structures in TBAB+TBAC mixed semi-clathrate hydrate systems. **M. Oshima**, M. Kida, Y. Jin, J. Nagao
- PHYS 426.** Microwave spectroscopy of cyclopropanecarboxylic acid and the cyclopropanecarboxylic acid-formic acid dimer. **A.M. Pejovias**, **W. Lin**, S.G. Kukulich
- PHYS 427.** Resonance Raman investigation of the interaction between aromatic dithiocarbamate ligands and CdSe quantum dots. **J.J. Grenland**, K. Gong, C. Lin, D.F. Kelley, **A.M. Kelley**
- PHYS 428.** Raman spectroscopic study of solvent-mediated electron-transfer chemical doping of graphene. **R.A. Dziatko**, I.M. Klein, J. Karten, B. Janicek, **A. Crowther**

- PHYS 429.** Amorphous solid water: Pulsed heating of buried  $N_2O_4$ . J.E. Stornberg, S. McKean, C. Larson, H. Reisler, C. Wittig
- PHYS 430.** Millimeter-wave spectroscopy of diketene: Determination of the rotational constants for the third quantum vibration ( $v_{24}$ ). P.M. Kirkconnell, V.L. Orr, B.K. Amberger, B.J. Esselman, R.C. Woods, R.J. McMahon
- PHYS 431.** Ultrafast conformational fluxionality of organometallic catalytic intermediate revealed by 2D IR spectroscopy. J. Wang, W. Xiong
- PHYS 432.** Quantum surface control for trapped Bose-Einstein-Condensates. Q. Wang
- PHYS 433.** Modified relaxation dynamics in coupled vibration-cavity polaritons. A.D. Dunkelberger, K. Fears, B.T. Spann, B.S. Simpkins, J. Owrutsky
- PHYS 434.** Structures and nuclear quadrupole coupling tensors of 1,2-dichloroethane, 1-chloro-2-fluoroethane and 2,3-dichloropropene studied using microwave spectroscopy and computational chemistry. A.S. Dikkumbura, E.R. Webster, R.E. Dorris, R.A. Peebles, S.A. Peebles, N.A. Seifert, B.H. Pate
- PHYS 435.** Withdrawn.
- PHYS 436.** Effect of small, polar organics on the domain structures of dipalmitoylphosphatidylcholine (DPPC) monolayers during compression. C.G. Israel, H.C. Allen
- PHYS 437.** Using Raman spectroscopy to determine thiol functions and thiol-mediated redox equilibria. L.G. Frenzel-Sulyok, C.H. Londergan
- PHYS 438.** Effect of a second halogen atom on the nature of intermolecular interactions in protic acid-haloethylene bimolecular complexes. H.O. Leung, M.D. Marshall, A.J. Lee, H.K. Tandon
- PHYS 439.** Photoelectron-photofragment coincidence studies of cold negative ions. B.B. Shen, Y. Benitez, K. Lunny, R.E. Continetti
- PHYS 440.**  $\pi$ -stacking of pyrene is concentration dependent and affects excimer formation kinetics. A. Durff, A.D. Hanlon, B.H. Milosavljevic
- PHYS 441.** Resonant pump-probe spectroscopic measurements of terahertz frequency phonons in solid samples. B. Dastrup
- PHYS 442.** Use of second harmonic generation for nondestructive testing of aluminum alloys. A. Farnsworth, S. Averett, D. Broderick, J.E. Patterson
- PHYS 443.** TA, DSC and photophysical study of phase transitions in glycerol-water mixture. B.B. Saad, A. Harris, P. Venugopal, B.H. Milosavljevic
- PHYS 444.** Potential light-induced risks associated with expanding the genetic alphabet. B. Ashwood, M. Pollum, C. Crespo-Hernández
- PHYS 445.** Solution dynamics of iron and osmium pentacarbonyl in halogenated solvents. C.P. Baryames, C. Laperle
- PHYS 446.** Microwave spectrum and molecular structure of the argon-*cis*-1,2-dichloroethylene complex. M.D. Marshall, H.O. Leung, C.J. Nelson, L.H. Yoon
- PHYS 447.** Predicting the photosensitivity of photosensitive drugs. J. Andrews, A. Bills
- PHYS 448.** Reaction kinetics of the CN radical with methyl bromide reaction. M. Hodny, J.F. Hershberger
- PHYS 449.** Characterization of SCN vibrational probe group depth dependence in poly-L transmembrane peptides. S.T. Gebre, C.H. Londergan
- PHYS 450.** Temperature and confinement effects on the spectral properties of PRODAN indicate that it can be used as a luminophore for liquid-solid phase transitions. C. Somerville, B.H. Milosavljevic
- PHYS 451.** Effect of the substitution of tryptophan for phenylalanine in dipeptides. M.A. Shebel, J.A. Thomas
- PHYS 452.** Withdrawn.
- PHYS 453.** DSC, IR, rheological & photophysical study of phase transitions in poly(propylene glycol) - water binary mixture. S.D. Lovrinic, C. Malls, B.H. Milosavljevic
- PHYS 454.** Facile approaches of new biosensor using system of enzymatic and analytical techniques. Y. Lo, E.J. Parish, T. Wei, H. Honda
- PHYS 455.** Predicating photosensitivity in pharmaceutical drugs. A. Bills, J. Kellerson
- PHYS 456.** Dynamic and mechanism of hole-transport in DNA-hairpin model systems. F.D. Lewis, A.K. Mishra
- PHYS 457.** Photoinduced charge transport in DNA. A. Singh, R. Young, M.R. Wasielewski, F.D. Lewis
- PHYS 458.** Terahertz spectra of DNA nucleotides. D. Wei, M. Zhang, S. Yan
- PHYS 459.** Understanding virulence in *Mycobacterium tuberculosis*: Characterizing cofactor assembly in the novel Mn/Fe lipid oxidases. N. Trivelas, E.K. Miller, P.T. Mauger, H.S. Shafaat
- PHYS 460.** Influence of  $Ca^{2+}$  vs  $Mg^{2+}$  binding to negatively charged phosphatidic acid monolayers studied by infrared reflection-absorption spectroscopy and surface tensiometry. T. Zhang, M.G. Catcart, H.C. Allen
- PHYS 461.** Protonation states of oxygenic ligands in the non-heme iron dioxxygenase, TauD. C. John, G. Swain, R.P. Hausinger, D.A. Proshlyakov
- PHYS 462.** Proton pumping and water exit pathway in B-type cytochrome c oxidase from thermus thermophilus. L. Yang, Å.A. Skjevik, W. Han Du, L. Noodleman, R.C. Walker, A.W. Goetz
- PHYS 463.** Development of FRET assays for investigating the interaction between fibroblast growth factor (FGF) and its receptor (FGFR). M. Mohale
- PHYS 464.** BOMD calculations elucidate effect of temperature on  $Na^+$ (tryptamine)  $(H_2O)_{1-2}$  cluster ions. J. Toberman, J. Beck
- PHYS 465.** Investigation and characterization of membrane protein folding in small unilamellar vesicles (SUVs) and nanodiscs. D.K. Asamoto, G. Kang, J.E. Kim
- PHYS 466.** Interactions of beta scorpion toxin with Nav1.6 sodium channels. D.W. Ball, W.R. Martin
- PHYS 467.** Unraveling electron transfer pathways in cryptochromes. R.N. Tazhigulov, K.B. Bravaya
- PHYS 468.** Probing DNA interactions with carboplatin utilizing surface-enhanced Raman scattering. S. Khan, N. Mirsaleh-Kohan
- PHYS 469.** On the origin of sugar selectivity by DNA polymerase. H. Yoon, A. Warshel
- PHYS 470.** Dependence of water exchange values and thermodynamic quantities on DNA binding mode and sequence. R. Kenney, K. Buxton, S. Glazier
- PHYS 471.** Dynamic structure of alpha-synuclein bound to micelles and vesicles as reported by IR spectra site-specific SCN probe groups. D.M. Konstantinovskiy, C.H. Londergan
- PHYS 472.** Investigating dynamic protein-protein binding interactions in the Nipah and Hendra virus ntail-XD complexes using the cyanylated cysteine vibrational probe. R.N. King, M. Khromava, R.B. Wai, C.H. Londergan
- PHYS 473.** Surface-enhanced Raman scattering of cisplatin derivatives: Carboplatin, oxaliplatin and nedaplatin. M. Torres, M. Duplanty, N. Mirsaleh-Kohan
- PHYS 474.** Influence of damaged mRNA on codon:anticodon selectivity in the ribosomal decoding center. L. Albrecht, S.D. Wetmore
- PHYS 475.** Activation properties of the association and dissociation of doxorubicin and DNA. E. Curtis, A. Hill, S. Glazier
- PHYS 476.** Computational study of spin crossover in the  $Fe_2S_2$ -ferredoxin active site model. A.O. Lykhin, S.A. Varganov
- PHYS 477.** *E.coli* RNA polymerase activity under crowding. S. Chung, E. Lerner, Y. Jin, Y. Alhadid, S. Kim, C.M. Knobler, W.M. Gelbart, S. Weiss
- PHYS 478.** Comparative study of gold nanoparticles coated with human serum albumin as drug carriers. S. Sulaiman, O. Abou-Zied
- PHYS 479.** Rupture of a graphene membrane under an electric field using DFTB. K. Reiss, J. Jakowski, J.W. Mazza
- PHYS 480.** Absorbance and fluorescence properties of bis(benzimidazole)perylene dyes in polysiloxane matrix containing gold nanoparticles. N. Barashkov, A. Mantel, A. Aldongarov, I. Irgibaeva
- PHYS 481.** On-grey-off transitions in core/multi-shell quantum dots. P. Bajwa, F. Gao, C.D. Heyes
- PHYS 482.** Modification of titanium dioxide by mono- and bimetallic nanoparticles to improve the activity of the photocatalytic reduction of carbon dioxide by water vapor. M. Ovcharov, V. Shvalagin, T. Sakhno, N. Barashkov, V. Granchar
- PHYS 483.** Second harmonic generation studies on plasmonic nanoparticles for light-mediated drug delivery. B.P. Kruger, R. Kumal, M. Abu-Laban, T. Karam, C. Landry, D. Hayes, L.H. Haber
- PHYS 484.** Withdrawn.
- PHYS 485.** Effect of thiol adsorption on the surface reconstruction of Au(111) using periodic DFT. L.E. Eddy, F. Tielsen
- PHYS 486.** Photopolymerization of guest molecules in host urea inclusion complexes resulting in C-C bond formation. P. McLaughlin, B.S. Hudson
- PHYS 487.** Promoting molecular planarity and solid state state  $\pi$ -stack formation in conjugated organic materials. P.T. Pham, M. Bader
- PHYS 488.** Direct basis approach to nonorthogonality in second quantization: Theory and application. Z. Hu, M.A. Ratner, T. Seideman
- PHYS 489.** Withdrawn.
- PHYS 490.** Fluorescent liquid crystal of bay-substituted perylene bisimide. S. Herbst, P. Leowanawat, M. Lehmann, F. Wuerthner
- PHYS 491.** Room temperature phosphorescence from organic nanocrystals. E. Moses, G. Piland, C.J. Bardeen
- PHYS 492.** Detecting and communicating material damage using embedded ultrasmall CdSe quantum dots. T. Frecker, C. Brubaker, I. Njoroge, G. Jennings, D. Adams, S. Rosenthal
- PHYS 493.** Characterizing the electronic states of gold monosulfide, AuS. T.D. Varberg, B. Pearlman, I. Wyse, D. Kokkin, R. Zhang, T.C. Steimle
- PHYS 494.** Correlating photoluminescence and particle morphology of individual indium phosphide quantum dots using fluorescence and electron microscopy. K. Reid, J.R. McBride, S. Rosenthal
- PHYS 495.** Charge effect on adsorption onto colloidal silica surfaces: An *in situ* laser photolysis study. S. Bevilacqua, N. Long, E. Piechota, B.H. Milosavljevic
- PHYS 496.** Effect of Gemini surfactants on clay nanocomposite formation using hydrophilic polymers. R. Hussein, N. Shabestary
- PHYS 497.** Ion insertion barriers in prototypical lithium-ion batteries. L. Raguetta
- PHYS 498.** Modeling sodium battery electrolytes and electrode interfaces at varying concentration using classical molecular dynamics. J. Wahlers, R.P. Jörn, R. Kumar, D.G. Kuroda
- PHYS 499.** Investigating the fluxional nature of  $Mo(PH_3)_3H_2$  and implications for hydrogenation catalysis. D.L. Reese, R. Steele
- PHYS 500.** Development of porphyrin-thiazolothiazole donor-acceptor materials for solar energy conversion. K. Ren, D.M. Marin, J.M. Kolesar, S.J. Hall, N.G. Grubich, M.G. Walter
- PHYS 501.** Multiscale simulations of novel photovoltaic materials. L. Meng
- PHYS 502.** Monitoring exciton diffusion transport in long alkyl chain porphyrin films for photovoltaics application. M. Kaushal, A. Ortiz, G. Singh, T. Lee, M. Walter
- PHYS 503.** Real-time electronic dynamics in  $CH_3NH_3PbI_3$  perovskite. T. Nguyen, J. Parkhill
- PHYS 504.** Probing interfacial electron transfer dynamics in semiconductor-chromophore assemblies. J. Miller, J.K. McCusker
- PHYS 505.** Bright fission: Singlet fission into a pair of emitting states. D. Casanova
- PHYS 506.** Broadband transient absorption of iron pyrite. S.A. Sorenson, J. Patrow, J.M. Dawlaty
- PHYS 507.** Tuning charge-transfer in fullerene: Molecular cluster solid-state materials. M.V. Paley, N. Patel, E. O'Brien, B. Choi, X. Roy, A. Crowther
- PHYS 508.** Application of chromophoric dyes with applied bias to increase photoconversion efficiency of dye sensitized solar cells. C.A. Sweet, C.R. Rockwell, A.R. McCabe, B.S. Sheetz, C.J. Timpson, C. Murphy

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- PHYS 509.** Effects of disorder on the dissociation of the interfacial charge-transfer exciton in organic donor-acceptor blends. **L. Shi, C. Lee, A. Willard**
- PHYS 510.** How singlet fission depends on crystal morphology. **G. Piland, C.J. Bardeen**
- PHYS 511.** Solution structures of highly active molecular Ir water-oxidation catalysts from density functional theory combined with high-energy x-ray scattering and EXAFS spectroscopy. **K.R. Yang, A.J. Matula, G. Kwon, J. Hong, J.M. Thomsen, G.W. Brudvig, R.H. Crabtree, D.M. Tiede, L.X. Chen, V.S. Batista**
- PHYS 512.** Optimization of energy transfer in DNA-dye excitonic circuits. **W. Bricker, N.P. Sawaya, R. Veneziano, A. Aspuru-Guzik, M. Bathe**
- PHYS 513.** Withdrawn.
- PHYS 514.** Fluorescence investigation of aggregation behavior of betanin on nano-porous films of titanium dioxide and zirconium dioxide. **N. Treat, J. McHale**
- PHYS 515.** Can disorder enhance incoherent exciton diffusion? **E.M. Lee, W.A. Tisdale, A.P. Willard**
- PHYS 516.** Effect of transmitter dipole moment on the upconversion efficiency in hybrid inorganic-organic nanocrystal-molecule systems. **P. Xia, M. Tang**
- PHYS 517.** Withdrawn.
- PHYS 518.** Plasmonic dye-sensitized solar cells: Evaluating the efficiency, observing possible dye degradation, and developing a screening assay for dyes. **J.M. Wiest**
- PHYS 519.** Heterogeneous reaction kinetics in a photomechanical molecular crystal. **F. Tong, C.J. Bardeen**
- PHYS 520.** Detailed and coarse-grained simulations of aggregating charged ligand-coated gold nanoparticles. **G. Chong, R. Hernandez**
- PHYS 521.** Synchrony transitions due to dynamical quorum sensing in single-cathode multi-anode nickel dissolution system. **M.J. Hankins, I.Z. Kiss**
- PHYS 522.** *Ab initio* kinetic analysis of acryloyl and butadienyl radicals with atomic and molecular oxygen. **P. Winter, A.L. Cooksy**
- PHYS 523.** Theoretical study of geometrical, spectroscopic and spin-spin interatomic interactions in ruthenium complexes and some selected organic molecules. **A.A. Adeniji, P.A. Ajibade**
- PHYS 524.** Quantum computation of substituted effect on amide. **Y. Wang**
- PHYS 525.** Anharmonic vibrational spectroscopy calculations of large molecules. **X. Cheng, R. Steele**
- PHYS 526.** Computational IR spectroscopy for detecting the endohedral complexes  $M@C_{60}$  ( $M = Li, Na, K$ ) in stellar and interstellar environments. **S. Ahmadvand**
- PHYS 527.** Novel approaches to the computational chemistry and computer-assisted application of MNDO calculation for sterols. **E.J. Parish, W. Huang, H. Honda, T. Wei**
- PHYS 528.** Non-linear properties of chromophores in solution using equation-of-motion coupled cluster (EOM-CC) and effective fragment potential (EFP): A QM/MM approach. **K. Nanda, A. Krylov**
- PHYS 529.** Improving far-UV CD prediction with the dipole interaction model. **A.C. Jungong, R. Nori, I.V. Uporov, F.N. Ngassa, E.R. Aushof, E. Holt, K.A. Thomasson**
- PHYS 530.** Electronic structure calculations aid in the interpretation of  $^{19}F$  NMR chemical shifts. **C. Kasireddy, J. Bann, K. Mitchell-Koch**
- PHYS 531.** Direct measurement of carrier diffusion in lead halide perovskite single crystals. **O.E. Semonin, G. Elbaz, D. Straus, C.R. Kagan, X. Roy, J.S. Owen**
- PHYS 532.** *Ab initio* multiple spawning method for intersystem crossings: Spin-forbidden transitions between  $^3B_1$  and  $^1A_1$  states of  $SiH_2$ ,  $GeH_2$ . **D. Fedorov, S.A. Varganov**
- PHYS 533.** Advances in the software for simulating quantum nonadiabatic dynamics. **A.V. Akimov**
- PHYS 534.** Light interaction with live molecular junctions under the bias. **A. Morteza Najarian, R.L. McCreery**
- PHYS 535.** Mixed quantum and classical simulation of the hydrated electron: Temperature dependence in resonance Raman spectra, excited states relaxation and whether the electron resides in a cavity. **C. Zhou, E. Farr, B.J. Schwartz**
- PHYS 536.** Toward a complete description of ion hydration from the gas to the condensed phase using many-body potentials. **P. Bajaj, F. Paesani**
- PHYS 537.** Development of multipolar polarizable force field for molecular dynamics simulations of carbonate-based electrolytes. **O.N. Starovoytov**
- PHYS 538.** i-TTM model for *ab initio*-based ion-water interaction potentials: Alkali-water and alkali-earth-water potential energy functions. **M. Riera Riambau, F. Paesani**
- PHYS 539.** Physicochemical properties of mixed ionic Liquids: Molecular dynamics study of its structural organization. **R. Ormazabal-Toledo, P. Fuentealba**
- PHYS 540.** New equation of state for oligomeric particles modeled by dissipative particle dynamics. **R. Hembree, S.N. Jamadagni, J.I. Siepmann**
- PHYS 541.** Simulations of reactivity at complex interfaces: Catalytic conversion of biomass derived alcohols at  $Pt/H_2O$  interface. **B. Schweitzer, K. Li, C. Michel, S. Steinmann, P. Sautet**
- PHYS 542.** Potential energy surface calculations for biological water bridge proton transfer systems. **C.P. Schultz, J.W. Mazuza**
- PHYS 543.** Molecular dynamics studies of *Candida antarctica* lipase B enzyme dynamics and solvent dynamics at the enzyme interface. **J.N. Dahanayake, K. Mitchell-Koch**
- PHYS 544.** Propagator based adaptive configuration interaction method. **T. Zhang, F.A. Evangelista**
- PHYS 545.** Studying the kinetic properties of small RNA molecules using Markov state models. **G. Pinamonti, S. Bottaro, F. Noe, G. Bussi**
- PHYS 546.** Calculation of guests binding to  $\beta$ -cyclodextrin: From thermodynamics to kinetics. **Z. Tang, C. Chang**
- PHYS 547.** Design of new disulfide-based compounds for the improvement of self-healing materials. **J. Matxain, J.M. Asua, F. Ruiperez**
- PHYS 548.** Exploring the inhomogeneity of the hydrogen bond network in liquid water through many-body molecular dynamics. **S. Straight, F. Paesani**
- PHYS 549.** On the breakdown of linear response theory: An investigation of Gaussian statistics and the dipole flip model. **A. Schile, B. Laird, W. Thompson**
- PHYS 550.** Liquid-liquid critical point of a water model including explicit three-body interactions. **Y. Ni, J.L. Skinner**
- PHYS 551.** Deconstructing the "water finger": A reexamination of water-organic ion transfer. **J.J. Karnes, I. Benjamin**
- PHYS 552.** Detailed balance and nonadiabatic dynamics. **N. Bellonzi, J.E. Subotnik**
- PHYS 553.** Detailed kinetic modeling of processes relevant to fusion energy. **M. Mehl, M. Armstrong, J.M. Zaugg, J.C. Crowhurst, H.B. Radousky, E. Stavrou**
- PHYS 554.** Fully quantum mechanical TDDFT for giant gold clusters with up to 10,000 electrons with stochastic TDDFT. **S. Hernandez, R. Baer, E. Rabani, J.Q. Dam, A.H. Nguyen, A.S. Seshappan, Z. Sun, D. Neuhauser**
- PHYS 555.** Adaptive configuration interaction method for constructing compact wavefunctions. **J.B. Schriber**
- PHYS 556.** Energy landscape of zirconia phase transitions. **S. Guan, X. Zhang, Z. Liu**
- PHYS 557.** Density functional tight binding with ScalAPACK for efficient electronic structure calculations. **J.J. Blaziejewski, J. Jakowski, J.W. Mazuza**
- PHYS 558.** DFT insights into mechanisms of brightening of CdSe quantum dots by hydride. **L. Lystrom, S. Kilina, S. Ivanov**
- PHYS 559.** Withdrawn.
- PHYS 560.** Studies on the relationship between internal energy and state of ideal gas. **H. An, X. Yao, G. Yang, J. Hou, T. Niu**
- PHYS 561.** Reaction rate theory of coordination number: An application to ion solvation. **S. Roy, M.D. Baer, C.J. Mundy, G.K. Schenter**
- PHYS 562.** On the multireference character of transition metal complexes. **J.C. Plascencia, J. Wang, C. Peterson, A.K. Wilson**
- PHYS 563.** Modeling of lithium deposition and dissolution during battery cycling. **C. Wang, T.F. Miller**
- PHYS 564.** Dynamics of the  $F + HOCH_3 \rightarrow HF + OCH_3$  reaction. **A.W. Ray, B.B. Shen, R. Otto, R.E. Continetti**
- PHYS 565.** Investigation of small molecules with the multireference correlation consistent composite approach (MR-ccCA). **R.J. Weber, A.K. Wilson**
- PHYS 566.** Comparison of DFT functionals for the structural prediction of lanthanide species. **S.H. Yuwono, R.J. Weber, G. Schoendorff, A.K. Wilson**
- PHYS 567.** Density-functional computation of strongly correlated systems. **J. Kong, E. Proynov**
- PHYS 568.** New weighting scheme in simulated tempering minimizing round-trip time between a pair of conformational states. **Q. Qiao, X. Huang**
- PHYS 569.** Intrinsic effects of glycosylation on alpha-helix stability. **S. McHugh, J. Rogers, Y. Lin**
- PHYS 570.** Numerical calculation of densities of states and partition functions. **D. Calderini, D. Skuterich, V. Barone**
- PHYS 571.** Withdrawn.

## THURSDAY MORNING

## Section A

San Diego Convention Center  
Room 29A

**Computer Simulations & Long-Time Kinetics of Molecular Events**

R. Elber, R. M. Levy, C. F. Wong, D. M. Zuckerman, *Organizers*

D. E. Makarov, *Presiding*

**8:00** **PHYS 572.** Dynamics of dopamine transporters: Insights from simulations at multiple scales. **M.H. Cheng, C. Kaya, A. Sorkin, J.R. Faeder, I. Bahar**

**8:30** **PHYS 573.** Free energy calculations and reaction coordinates from transition path sampling of enzymatic reactions. **S.D. Schwartz**

**9:00** Intermission.

**9:15** **PHYS 574.** Solvation thermodynamics of biosolutes in mixed protecting-denaturing osmolytes. **P. Ganguly, N. van der Vegt, J.E. Shea**

**9:30** **PHYS 575.** Development of a multi-scale sampling methodology to examine the favored ligand binding pathways of influenza neuraminidase. **A.W. Van Wynsberghe**

**9:45** **PHYS 576.** Damage recognition and base extrusion strategies of DNA repair glycosylase enzyme. **B. Kossmann, I.N. Ivanov**

**10:00** **PHYS 577.** Bending and base step flexibilities of normal, methylated, and damaged DNA. **A. Van Der Vaart**

**10:15** **PHYS 578.** Molecular stripping in the NF $\kappa$ B/I $\kappa$ B/DNA genetic regulatory network. **D. Potoyan, P.G. Wolynes**

**10:30** Intermission.

**10:45** **PHYS 579.** Replica exchange multiscale CFD-MD integrator. **A.V. Popov, R. Hernandez**

**11:00** **PHYS 580.** Generalized manning model captures the RNA ion atmosphere. **U. Mohanty**

**11:15** **PHYS 581.** Wigner phase space distribution via classical adiabatic switching. **A. Bose, N. Makri**

**11:30** **PHYS 582.** Conformationally gated charge transfer in DNA three-way junctions. **Y. Zhang, C. Liu, D.N. Beratan**

## Section B

San Diego Convention Center  
Room 28C

**Decoding the Spectroscopic Signatures of Large Amplitude Motions: Challenges & Opportunities for Theory & Experiment**

Z. Bacic, M. A. Johnson, *Organizers*

S. S. Xantheas, *Presiding*

**8:00** **PHYS 583.** Isotopic and tunneling patterns in water clusters. **J. Richardson, C. Perez, Z. Kisiel, B. Temelso, G.C. Shields, A. Reid, D. Wales, S. Athorpe, L. Evangelisti, S. Lobsiger, B.H. Pate**

**8:40** **PHYS 584.** Infrared spectroscopy of metal-CO $_2$  complexes: Candidates for large amplitude vibrations. **M.C. Thompson, J. Weber**

**Technical program information known at press time.**

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**9:20 PHYS 585.** Large amplitude motions on the S<sub>1</sub> electronic surface of acetylene. R. Field

**10:00** Intermission.

**10:20 PHYS 586.** Large amplitude motions in complexes of carboxylic acids with water: Rotational spectroscopic and *ab initio* studies. E. Schnitzler, B. Zenchyzen, S. Ghosh, J. Thomas, Y. Xu, W. Jaeger

**11:00 PHYS 587.** Using contracted basis functions and the Lanczos algorithm to compute spectra of exible Van der Waals dimers. T. Carrington, X. Wang

## Section C

San Diego Convention Center  
Room 28D

### Electronic Structure & Dynamics of Metastable States

K. B. Bravaya, K. D. Jordan, *Organizers*

J. Parkhill, *Presiding*

**8:00 PHYS 588.** Role of resonances in vibrational excitation of polyatomic molecules. R. Curik, P. Carsky, M. Allan

**8:40 PHYS 589.** Resonances in electron-molecular ion scattering. A. Orel, A. Larson

**9:20 PHYS 590.** Symmetry lowering in decay dynamics of transient molecular anions. J. Fedor, J. Kocisek

**9:40** Intermission.

**10:00 PHYS 591.** Computational modeling of resonant vibrational excitation via electron impact. M.F. Falcetta

**10:40 PHYS 592.** Electron-induced reaction dynamics of halogenated hydrocarbons on the Cu(110) surface. A.F. Izmaylov

**11:20 PHYS 593.** New developments in non-Hermitian Hartree-fock for shape resonances in molecules. A. White, C.W. McCurdy, M.P. Head-Gordon

## Section D

San Diego Convention Center  
Room 28E

### Frontiers in Solar Light Harvesting Processes

T. Krauss, A. Mohite, O. V. Prezhdo, S. Tretiak, *Organizers*

D. Kilin, *Presiding*

**8:00 PHYS 594.** Progress in solar water splitting. B.A. Parkinson

**8:40 PHYS 595.** Impact of dissociated water at photocatalytic aqueous semiconductor interfaces. M.S. Hybertsen

**9:20 PHYS 596.** Efficient computational screening tool for Ru(II) light harvesters. L.A. Fredin, T.C. Allison

**9:40** Intermission.

**10:05 PHYS 597.** Trapping and dynamics of excess electrons at TiO<sub>2</sub> anatase surfaces and interfaces. A. Selloni

**10:45 PHYS 598.** Polynuclear Ru-based metal complexes for energy and electron transfer. L. Baraldo, V.D. Kleiman

**11:25 PHYS 599.** What makes the photocatalytic CO<sub>2</sub> reduction on n-doped Ta<sub>2</sub>O<sub>5</sub> efficient: insights from nonadiabatic molecular dynamics. A.V. Akimov, R. Jinnouchi, R. Asahi, O.V. Prezhdo

## Section E

San Diego Convention Center  
Room 29B

### Physical Chemistry of Complex Environmental Interfaces

*Cosponsored by COLL*

V. H. Grassian, G. M. Nathanson, *Organizers*

H. C. Allen, *Presiding*

**8:00 PHYS 600.** Far infrared spectra of neutral gas phase peptides: Signatures from combined experiment and theory. M.P. Gaigeot

**8:20 PHYS 601.** Formation of reactive oxygen species by atmospheric aerosols in water. M. Shiraiwa

**9:00 PHYS 602.** Experimental and theoretical studies of atomic oxygen reactions with terminal alkenes: Relevance of the formaldehyde product channel for atmospheric organic aerosol growth. P. Casavecchia, G. Vanuzzo, N. Balucani, F. Leonori, D. Stranges, S. Falcinelli, C. Cavallotti

**9:20 PHYS 603.** OCEANFILMS: A process model for the organic enrichment of marine sea spray particle. S. Burrows

**10:00** Intermission.

**10:20 PHYS 604.** Surface propensity and binding of Mg<sup>2+</sup>, Ca<sup>2+</sup>, SO<sub>4</sub><sup>2-</sup>, HSO<sub>4</sub><sup>-</sup>, and Cl<sup>-</sup> at the air/water Interface, a proxy for atmospheric aerosol surfaces. H.C. Allen, D. Verreault, W. Hua, E. Adams, T. Zhang, B.A. Wellen

**11:00 PHYS 605.** Linking size-dependent 3-D morphology and physicochemical properties of substrate-deposited sea spray aerosol particles. A.V. Tivanski

**11:40 PHYS 606.** Short range catalyst-surface interactions revealed by heterodyne two dimensional sum frequency generation spectroscopy. J. Wang, Y. Li, M.L. Clark, C.P. Kubiak, W. Xiong

## Section F

San Diego Convention Center  
Room 29C

### Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials

D. Eisele, A. P. Willard, *Organizers*

B. M. Discher, *Presiding*

**8:00 PHYS 607.** From dimers to self-assembled molecular nanotubes: Challenges for theory. A. Stradomska

**8:30 PHYS 608.** Living on the edge: Tuning supramolecular interactions to design two-dimensional organic crystals near the boundary of two stable structural phases. B. Hirsch, K.P. McDonald, B. Qiao, A.H. Flood, S.L. Tait

**8:50 PHYS 609.** Self-assembly of hierarchical biomorphs from crystalline nanorods. E. Nakouzi, P. Knoll, Y. Ghoussoub, O. Steinbock

**9:10 PHYS 610.** Atomistic simulations of the formation of perylene-based supramolecular complexes in aqueous solution. N. Hansen

**9:30** Intermission.

**9:40 PHYS 611.** Light harvesting in purple bacteria benefits more from a favorable energy landscape than from coherent delocalization. S. Baghbanzadeh, I. Kassal

**10:10 PHYS 612.** Withdrawn.

**10:30 PHYS 613.** Effective optoelectrical switching by using pseudo-single crystal of monolayer array of 2D polymer-plasmonic nanoparticles system. M.A. Mahmoud

**10:50 PHYS 614.** Enol tautomeric polymorphism of barbituric acid: The role of zero point energy in stability. B.S. Hudson, M. Marshall, V. Lopez, D.G. Allis

## Section G

San Diego Convention Center  
Room 29D

### Towards Predictive Calculations in Strongly Correlated Molecules & Materials

T. C. Berkelbach, E. Neuscamman, *Organizers*

D. R. Reichman, *Presiding*

**8:00 PHYS 615.** Electrodynamics calculations of ultrafast energy transfer processes in quantum dots. A. Bande

**8:45 PHYS 616.** Predicting atomistic morphologies and charge-transport of [5]-[12] cycloparaphenylene. I. Yavuz, J. Lin, S.A. Lopez, E. Darzi, R. Jasti, K.N. Houk

**9:10 PHYS 617.** Attosecond electronic band dynamics. S.R. Leone

**9:55** Intermission.

**10:15 PHYS 618.** Non-equilibrium atomic limit and divide-and-conquer method for nanoscale simulations. Y. Gao, M.A. Ochoa, M. Galperin

**10:40 PHYS 619.** Simulation of electron transport in molecular junctions using the multilayer multiconfiguration time-dependent Hartree method. M. Thoss, H. Wang

**11:25 PHYS 620.** Mixed stack charge-transfer crystals: New perspectives for old materials. A. Girlando

## Section H

San Diego Convention Center  
Room 30A

### Physical Principles in Functional Nanoscience: Symposium in honor of Mostafa A. El-Sayed

P. K. Jain, C. F. Landes, S. Link, *Organizers*

B. Nikoobakht, *Presiding*

**8:00 PHYS 621.** Obtaining exact transition state theory rates without perturbation theory. R. Hernandez

**8:35 PHYS 622.** One-way molecular excitations: Topological insulator analogues for excitons and plexitons. J. Yuen Zhou

**8:55 PHYS 623.** When small is different: Nanoscale computational microscopy. U. Landman

**9:30 PHYS 624.** Predicting sintering resistance for nanoparticles on amorphous silica supports. C. Ewing, K. Johnson, G. Vesper, J.J. McCarthy, D. Lambrecht

**9:50** Intermission.

**10:10 PHYS 625.** Quantum plasmonics and hot-electron induced processes. P.J. Nordlander

**10:45 PHYS 626.** Theory of plexiton donor-acceptor energy transfer. Z. Hu, R. Leon Montiel, J. Yuen Zhou

**11:05 PHYS 627.** Resolving energy transfer dynamics in plasmonic bowtie nanocavity arrays. C. Deeb

**11:40 PHYS 628.** Electron energy-loss spectroscopy calculation in finite-difference time-domain package: EELS-FDTD. N. Large, A. Manjavacas, M. Zhang, S.X. Wang, P.J. Nordlander

## Big Data Science

### Accessing Chemical Space & Better Modeling

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

### Computer-Aided Drug Design

#### New Modality Therapeutics

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVIR and PHYS*

### Quantum Mechanics

*Sponsored by COMP, Cosponsored by PHYS*

## THURSDAY AFTERNOON

### Section A

San Diego Convention Center  
Room 29A

### Computer Simulations of Thermodynamics & Long-Time Kinetics of Molecular Events

R. Elber, R. M. Levy, D. M. Zuckerman, *Organizers*

C. F. Wong, *Organizer, Presiding*

**1:30 PHYS 629.** Exploring photo-induced electron transfer leading to "oxidative redding" in fluorescent proteins. A. Acharya, A. Kolomeisky, A. Krylov

**1:45 PHYS 630.** Molecular dynamics studies of the effects of drug-resistant mutations of EGFR on inhibitor binding affinities and the drug target selectivity profiles. J. Park, J. McDonald, R. Pettey, K.N. Houk

**2:00 PHYS 631.** Sequence-level prediction and control of the production of a membrane protein. M. Niesen, S.S. Marshal, W.M. Clemons, T.F. Miller

**2:15 PHYS 632.** Molecular simulation of concentration-dependent interactions of hydrophobic drugs with cellular membrane. M. Kang, S. Loverde

**2:30** Intermission.

**2:45 PHYS 633.** Quantum-mechanical path integral simulations of ferrocene-ferrocenium charge transfer in solution. P.L. Walters, N. Makri

**3:00 PHYS 634.** Molecular dynamics simulations of stacked DNA base surrogates. A. Mazaheripour, C. Markegard, J. Jocson, A.M. Burke, M.N. Dickson, A.A. Gorodetsky, H. Nguyen

**3:15** Intermission.

**3:30 PHYS 635.** Sampling rare events in molecular simulations: Heterogeneous ice nucleation – a case study. R. DeFever, W. Judge, B. Glatz, S. Sarupria

**3:45 PHYS 636.** Computational study on the catalytic role of the magnesium ions in the active site of the DNA Polymerase  $\beta$ . R.A. Matute, A. Warshel

**4:00 PHYS 637.** Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates. N.E. Zimmermann, B. Vorselaars, D. Quigley, B. Peters

**4:15 PHYS 638.** Effect of single and multiple types of bases on aerosol formation rates. B. Temelso, F. Morrison, G. Kim, N. Appiah-Padi, S. Janitschke, D. Speer, G.C. Shields

**4:30 PHYS 639.** Multiscale modeling of the chromatin fiber. T. Schlick

## Section B

San Diego Convention Center  
Room 28C

### Decoding the Spectroscopic Signatures of Large Amplitude Motions: Challenges & Opportunities for Theory & Experiment

Z. Bacic, M. A. Johnson, *Organizers*  
E. Garand, *Presiding*

- 1:30 PHYS 640.** Vibrational signatures of electronic properties in energy and biology. R. Steele
- 2:10 PHYS 641.** Nuclear and electronic quantum effects in hydrogen bonded systems. T. Markland
- 2:50 PHYS 642.** Path integral simulations and spectra of weakly bound complexes. P. Roy
- 3:30** Intermission.
- 3:50 PHYS 643.** Vibrational signatures of large amplitude motions in  $\text{H}_3\text{O}^+$  bound to 18-Crown-6 using cryogenic ion vibrational predissociation spectroscopy. F.S. Menges, S. Craig, C. Duong, M.A. Johnson
- 4:10 PHYS 644.** Computing anharmonic vibrational spectra for polycyclic aromatic hydrocarbons: Naphthalene, anthracene, and tetracene. T.J. Lee, C.J. Mackie, A. Candian, X. Huang, A.G. Tielens, E. Maltseva, A. Petrigiani, J. Oomens, W.J. Burna
- 4:30 PHYS 645.** Unimolecular dynamics and reactant density of states for ion-molecule clusters. W.L. Hase
- 5:10 PHYS 646.** Spectroscopic signature of the hydrated proton reveal its solvation structure in aqueous solution. E. Pines

## Section C

San Diego Convention Center  
Room 28D

### Electronic Structure & Dynamics of Metastable States

K. B. Bravaya, K. D. Jordan, *Organizers*  
A. F. Izmaylov, *Presiding*

- 1:30 PHYS 647.** Complex-absorbing potentials in equation-of-motion coupled-cluster theory. T. Jagau
- 2:10 PHYS 648.** Development and application of the complex scaled multiconfigurational spin tensor electron propagator method (CMCSTEP) for determining electron-atom/molecule resonances. D. Yeager
- 2:50 PHYS 649.** Calculations of metastable states of molecules and molecular clusters using self-interaction corrected DFT. H. Jonsson
- 3:10** Intermission.
- 3:30 PHYS 650.** Electronic structure theories employing complex potentials to describe electron transport and metastable states. M. Ernzerhof
- 4:10 PHYS 651.** Long-range exact exchange DFT for giant systems using stochastic exchange. D. Neuhauser, E. Rabani, R. Baer
- 4:50 PHYS 652.** Realtime, black-box simulation of pump probe spectra with decay. J. Parkhill

## Section D

San Diego Convention Center  
Room 28E

### Frontiers in Solar Light Harvesting Processes

T. Krauss, A. Mohite, O. V. Prezhdo, S. Tretiak, *Organizers*  
A. V. Akimov, *Presiding*

- 1:30 PHYS 653.** Influence of extended solvation structure upon TDDFT absorption spectra determined using intermolecular network theory and both classical and quantum mechanical treatments of nuclei. A.E. Clark, T. Markland, C. Isborn
- 2:10 PHYS 654.** Nonadiabatic Excited-State Molecular Dynamics: On-the-Fly Reduction of Excited States. T. Nelson, S. Fernandez-Alberti, S. Tretiak
- 2:50 PHYS 655.** Addressing the second derivative coupling in nonadiabatic molecular dynamics simulation. G. Meek, B.G. Levine
- 3:10** Intermission.
- 3:35 PHYS 656.** Plexciton resonant energy transfer. J. Yuen Zhou
- 3:55 PHYS 657.** Calculating non-linear properties of closed- and open-shell species with EOM-CCSD: Theory and examples. K. Nanda, A. Krylov
- 4:15 PHYS 658.** Semiconductors used in photovoltaic and photocatalytic devices: Insight from DFT based calculations. T. Le Bahers, S. Melissen, P. Sautet, K. Takanahe
- 4:35 PHYS 659.** Simulation of realistic electronic spectra bandshapes of chromophoric systems relevant for solar light harvesting. M. Biczysko, J. Bloino

## Section E

San Diego Convention Center  
Room 29B

### Physical Chemistry of Complex Environmental Interfaces

*Cosponsored by COLL*

V. H. Grassian, *Organizer*  
G. M. Nathanson, *Organizer, Presiding*

- 1:30 PHYS 660.** Propensity of acids and bases to the air-water interface: A consensus in the making. C.J. Mundy, M.D. Baer, D. Tobias
- 2:10 PHYS 661.** Surface propensity of the self-ions of water: A Lewis Study. C. Bai, J. Herzfeld
- 2:30 PHYS 662.** Development of single particle pH and SERS as methods to study organic and inorganic species and reactions in atmospheric particles and model system. A.P. Ault, R.L. Craig, A. Bondy, J.D. Rindelaub, L. Nandy, C. Dutcher, P.B. Shepson
- 3:10** Intermission.
- 3:30 PHYS 663.** Spectroscopic signatures of divalent metal binding motifs to long chain acids under microhydration. M.A. Johnson
- 4:10 PHYS 664.** Unraveling the complex nature of bulk and surface hydrated electrons in conventional and non-conventional ways. P. Jungwirth
- 4:30 PHYS 665.** Studies of the structure, dynamics and collisions of single nanoparticles. R.E. Continetti
- 5:10 PHYS 666.** Liquid-jet XPS and MD simulations of depth dependent concentration profiles at the liquid/vapor interface of aqueous propanol solutions. M. Makowski, J.M. Langford, R.P. Galhenage, H. Bluhm, J.C. Hemming

## Section F

San Diego Convention Center  
Room 29C

### Towards Predictive Calculations in Strongly Correlated Molecules & Materials

T. C. Berkelbach, E. Neuscarman, *Organizers*  
D. Zgid, *Presiding*

- 1:30 PHYS 667.** On couplings and excimers: Lessons from studies of singlet fission in covalently linked dimers. X. Feng, A. Krylov
- 2:15 PHYS 668.** Accurate excitation energies for systems with near-degeneracies. D. Lambrecht
- 2:40 PHYS 669.** Charged and neutral excitations in organic systems from first principles. J. Neaton
- 3:25** Intermission.
- 3:45 PHYS 670.** Self-consistent, correlated dynamics for small-gap molecules. J. Parkhill
- 4:10 PHYS 671.** Quantum Monte Carlo for excited states in complex environments. C. Filippi
- 4:55 PHYS 672.** Excited molecular electronic states with open quantum systems on a quantum computer. J. McClean, M. Schwartz, C. Macklin, I. Siddiqi, W. Dejong, J. Carter

## Section G

San Diego Convention Center  
Room 29D

### Physical Principles in Functional Nanoscience: Symposium in honor of Mostafa A. El-Sayed

P. K. Jain, S. Link, *Organizers*

C. F. Landes, *Organizer, Presiding*

- 1:30 PHYS 673.** New directions in research with anisotropic metal nanoparticles and their optical properties. G.C. Schatz
- 2:05 PHYS 674.** Enabling next generation quantum dots by correlation of photophysics and atomic structure. J.R. McBride, N. Orfield, K. Reid, S. Rosenthal
- 2:25 PHYS 675.** Tailoring chromophore dark states for improved fluorescence microscopy. R. Dickson
- 3:00 PHYS 676.** Far-field superresolution detection of plasmonic near-fields. R. Boutelle, D. Neuhauser, S. Weiss
- 3:20** Intermission.
- 3:40 PHYS 677.** Strategies for reducing blinking in quantum dots while maintaining as small a size as possible: Insights from multiparametric Studies. C.D. Heyes
- 4:15 PHYS 678.** Withdrawn.
- 4:35 PHYS 679.** Non-plasmonic hot electrons from exciton-to-hot electron upconversion in doped quantum dots for enhanced photochemistry. D. Son

## Big Data Science

### Interpreting Pharmacology

*Sponsored by MPPG, Cosponsored by BIOL, CINF, COMP, MEDI and PHYS*

### Elucidation of Mechanisms & Kinetics on Surfaces

*Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS*

### Quantum Mechanics

*Sponsored by COMP, Cosponsored by PHYS*

## POLY

## Division of Polymer Chemistry

M. Jeffries-El, T. White and C. Lipscomb, *Program Chairs*

### OTHER SYMPOSIA OF INTEREST:

Eli Pearce Memorial Symposium  
(see IAC, Tue)

### SOICIAL EVENTS:

**Luncheon**, 12:00 PM: Sun, Mon

**Breakfast**, 7:30 AM: Tue

**Reception**, 6:00 PM: Tue

**Reception**, 5:30 PM: Wed

## SUNDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Santa Rosa

### Applications of Polymer Surfaces & Interfaces

### New Processes & Surface Functionalization

*Cosponsored by COLL and PMSE*

S. T. Iacono, J. M. Mabry, A. Tuteja, *Organizers*,  
*Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 1.** Surface modification of oxide-free metal and hydrogenated metal substrates with trihydrosilanes. B. Arkles

**8:35 POLY 2.** Visible light-driven proton pumps utilizing photoacid molecules and polymeric nanopore scaffolds. C. Sanborn, S. Ardo

**8:55 POLY 3.** Pyrene-modified polyelectrolytes/MWNT multilayer thin films extinguish flames on polyurethane foam. K. Holder, A. Cain, M. Plummer, B. Stevens, P. Odenborg, A.B. Morgan, J.C. Grunlan

**9:15 POLY 4.** Hierarchical comb brush architectures via sequential light-mediated controlled radical polymerizations. B. Narupai, J.E. Poelma, C.W. Pester, J.W. Kramer, P. Clark, C.J. Hawker

**9:35 POLY 5.** Tightly-bound PVAc on silica: Different from bulk polymer? F.D. Blum, H. Mortazavian, B. Hetayothin

**10:05** Intermission.

**10:15 POLY 6.** Unusual morphologies of poly(vinyl alcohol) thin films adsorbed on polydimethylsiloxane substrates. A. Karki, L. Nguyen, B. Sharma, K. Lim, Y. Yan, W. Chen

**10:45 POLY 7.** Enhanced dielectric breakdown strength in epoxy based nanodielectrics. M.H. Bell, T. Krentz, L. Schadler, J. Nelson, B.C. Benicewicz, H. Hillborg, S. Zhao

**11:05 POLY 8.** Mechanical characterization of copper thin films on polydopamine-functionalized polymer substrates. D. Merkel, C.M. Yakaacki, R. Rorrer, C. Frick

**11:25 POLY 9.** Escaping the tyranny of carbothermal reduction: Conversion of biowaste silica to alkoxy silanes without using silicon. R.M. Laine, V. Popova

**11:45 POLY 10.** F<sup>-</sup> catalyzed reactions at silicon as a route to hybrid materials. R.M. Laine, Y. Kim, D.J. Krug, J.C. Fugral, M.Z. Asuncion

## Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

## Sustainable Polymers, Processes &amp; Applications

Cosponsored by PMSE

D. Boday, J. H. Wang, *Organizers, Presiding*  
K. M. Desai, *Presiding*

8:00 Introductory Remarks.

8:05 **POLY 11.** Ring-opening polymerization of cyclic hemiacetal esters for the preparation of degradable polymers. **M.A. Hillmyer**

8:35 **POLY 12.** Use of cottonseed proteins in adhesive applications. **H. Cheng**, M.K. Dowd, Z. He

9:05 **POLY 13.** Fully renewable pressure-sensitive adhesive system. **S. Lee**, Y. Kim, J. Shin

9:25 Intermission.

9:45 **POLY 14.** The PHAome. **G. Chen**

10:15 **POLY 15.** Synthesis of hybrid molecular brushes with chitosan backbone in biphasic reaction. **M. Chawathe**, A. Patel, S. Jonnalagadda, A. Sidorenko

10:35 **POLY 16.** Highly porous poly(urethane urea) monoliths from renewable resource polymers through emulsion templating. **T. Bialystocki**, L. Avraham, I. Offen, **M.S. Silverstein**

10:55 Concluding Remarks.

## Section C

Marriott Marquis San Diego Marina  
San Diego Ballroom C

## Polymer Applications &amp; Characterization in Medical Devices Industry

X. Liu, J. Slager, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **POLY 17.** Biodegradable polymers derived from fatty acids, saccharides and amino acids. **A.J. Domb**

8:50 **POLY 18.** Biomedical applications of polymers made from natural compounds. **Y. Jia**, K. Wang, F. Le Dévédec, S. Strandman, M. Gauthier, J. Gautrot, **J.X. Zhu**

9:20 Intermission.

9:35 **POLY 19.** Restructuring polymers for medical devices via nano-confinement in and subsequent release from cyclodextrin and urea inclusion compounds. **A.E. Tonelli**

10:05 **POLY 20.** Adipomesh a novel adipocyte growth promoting scaffold. **E. Kallick**, S. Li, A. Aballay, H. Edington, **S. Averick**

10:35 **POLY 21.** Optimization of methacrylic acid based pH-responsive hydrogels for the oral delivery of therapeutic proteins. **S. Steichen**, C. O'Connor, N. Peppas

11:05 **POLY 22.** Characterization of hyaluronic acid and gelatin using asymmetric flow field fractionation with advanced detections. **W. Gao**, X.M. Liu, X. Lu

## Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

## Polymer Additive Manufacturing: Materials, Processes &amp; Simulation

T. E. Long, *Organizer*

R. C. Advincula, J. M. Desimone, *Organizers, Presiding*

8:00 **POLY 23.** 3D printing functional objects with mask projection microsteerolithography: Expanding the polymer toolbox. **J. Serrine**, A. Pekkanen, N. Chartrain, A. Schultz, C. Williams, **T.E. Long**

8:30 **POLY 24.** Additive approach for improving block resistance in coatings. **P.S. Majumdar**, M.R. Winkle, S. Fitzwater, M.B. Clark, A. Krasovskiy, S. Ibbitson

9:00 **POLY 25.** New polymer materials for additive manufacturing and understanding failure modes. **R.C. Advincula**

9:30 Intermission.

9:45 **POLY 26.** Fundamental characterization of soft matter 3D printing processes. **J. Seppala**, K.E. Hillgartner, C.S. Davis, K. Migler

10:15 **POLY 27.** Improving inter-filament interlayer interfaces in 3-D printing of polymers. **E. Duranty**, N. Levenhagen, M. Stark, **M.D. Dadmun**

## Section E

Marriott Marquis San Diego Marina  
Mission Hills

## Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Scott D. Allen, Geoffrey W. Coates &amp; Anthony R. Eisenhut

## Starting a Company on University Technology

Cosponsored by PROF and SCHB

S. Allen, *Organizer*

S. R. Turner, *Organizer, Presiding*

9:00 **POLY 28.** Patterning methods for flexible electronics: A startup company in a startup industry. **C.K. Ober**

9:30 **POLY 29.** PPL (the smallest polyolefins company in the world) - from start-up to scale-up. **L.R. Sita**

10:00 **POLY 30.** Path to an early stage material science start-up company. **G.G. Rodriguez-Calero**

10:30 Intermission.

10:45 **POLY 31.** Performance without permanence: Recyclable thermosets & the future of energy efficient transportation. **S. Pastine**

11:15 **POLY 32.** Commercial aspects of atom transfer radical polymerization. **K. Matyjaszewski**

## Section F

Marriott Marquis San Diego Marina  
Catalina

## Responsive Nanostructures &amp; Nanocomposites

Y. C. Simon, *Organizer*

E. B. Berda, J. Foster, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **POLY 33.** Synthesis and applications of redox-responsive highly branched polymers. **N.V. Tsarevsky**, H. Han, H. Tang, Z. Wang, S.R. Woodruff

8:35 **POLY 34.** Thermoresponsive hyperbranched polymers with low polydispersity and segmented structure. **Y. Shi**, **H. Gao**

9:05 **POLY 35.** Stimuli-responsive gibbous and inverse-gibbous colloidal nanoparticles in gear-like assemblies. **C. Lu**, **M.W. Urban**

9:35 Intermission.

9:50 **POLY 36.** Stimuli-responsive polymers, nanostructures and macroscopic cross-linked networks. **K.L. Wooley**

10:20 **POLY 37.** Responsive and "switchable" cellulose nanocrystal hybrid materials. **Z. Hu**, K.H. Kan, E.D. Cranston, R.H. Pelton

10:50 **POLY 38.** Macromolecular structure and aggregate response in block copolymer solution assemblies. **R.B. Grubbs**, Z. Sun

## Section G

Marriott Marquis San Diego Marina  
Del Mar

## General Topics: New Synthesis &amp; Characterization of Polymers

D. Garcia, *Organizer*

R. P. Viggiano, Z. Zhou, *Presiding*

8:00 **POLY 39.** Macrostructures: How can we characterize the complete chain architectures of polymers? **R. Gurarslan**, **A.E. Tonelli**

8:20 **POLY 40.** NMR study of the separation mechanism of polyethylene-*o*-ctene block copolymer by HT-LC with graphite. **Z. Zhou**, M.D. Miller, D. Lee, R. Cong, C. Klinker, T. Huang, C. Li Pi Shan, W. Winniford, A. DeGroot, L. Fan, T. Karjala, K. Beshah

8:40 **POLY 41.** Monte Carlo simulations of copolymers in liquid chromatography at the critical condition utilizing different pore shapes. **K.N. Struk**, M. Hoffmann, M.R. Schure, J.I. Siepmann

9:00 **POLY 42.** Structure and properties of crystalline-crystalline block copolymers prepared by living organometallic catalysts. **R. Di Girolamo**, C. De Rosa, F. Auremma, G. Talarico, C. Santillo, I. Pierro, C. Cioce, G.W. Coates

9:20 **POLY 43.** Thermal and mechanical properties of linear ABC polymers for application in proton exchange membranes. **C. Hager**, M. Quast, A. Mueller

9:40 **POLY 44.** Innovative TG-GC-MS methods for thermal degradation studies of polymers. **K. Lilova**

10:00 **POLY 45.** Ion conduction in polyvinylidene fluoride (PVDF)/MXene nanolayers membrane for water treatment applications. **M.K. Hassan**, A. Ali, K. Rasool, K.A. Mahmoud

10:20 **POLY 46.** Synthesis and characterization of polysulfone-poly(N,N-diallylammonium salt) block copolymers for polymer electrolyte membranes. **D.J. Strasser**, D.M. Knauss

10:40 **POLY 47.** Sub-10 nm domain spacing within nanostructured, microphase-separated organic thin films of low molecular weight, *atactic* poly( $\alpha$ -olefin)-sugar hybrid conjugates. **T.S. Thomas**, L.R. Sita

11:00 **POLY 48.** Synthesis and characterization of cardo-diamine containing polyimide aerogels. **R.P. Viggiano**, J. Williams, M. Meador

11:20 **POLY 49.** Precision polyolefins from substituted cyclopentenes. **W.J. Neary**, **J.G. Kenemur**

11:40 **POLY 50.** Opposite effects of a singlet oxygen quencher on photochemical degradation of dicyano-substituted poly(phenylenevinylene)s with different side chains. **L.P. Sanow**, J. Sun, C. Zhang

## Biomass &amp; Polymer Extrusion, Composite &amp; Reaction Technologies: New Insights, Future Potential &amp; Principles to Practice

Sponsored by CELL, Cosponsored by PMSE and POLY

## New Horizons in Sustainable Materials

## Nanocellulose

Sponsored by CELL, Cosponsored by DAC $\ddagger$  and POLY

## SUNDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
Santa Rosa

## Applications of Polymer Surfaces &amp; Interfaces

## New Processes &amp; Surface Functionalization

Cosponsored by COLL and PMSE

S. T. Iacono, J. M. Mabry, A. Tuteja, *Organizers, Presiding*

1:00 **POLY 51.** Recent advances in fluoropolymer chemistry at Clemson University. **X. Liu**, D. Hercules, C.A. Parrish, S.P. Belina, A. Matsnev, I. Sharif, D.D. Des Marteau, **J.S. Thrasher**

1:30 **POLY 52.** Interfacial encapsulated graphene with self-assembled diblock copolymers. **H. Tran**, H.M. Bergman, C. Dean, L.M. Campos

1:50 **POLY 53.** Non-isocyanate approach for the synthesis of polyurethane fouling release coatings. **M.M. Pade**, J. Benda, D.C. Webster, S. Stafslien, L. VanderWal

2:10 **POLY 54.** Impact of architecture and substrate interfacial interactions on the preparation and stability of ordered monolayers of polymer grafted nanoparticle. **J. Che**, K. Park, C.A. Grabowski, J. Kelley, H. Koerner, R.A. Vaia

2:30 **POLY 55.** Modification of carbon surfaces with hyperbranched polymer for developing novel catalyst materials. **Y. Nabae**, J. Liang, T. Hayakawa, M. Kakimoto

3:00 Intermission.

3:10 **POLY 56.** Interface-enforced complexation between copolymer blocks. **A. Steinschulte**, W. Xu, F. Draber, P. Hebbeker, A. Jung, D. Bogdanovski, S. Schneider, V.V. Tsukruk, F. Plamper

3:30 **POLY 57.** Copolymer of hyperbranched polystyrene and poly(*N*-isopropylacrylamide) as a thermo-responsive biomaterial for cell sheet recovery. **Y. Sudo**, Y. Nabae, T. Hayakawa, M. Kakimoto

3:50 **POLY 58.** Effect of DexPEG hydrogel cross-link density on the preparation of giant unilamellar vesicles. **A. Kros**

4:20 **POLY 59.** Toward rationally designed, additively manufactured carbon fiber composites with optimized mesostructures. **J.P. Lewicki**

4:50 **POLY 60.** Silicone Elastomers with Discrete Compartments. **A. Skov**, P. Mazurek

## Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

**Sustainable Polymers,  
Processes & Applications**

*Cosponsored by PMSE*

D. Boday, J. H. Wang, *Organizers*

H. Cheng, M. A. Hillmyer, *Presiding*

1:00 Introductory Remarks.

1:05 **POLY 61.** Functional polycarbonates: A broadly useful biodegradable polymer platform. J.L. Hedrick

1:35 **POLY 62.** Development of functionalizable and biodegradable poly(D-glucose carbonate)s as emerging nanomaterials toward biomedical applications. L. Su, J. Fan, H. Wang, T. Gustafson, F. Zhang, K.L. Wooley

1:55 **POLY 63.** New monomers and catalysts for sustainable non-isocyanate polyurethanes. R. Lambeth

2:15 **POLY 64.** Non-isocyanate polyurethanes based on 6-membered cyclic carbonates. S. Mathew, R.H. Lambeth

2:35 Intermission.

2:55 **POLY 65.** Renewable and recyclable polyesters by ring-opening polymerization of bio-derived non-strained lactones. E.Y. Chen

3:25 **POLY 66.** Completely recyclable biopolymers with linear and cyclic topologies via ring-opening polymerization of  $\gamma$ -butyrolactone. M. Hong, E.Y. Chen

3:45 **POLY 67.** Dynamic bulk materials through tunably dynamic boronic ester bonds. J. Chung, O. Cromwell, Z. Guan

4:05 Concluding Remarks.

## Section C

Marriott Marquis San Diego Marina  
Balboa

**Industrial Research at the  
Interface of Inorganic Chemistry  
& Polymer Science**

*Cosponsored by BMGT and INOR#*

N. S. Radu, L. Stratton, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 **POLY 68.** Catalyst development for a HCN-free methyl methacrylate synthesis. T. Foskey, L. Huffman, D. Arriola, J. Briggs

1:35 **POLY 69.** Some current microscopy techniques used for characterization of inorganic fillers in tire compounds. B.D. Korth

2:05 **POLY 70.** From synthetic developments to applications: Hexahydrotriazines as a materials platform for industrial solutions. R.J. Wojtecki, G.O. Jones, T.G. Zimmerman, A.Y. Yuen, D. Boday, J.L. Hedrick, J.M. Garcia

2:35 **POLY 71.** Inorganic phosphate performance coatings. A.S. Wagh

## Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

**Polymer Additive Manufacturing:  
Materials, Processes & Simulation**

R. C. Advincula, J. M. Desimone, *Organizers*

T. E. Long, *Organizer, Presiding*

J. M. Messman, *Presiding*

1:00 **POLY 72.** Generation of thermotropic liquid crystalline polymer thermoplastic composite filaments and their processing in fused filament fabrication. D.G. Baird, M. Ansari, C. Mansfield, C. Qian

1:30 **POLY 73.** Synthesis of well-defined poly(propylene fumarate) oligomers for photocrosslinked 3D printing. M. Becker

2:00 **POLY 74.** Oxygen-inhibition lithography for the fabrication of multipolymeric structures and multifunctional devices. A. Vitale, M. Quaglio, A. Chiodoni, K. Bejtka, M. Cocuzza, C. Pirri, R.M. Bongiovanni

2:30 **POLY 75.** Novel thermosetting polymers for reducing anisotropy in fused filament fabrication 3D printing. K. Yang, B.R. Lund, R. Smaldone, W. Voit

## Section E

Marriott Marquis San Diego Marina  
Mission Hills

**Kathryn C. Hach Award for  
Entrepreneurial Success: Symposium  
in honor of Scott D. Allen, Geoffrey  
W. Coates & Anthony R. Eisenhut**
**Starting a Company on  
University Technology**

*Cosponsored by PROF and SCHB*

S. Allen, *Organizer*

S. R. Turner, *Organizer, Presiding*

1:00 **POLY 76.** Translating basic science into products and the role of diversity in making that happen: The launching of carbon3D. J.M. Desimone

1:30 **POLY 77.** Reflection on my experience to commercialize lab inventions. Z. Bao

2:00 **POLY 78.** Integrated materials systems for chemical sensing. T.M. Swager

2:30 Intermission.

2:45 **POLY 79.** Success stories in commercial functional materials - from haircare to pharmaceuticals. C.J. Hawker

3:15 **POLY 80.** Fundamental to commercial chemistry. R.H. Grubbs

3:45 **POLY 81. Award Address** (Kathryn C. Hach Award for Entrepreneurial Success sponsored by the Kathryn C. Hach Award Fund). Converting pollutants into polymers and specialty chemicals. S. Allen, G.W. Coates, A. Eisenhut

## Section F

Marriott Marquis San Diego Marina  
Catalina

**Responsive Nanostructures  
& Nanocomposites**

E. B. Berda, *Organizer*

J. Foster, Y. C. Simon, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 **POLY 82.** Selective response and actuation in polymer hydrogels. B.D. Olsen, M. Gkikas, S. Tang, C. Edwards

1:35 **POLY 83.** Thiol-triggered hydrogen-sulfide releasing gels. J.B. Matson, Y. Qian, J. Carter

2:05 **POLY 84.** Synthesis and blending of magneto-responsive colloidal polymers: Observation of mesoscopic phase separation. J. Pyun

2:35 Intermission.

2:50 **POLY 85.** Responsive peptide block polymer assembly: ABA, ABC and star triblocks. G. Strange, I. Smith, C. Machado, D.A. Savin

3:20 **POLY 86.** Low-power photon upconversion through triplet-triplet annihilation in nanostructured polymers. C. Weder, R. Vadrucchi, S. Lee, D. Thevenaz, Y.C. Simon

3:50 **POLY 87.** Large low temperature thermoelectric power factor, that rivals inorganic semiconductors, from completely organic nanocomposite multilayer thin films. J.C. Grunlan, C. Yu

## Section G

Marriott Marquis San Diego Marina  
Del Mar

**Paul J. Flory Polymer Education  
Award: Symposium in honor  
of Kenneth B. Wagener**

M. Jeffries-El, T. J. White, *Organizers*

E. B. Berda, *Presiding*

1:00 **POLY 88.** Chemistry and ken's way. E.B. Berda

1:15 **POLY 89.** New polymers with functional group containing semi-rigid alternating copolymers. S.R. Turner, J. Huang, N. Nezamabadi

1:45 **POLY 90.** Catalysis for monomer and polymer synthesis. R.M. Waymouth

2:15 **POLY 91.** History of SCKs as an interdisciplinary educational tool, including the Butler Laboratory. K.L. Wooley

2:45 Intermission.

3:00 **POLY 92.** Deformation mechanisms of block copolymers. E.L. Thomas

3:30 **POLY 93.** Translating university research to the marketplace. J.M. Desimone

4:00 **POLY 94.** Synthesis of polymers with controlled structures. R.H. Grubbs

4:30 **POLY 95.** Teaching and building a polymer laboratory at the University of Florida. K.B. Wagener

**Discussions with the President's  
Task Force on Employment**

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

**Biomass & Polymer Extrusion,  
Composite & Reaction Technologies:  
New Insights, Future Potential  
& Principles to Practice**

*Sponsored by CELL, Cosponsored by PMSE and POLY*

**New Horizons in Sustainable Materials**
**Lignocellulosics**

*Sponsored by CELL, Cosponsored by DAC‡ and POLY*

## SUNDAY EVENING

**My Comments to the President's  
Task Force on Employment**

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

**My Experience with & Advice for  
Improving Diversity in Chemistry**

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

**My Experiences in & Advice for  
Organic Chemistry Courses**

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## MONDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Rancho Santa Fe 1 & 2

**Frederic Stanley Kipping Award  
in Silicon Chemistry: Symposium  
in honor of Michael A. Brook**

*Cosponsored by PMSE*

P. Zelisko, *Organizer, Presiding*

A. K. Franz, *Presiding*

8:00 Introductory Remarks.

8:10 **POLY 96.** Surface energy, structure, and silicon: Wetting-resistant surfaces from less-familiar compounds. J.M. Mabry, A.J. Guenther, A. Tuteja, S.T. Iacono, A. Kota, R. Campos, S.M. Ramirez, T.S. Haddad, R. Stone, Y.J. Diaz

8:35 **POLY 97.** Synthesis and properties of siloxane-containing phospholipids. M.B. Frampton, D. Marquardt, G. Pabst, P.M. Zelisko

9:00 **POLY 98.** Silicon and silicone chemistry with an eye toward surfaces. T.J. McCarthy

9:25 **POLY 99.** Functionalised silica nanoparticles: Towards durable super hydrophobic coatings. G.G. Durand, A. Taylor, N. Sid, M. Alvarez

9:50 Intermission.

10:10 **POLY 100.** Silicon wettability aspects. M.J. Wilson

10:35 **POLY 101.** Anti-fouling silicones prepared with PEO-silane amphiphiles. M. Grunlan, M.A. Rufin, M. Hawkins

11:00 **POLY 102. Award Address** (Frederic Stanley Kipping Award in Silicon Chemistry sponsored by The Dow Corning Corporation). Designing silicones to control interfaces. M.A. Brook, Y. Chen, B. Macphail, L. Zepeda-Velasquez, J.B. Grande, A. Fatona, J. Moran-Mirabal, M. Whinton, M.F. Khan

## Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

**Sustainable Polymers,  
Processes & Applications**

*Cosponsored by PMSE*

D. Boday, J. H. Wang, *Organizers*

E. Y. Chen, J. L. Hedrick, *Presiding*

8:00 Introductory Remarks.

8:05 **POLY 103.** Progress towards sustainable polyurethanes and polycarbonates built from bio-based chemicals. D.S. Wardius, G. Behnken, F. Buckel, B. Sanchez, N. Rahmen, N. Meine, J. Schutte

8:35 **POLY 104.** Sustainable chemically recyclable polyurethanes. D.K. Schneiderman, M. Vanderlaan, D. Batiste, A.M. Mannion, T.R. Panthani, M.A. Hillmyer

8:55 **POLY 105.** Synthesis of biorenewable and water degradable polyesters from itaconic acid. P. Qi, S.A. Miller

9:15 **POLY 106.** High molecular weight sustainable polymers and thermoplastic elastomers from resin acids via living ring-opening metathesis polymerization. M.S. Ganewatta, L. Yuan, M. Rahman, W. Ding, M.L. Robertson, C. Tang

9:35 Intermission.

9:55 **POLY 107.** Renewable thermoplastic materials from polysaccharides. B. Zhou, J.H. Wang, Q. Jia



**10:25 POLY 108.** Super-strong, transparent polyamides derived from renewable aromatic amino acid. **T. Kaneko**, M. Okajima, S. Tateyama, N. Takaya

**10:45 POLY 109.** Improving epoxy resin fracture toughness through biobased cashew nutshell liquid resin for high viscosity applications. **A. Maiorana**, L. Ren, G. Lo Re, S. Spinella, C.Y. Ryu, P. Dubois, R.A. Gross

**11:05** Concluding Remarks.

## Section C

Marriott Marquis San Diego Marina  
Solana

### Polymer Applications & Characterization in Medical Devices Industry

X. Liu, J. Slager, *Organizers, Presiding*

**8:00 POLY 110.** Probing the morphology, hydration, mechanics and tribology of biomedical coatings with environmental AFM. **G.D. Haugstad**

**8:30 POLY 111.** Morphological variations in poly (L-Lactic Acid) (PLLA) vascular scaffolds for the treatment of coronary heart disease (CHD). **K. Ramachandran**, A. Allianou, M. Kossuth, J.P. Oberhauser, J.A. Kornfield

**9:00 POLY 112.** Molecular weight analysis of implanted polyurethane insulated cardiac leads: Role of alliphantane linkages. **E. Chen**, A.D. Padsalgikar

**9:30** Intermission.

**9:45 POLY 113.** Use of ion exchange resins in pharmaceutical formulations. **A. Gehris**

**10:15 POLY 114.** Mechanical performance of surface porous PEEK for orthopaedic applications. **D. Safranski**, N. Evans, B. Torstrick, W.A. Chang, S. Laffoon, C.S. Lee, K. Gall, A.S. Lin, R. Guldberg

**10:45 POLY 115.** Characterization of novel degradable polymers for drug delivery applications. **J. Slager**

**11:15** Concluding Remarks.

## Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

### ACS Award in Polymer Chemistry: Symposium in honor of Edmund M. Carnahan

P. D. Hustad, *Organizer, Presiding*

**8:00 POLY 116.** Tuning ethylene/1-octene selectivity during olefin polymerization reactions with molecular catalysts. **J. Klosin**

**8:30 POLY 117.** FI Catalysts for developing new materials and catalysis. **H. Makio**

**9:00 POLY 118.** Group IV polyolefin catalysts supported by bidentate nitrogen-based ligands. **P.P. Fontaine**

**9:30 POLY 119.** Activation and reactivity of group(IV) metal-pyridylamido catalysts for olefin polymerization as disclosed by NMR studies. **A. Macchioni**, C. Zuccaccia

## Section E

Marriott Marquis San Diego Marina  
Balboa

### Excellence in Graduate Polymer Research

*Cosponsored by PRES, PROF, SOCED and YCC*  
*Financially supported by POLY IAB; Tosoh; Wiley*

C. J. Ellison, T. E. Long, *Organizers*

H. Cheng, C. J. Landry-Coltrain, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 120.** Synthesis and dipolar assembly of tetrapod functional colloidal monomers: Colloidal polymers with giant T-butyl groups. **N.G. Pavlopoulos**, J. Pyun

**8:35 POLY 121.** Synthesis of star-like and brush polymers via grafting-through of macromonomers by ATRP. **P. Krys**, H. Cho, K. Szczesniak, H. Schröder, S. Park, S. Jurga, M.J. Buback, K. Matyjaszewski

**9:05 POLY 122.** Assembly of branched polymers into responsive 2D and 3D microstructure. **W. Xu**, V.V. Tsukruk

**9:35** Intermission.

**9:50 POLY 123.** Optimizing surface treatments for the directed self-assembly of silicon-containing block copolymers. **G. Blachut**, S. Sirard, M. Maher, Y. Asano, Y. Someya, A. Lane, W. Durand, R. Gronheid, D. Hymes, C.J. Ellison, C.G. Willson

**10:20 POLY 124.** Enhanced supramolecular self-assembly of P3HT by copolymerization with methacrylate attached liquid crystalline mesogens. **T.M. Kekunawela Pathirana**, M.P. Bhatt, H. Magurudeniya, E.S. Rainbolt, M.C. Biewer, M.C. Stefan

**10:50 POLY 125.** Long range ordering of poly(3-hexylthiophene) in fluids and films: Effects of self-assembly techniques on liquid crystallinity, material properties and device performance. **N. Kleinhenz**, N. Persson, Z. Xue, P. Chu, G. Wang, Z. Yuan, D. Choi, M. Chang, E. Reichmanis

**11:20** Concluding Remarks.

## Section F

Marriott Marquis San Diego Marina  
Catalina

### Responsive Nanostructures & Nanocomposites

J. Foster, *Organizer*

E. B. Berda, Y. C. Simon, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 126.** Effects of copolymer structure and solution properties on antimicrobial activity of RAFT synthesized peptide mimics. **S.E. Morgan**, B. Abel, S.E. Goetz, L.C. Paslay, G.S. Sahukhal, M.O. Elasri, C.L. McCormick

**8:35 POLY 127.** Polypeptide nanoparticles for ocular drug delivery. **N.R. Cameron**

**9:05 POLY 128.** Cellulose nanocomposites and the role of surface chemistry. **J.P. Youngblood**, R. Moon, S. Peng, Y. Yoo

**9:35** Intermission.

**9:50 POLY 129.** Responsive shape-memory porous polymers and hydrogel-filled polymers: Templating within nanoparticle-stabilized emulsions. **C. Warwar Damouny**, I. Gurevitch, **M.S. Silverstein**

**10:20 POLY 130.** Stimuli-responsive polymeric materials that transform molecular detection events into autonomous reconfiguration of materials at the nano- and eventually macro-scale. **S.T. Phillips**

**10:50 POLY 131.** Incorporating Diels-Alder chemistry to prepare thermally-responsive materials. **M. Markmann**, M.R. Martinez, T. Schoch, R.G. Johnson, E.G. Wilborn, K.S. Barcus, E.D. Crenshaw, **P.J. Costanzo**

## Section G

Marriott Marquis San Diego Marina  
Del Mar

### General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*

G. M. Policastro, D. Siriwardane, *Presiding*

**8:00 POLY 132.** Efficient anticancer polymer prodrug nanoparticles from drug-initiated controlled/living radical polymerization. **Y. Bao**, D. Desmaele, S. Mura, C. Patrick, J. Nicolas

**8:20 POLY 133.** Role of polymer architecture on the activity of protein-polymer conjugates for the treatment of disease. **B. Tucker**, J.D. Stewart, J. Aguirre, L. Holliday, C.A. Figg, J.G. Messer, B.S. Sumerlin

**8:40 POLY 134.** From benchtop to human clinical trials: A successful imaging agent for detecting early-stage atherosclerosis. **A. McGrath**, E. Pressly, D. Klinger, Y. Liu, R. Laforest, D. Sultan, H. Luehmann, S. Schwarz, R. Gropler, P. Woodard, C.J. Hawker

**9:00 POLY 135.** Responsive polymeric nanoparticles designed for site-specific delivery in agriculture. **M. Hill**, E.M. Mackrell, C.P. Forsthoefel, S.P. Jensen, M. Chen, G.A. Moore, Z. He, B.S. Sumerlin

**9:20 POLY 136.** Peptide crosslinking strategies for increasing mechanical properties in degradable poly(ester ureas). **G.M. Policastro**, M. Becker, F. Lin

**9:40 POLY 137.** Design of degradable and non-degradable highly branched polymers based on liponic acid. **H. Tang**, N.V. Tsarevsky

**10:00 POLY 138.** PLLA-WS<sub>2</sub> nanocomposites for bioresorbable vascular scaffolds. **T. Di Luccio**, K. Ramachandran, J.A. Kornfield

**10:20 POLY 139.** Functional macromolecular platforms for sequence-defined polymers and multidrug-loaded nanoparticle chemotherapeutics. **J. Barnes**, H.V. Nguyen, D.J. Ehrlich, L. Liao, J. Liu, K.W. Young, F.A. Leibfarth, T.F. Jamison, J.A. Johnson

**10:40 POLY 140.** Polynorbomene-*g*-starch copolymers for small hydrophobic molecule encapsulation and release. **A. Sengupta**, J. Enem, J. Nettleton, P.M. Iovine

**11:00 POLY 141.** Deoxyribonucleic acid as a model for the design of functional, degradable polymers. **Y.T. Tsao**, K.L. Wooley

**11:20 POLY 142.** Molecular screws of polycarbodiimides from helix sense selective polymerization and their complexation. **D. Siriwardane**, O.V. Kullikov, B.M. Novak

**11:40 POLY 143.** Polyelectrolyte nanocages via crystal-forming miniemulsions. **B. Sun**, H. Sun, Y. Li, H. Cui, **C. Cheng**

### ACS Award in Applied Polymer Science: Symposium in honor of Thomas P. Russell

*Sponsored by PMSE, Cosponsored by POLY*

### Is There a Crisis in Organic Chemistry Education?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## New Horizons in Sustainable Materials

### Glycoscience

*Sponsored by CELL, Cosponsored by DAC† and POLY*

### ACS Award for Creative Invention: Symposium in honor of Antonio Facchetti

*Sponsored by PMSE, Cosponsored by POLY*

## MONDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Rancho Santa Fe 1 & 2

### Applications of Polymer Surfaces & Interfaces

### Composites, Brushes & Medical Devices

*Cosponsored by COLL and PMSE*

S. T. Iacono, J. M. Mabry, A. Tuteja, *Organizers, Presiding*

S. M. Ramirez, *Presiding*

**1:00 POLY 144.** Extremely low friction with hydrophilic brushes in water when segregated from a PDMS matrix. **S. Hvilsted**, I. Javakhishvili, K. Jankova, T. Roen, S. Lee

**1:30 POLY 145.** Property prediction with molecular dynamics simulations on graphene-epoxy coating materials. **L. Subramanian**

**1:50 POLY 146.** Interphase development in thermoset matrix composites. **J. Moller**, S. Barr, A. Ecker, T. Breitman, D. Nepal, R.J. Berry

**2:20 POLY 147.** Comparison of polymer brush solvation across grafting density regimes via vapor absorption measurements. **S.V. Orski**, R.J. Sheridan, K. Beers

**2:40 POLY 148.** Development and application of chain growth aromatic polyamide brushes. **S.G. Boyes**, F.C. Prehn

**3:10** Intermission.

**3:20 POLY 149.** Fabrication of bioactive surfaces with enhanced blood compatibility via a sequential co-immobilization strategy. **Q. Yu**, W. Zhan, H. Chen

**3:50 POLY 150.** Withdrawn.

**4:10 POLY 151.** Brushing off salt using new polymer brush membranes. **M. Sorci**, J.M. Imbrogno, J.J. Keating, J.E. Kilduff, G. Belfort

**4:30 POLY 152.** Deposition of functional polymers coatings onto parylene substrates for biomedical applications. **M. Gupta**, M. De Luna, C. Cheng

**5:00 POLY 153.** Ultrathin polymer coatings for the control of cell-surface interactions. **M. Henze**, O. Prucker, J. Rühle

### Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

### Sustainable Polymers, Processes & Applications

*Cosponsored by PMSE*

D. Boday, J. H. Wang, *Organizers*

G. Chen, D. S. Wardius, *Presiding*

**1:00** Introductory Remarks.

**1:05 POLY 154.** Modified vegetable oil as a styrene replacement in commercial unsaturated polyester resins for fiber-reinforced composites. **Y. Wu**, K. Li

**1:35 POLY 155.** Replacement of styrene with a food additive in commercial unsaturated polyester resins for fiber-reinforced composites. **Y. Wu, K. Li**

**1:55 POLY 156.** Effect of degree of functionality on properties of methacrylated bio-based resins and thermosets. **A.Z. Yu, D.C. Webster**

**2:15 POLY 157.** Highly functional cationic biobased resins for sustainable UV-curable coatings. **I. Hevus, D.C. Webster**

**2:35 Intermission.**

**2:55 POLY 158.** Soy-Based Resins and Fillers for Thermoset Composites. **C.R. Pugh, B. Mehta, P. Watt**

**3:25 POLY 159.** New lanthanide complexes for the polymerization of  $\alpha$ -methylene- $\gamma$ -butyrolactone to obtain biodegradable cross-linkable unsaturated polyesters. **P.I. Binda**

**3:45 POLY 160.** Monomers, polymers, and nanocomposites derived from plant oil as next-generation sustainable materials. **Z. Wang, L. Yuan, N.M. Trenor, C. Tang**

**4:05 Concluding Remarks.**

## Section C

Marriott Marquis San Diego Marina  
Solana

### Industrial Innovation in Polymer Chemistry: Sustainable Polymerization Feedstocks & Process Technology

*Cosponsored by BMGT*

*A. Meyer, Organizer*

*L. Pitet, Organizer, Presiding*

**1:00 POLY 161.** Bio based thermoplastic polyurethane. **G. Scholz**

**1:30 POLY 162.** Industrial applications of medium chain length poly(hydroxy alkanooates): From feedstock to finished article. **M. Mang**

**2:00 POLY 163.** Supramolecular structures for the precision release of therapeutics. **J.L. Hedrick, Y. Yang**

**2:30 POLY 164.** Commercial scale self-assembled polymer-pigment composites for waterborne coatings with high performance, improved eco-footprint and lower cost. **J. Bohling**

**3:00 Intermission.**

**3:15 POLY 165.** Development and life cycle assessment of organic photovoltaics. **B. Worfolk, A. Kapur, A.A. Johnston, K.B. Woody**

**3:45 POLY 166.** Flame resistant textiles for the 21st century: Sustainable solutions from theory to practice. **J.M. Spruell, W. Gerhardt**

**4:15 POLY 167.** Photoluminescent UV curable polymer-quantum dot composite as luminescent down-shifting layer for photovoltaics. **G. Draaisma, D.F. Reardon**

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

### ACS Award in Polymer Chemistry: Symposium in honor of Edmund M. Carnahan

*P. D. Hustad, Organizer, Presiding*

**1:00 POLY 168.** Focusing the HTE approach to polyolefin catalysis. **V. Busico**

**1:30 POLY 169.** Polydispersity in block copolymer self-assembly: From photonic polyethylene to advanced lithographic patterning. **P.D. Hustad, J.D. Weinhold, E. Garcia-Meitin, G.R. Marchand, J. Zhang, V. Ginzburg, P. Trefonas**

**2:00 POLY 170.** Mythology of single site polyethylene catalysts. **R.L. Kuhlman, C. Zuccaccia, A. Macchioni, A. Gies**

**2:30 POLY 171.** Cooperative catalytic properties of multinuclear electrophilic organometallic ensembles. **T.J. Marks**

**3:00 POLY 172.** Applications of olefin block copolymers. **G.R. Marchand, R. Barry, H. Boone, Y. Hu, S. Karande, K. Kummer, R. Laakso, C. Li Pi Shan, L. Maderjan, A. Montoya-Goni, J. Munro, K. Walton**

**3:30 POLY 173.** Chromophore-labeled gel permeation chromatography applied to the study of hafnium pyridylamide catalyzed polymerization of 1-octene in the presence of diethyl zinc. **B.J. Anding, E. Cueny, H. Johnson, C.R. Landis**

**4:00 POLY 174.** Award Address (ACS Award in Polymer Chemistry sponsored by ExxonMobil Chemical Company). Advances in olefin block copolymers. **E.M. Carnahan**

## Section E

Marriott Marquis San Diego Marina  
Balboa

### Excellence in Graduate Polymer Research

*Cosponsored by PRES, PROF, SOGED and YCC. Financially supported by POLY IAB; Tosoh; Wiley*

*H. Cheng, C. J. Landry-Coltrain, Organizers*

*C. J. Ellison, T. E. Long, Organizers, Presiding*

**1:00 Introductory Remarks.**

**1:05 POLY 175.** Sustainable urethane-based vitrimers. **J.P. Brutman, D.J. Fortman, C.J. Cramer, M.A. Hillmyer, W. Dichtel**

**1:35 POLY 176.** Biomass-derived polymers incorporating monolignols. **B. Upton, A.M. Kasko**

**2:05 POLY 177.** Multifunctional modification of cellulose ethers via olefin cross-methathesis followed by Thiol-Michael addition. **Y. Dong, K.J. Edgar**

**2:35 Intermission.**

**2:50 POLY 178.** Facile syntheses of polypeptide molecular brushes with two-dimensional controlled architectures. **J. Fan, Y. Borguet, L. Su, X. He, T.P. Nguyen, K.L. Wooley**

**3:20 POLY 179.** *In vitro* illustrations: Achieving activated fluorescence in cancer cells. **M. Burdette, R. Jenkins, I. Bandera, R. Powell, T. Bruce, X. Yang, Y. Wei, S.H. Foulger**

**3:50 POLY 180.** Engineering responsive matrices for controlled drug delivery: From bulk gels to nanogels. **Y. Liang, K.L. Kluck**

## Section F

Marriott Marquis San Diego Marina  
Catalina

### Responsive Nanostructures & Nanocomposites

*E. B. Berda, J. Foster, Y. C. Simon, Organizers*

*W. Gramlich, S. T. Schneebeli, Presiding*

**1:00 Introductory Remarks.**

**1:05 POLY 181.** Freeform light-responsive spirals. **S.T. Schneebeli, M. Sharafi, X. Liu, K.E. Murphy, Z. Weinert**

**1:35 POLY 182.** Modular assembly of spatiotemporally patternable, stimuli responsive hydrogels. **N. Dadoo, W. Gramlich**

**2:05 POLY 183.** *In situ* nanofiller formation in polymer nanocomposites. **D. Roth, L.E. Hanzly, J.R. Barone**

**2:35 Intermission.**

**2:50 POLY 184.** Quantifying the behavior of a new family of pH-responsive hydrogels. **S. Patil, P. Chaudhury, L. Clarizia, M.J. McDonald, E. Reynaud, P. Gaines, D.F. Schmidt**

**3:20 POLY 185.** Application of anthracene in the synthesis and functionalization of single-chain nanotechnology. **P. Frank, E.B. Berda**

**3:40 POLY 186.** Fabrication and applications of multiresponsive cyclic poly(phthalaldehyde) microcapsules prepared by internal phase separation. **S. Tang, M. Odarzenko, N.R. Sottos, S. White, J.S. Moore**

**4:00 POLY 187.** Traceless crosslinking and bilayer permeability tuning of polymer-somes self-assembled from responsive amphiphilic block copolymers. **S. Liu**

## Section G

Marriott Marquis San Diego Marina  
Del Mar

### Supramolecular Polymers: From Structure to Advanced Functionality

*L. Montero, W. Weng, Organizers*

*J. Foster, J. B. Matson, Organizers, Presiding*

**1:00 Introductory Remarks.**

**1:05 POLY 188.** Unusual photocharge generation in 1D confined organic semiconductor nanostructures. **H. Frauenrath, R. Hafner, R. Marty**

**1:35 POLY 189.** Self-assembly of pH-regulated supramolecular polymers in water. **H.C. Frisch, P. Ahlers, P. Besenius**

**2:05 POLY 190.** Stimuli-responsive supramolecular polymers. **C. Weder**

**2:35 Intermission.**

**2:50 POLY 191.** Doubly Charged Monomers for Enhanced Physical Crosslinking: Are two charges per repeating unit twice as good? **K. Zhang, K. Drummey, M. Tamami, S. Cheng, S. Hemp, R. Gao, A.E. Smith, T.E. Long**

**3:20 POLY 192.** Application of tetra aniline oligomers in functional single-chain nanoparticles and materials. **E.B. Berda**

**3:50 POLY 193.** Dynamic and self-healing polymer design via both supramolecular and dynamic covalent interactions. **Z. Guan**

### ACS Award in Applied Polymer Science: Symposium in honor of Thomas P. Russell

*Sponsored by PMSE, Cosponsored by POLY*

### Diversity-Quantification-Success?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### New Horizons in Sustainable Materials

#### Polysaccharide Materials

*Sponsored by CELL, Cosponsored by DAC and POLY*

### ACS Award for Creative Invention: Symposium in honor of Antonio Facchetti

*Sponsored by PMSE, Cosponsored by POLY*

### Undergraduate Research Posters

#### Polymer Chemistry

*Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED*

### Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza

*Sponsored by INOR, Cosponsored by ENVR, ORGN and POLY*

## MONDAY EVENING

### Section A

San Diego Convention Center  
Halls D/E

#### Sci-Mix

*M. Jeffries-Eli, C. Lipscomb, T. J. White, Organizers*

**8:00 - 10:00**

306-307, 311, 314, 318, 320-322, 333, 336-341, 343-344, 346-347, 352-353, 357-358, 361-364, 367-370, 373, 375, 381, 383, 385, 389-390, 395-397, 400, 402, 407-408, 411, 415, 417, 420, 422-424, 427-429, 433, 435, 437-439. See subsequent listings.

### Potpourri of Polymer Projects: Take a Byte out of the NGS

*Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB*

## TUESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom B

### Applications of Polymer Surfaces & Interfaces

#### Energy Conversion

*Cosponsored by COLL and PMSE*

*S. T. Iacono, J. M. Mabry, A. Tuteja, Organizers, Presiding*

*A. Sellinger, Presiding*

**8:00 POLY 194.** Tracking the transformation of lead halide complex into organic lead halide perovskite. **P.V. Kamat, J. Manser, S. Yoon**

**8:30 POLY 195.** Towards stable and efficient metal halide perovskite solar cells for hybrid tandems with silicon. **T. Leijtens, M.D. McGehee, C. Bailie, K. Bush, E. Hoke**

**9:00 POLY 196.** Influence of surfaces and interfaces on the grain morphology and electronic structures in perovskite solar cells. **J. Huang**

**9:30 POLY 197.** Characterization of PVDF-g-sulfonated polystyrene and PE-g-sulfonated polyarylsulfone proton exchange membranes for direct methanol fuel cells. **T.M. Chung, G. Zhang, C. Nam**

**10:00 POLY 198.** Morphology studies of contact optimization in organic electronic devices. **L.J. Richter, D. DeLongchamp, A.L. Briseno, H. Lee, C. McNeill, E. Gann, D.Y. Yoon, N. Shinn**

**10:30** Intermission.

**10:40 POLY 199.** Silicone high voltage insulation. **M.J. Owen**

**11:05 POLY 200.** Nano-membranes for lithium/sulfur batteries. **C.B. Bucur, N. Osada, J. Muldoon**

**11:30 POLY 201.** Main-chain liquid-crystalline elastomers using a two-stage thiol-acrylate reaction for shape-switching biomedical applications. **C.M. Yakacki, R. Volpe, M. Saed, A. Torbati, D. Merkel, C. Frick**

**11:55 POLY 202.** Liquid crystal elastomer composites with aligned, anisotropic fillers as multifunctional actuators. **T.H. Ware, J. Boothby, H. Kim**

**12:20 POLY 203.** Responsive surfaces prepared by programming liquid crystalline elastomers. **T.J. White, T. Ware, B. Kowalski**

## Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

### Sustainable Polymers, Processes & Applications

*Cosponsored by PMSE*

D. Boday, J. H. Wang, *Organizers*

K. Li, C. R. Pugh, *Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 204.** Study of dynamics at a composite interphase as a result of applied stress using fluorescence imaging. **J.W. Woodcock, R. Beams, S. Stranick, C.S. Davis, M. Zammarano, F. Vollrath, D. Shah, J.W. Gilman**

**8:35 POLY 205.** Enhancing the sustainability of glass-fiber reinforced epoxies. **C. Kuncho, W. Liu, J. Moeller, E. Reynaud, D.F. Schmidt**

**8:55 POLY 206.** Refining the design of sustainable polymers with octanol-water partition coefficients. **R.T. Mathers**

**9:15** Intermission.

**9:35 POLY 207.** Single-step and simultaneous plasticization and compatibilization process for compounding starch and polyolefins. **A. Chen, J.H. Wang, G. Wideman**

**10:05 POLY 208.** Step-growth polymerization of highly efficacious antimicrobial polymers for consumer care products. **M. Zhang, R. Ono, A. Engler, Y. Yang, J.L. Hedrick**

**10:25 POLY 209.** High temperature thermo-setting polyimides derived from sustainable, non-toxic polyamides. **B.G. Harvey, G.R. Yandek, A. Chafin, J. Lamb, M. Garrison**

**10:45 POLY 210.** Phosphorus flame retardants for polymeric materials from isosorbide bis-acrylate. **Y. Daniel, B.A. Howell**

**11:05** Concluding Remarks.

## Section C

Marriott Marquis San Diego Marina  
Del Mar

### Undergraduate Research in Polymer Science

#### Synthesis, Characterization & Engineering of Polymers

*Financially supported by University of Southern Mississippi; POLY IAB; Sabic*

J. Lott, S. E. Morgan, S. I. Nazarenko, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 211.** Dual functional flame retardants from a non-edible seed oil. **E.A. Ostrander, B.A. Howell**

**8:25 POLY 212.** Use of Diels-Alder chemistry to prepare molecular weight changing material. **M.R. Martinez, M. Markmann, T. Schoch, P.J. Costanzo**

**8:45 POLY 213.** Synthesis and characterization of activatable dyes for integration into polymer systems. **C. Vollbrecht, M. Wang, J.W. Gilman**

**9:05 POLY 214.** Investigation of microphase separation by atomic force microscopy in oligo(ethylene oxide) grafted oxanorbornyl diblock copolymers for use as lithium ion battery electrolyte supports. **T.J. Kolibaba, D.A. Waldow**

**9:25** Intermission.

**9:40 POLY 215.** Electrically conductive silk fibroin scaffolds for use as nerve conduits. **E. Sanders, S. Severt, A. Murphy**

**10:00 POLY 216.** Withdrawn.

**10:20 POLY 217.** Thermally responsive materials with dynamic topology based upon Diels-Alder chemistry. **R.G. Johnson, E.G. Wilborn, K.S. Barcus, E.D. Crenshaw, P.J. Costanzo**

**10:40 POLY 218.** Integrated synthetic and computational techniques for the design of poly[3]rotaxanes. **E.P. Bruckner, M.J. Hore, S.J. Rowan**

**11:00 POLY 219.** PEG containing thiol-ene network membranes for CO<sub>2</sub> separation: PEG units as dangling chains versus peg units in the backbone. **T.N. Haddock, R. Ramakrishnan, V. Vasagar, S.I. Nazarenko**

## Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

### General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*

W. C. Anderson, J. C. Worch, *Presiding*

**8:00 POLY 220.** Chain transfer polymerization of carbon dioxide, cyclohexene oxide and poly(dimethyl)siloxanes utilizing zinc based catalysts. **M. Reiter, A. Kronast, B. Rieger**

**8:20 POLY 221.** Introduction of redox-active catalysis to the polymerization of olefins. **W.C. Anderson, B.K. Long**

**8:40 POLY 222.** Highly active and syndiospecific zinc complexes for the immortal ring-opening polymerization of  $\beta$ -butyrolactone. **T. Ebrahimi, S. Hatzikiakos, P. Mehrkhodavandi**

**9:00 POLY 223.** Highly active neodymium catalyst for polymerization of dienes, vinyl monomers and ring opening polymerization of lactones. **R. Kularatne, D. Krang, A. Yang, M.C. Biewer, M.C. Stefan**

**9:20 POLY 224.** Synthesis of redox-active, fluorescent, and/or thermo-responsive viologen-containing polymers by atom transfer radical polymerization. **Z. Wang, N.V. Tsarevsky**

**9:40 POLY 225.** Phenol-modified methylaluminoxanes for the activation of a bis(imino)pyridine iron catalyst in ethylene oligomerization. **B. Jiang, J. Ye, J. Wang, Y. Yang, J. Zheng**

**10:00 POLY 226.** Structure-activity relationship on palladium phosphine-sulfonates for olefin-polar monomer copolymerization. **M. Kobayashi, M. Ano, H. Uchino, J. Hosoi, T. Tayano**

**10:20 POLY 227.** Breaking symmetry-rules for stereoselective polymerization catalysis. **G. Talarico, C. De Rosa, R. Di Girolamo, A.B. Muñoz-García, M. Pavone**

**10:40 POLY 228.** Metal-free atom transfer radical polymerization. **N.J. Treat, J. Read De Alaniz, B.P. Fors, C.J. Hawker**

**11:00 POLY 229.** Robust catalysts for catalyst-transfer polycondensation of monomers containing electron withdrawing groups. **J.C. Worch, Y. Qiu, K.J. Noonan**

**11:20 POLY 230.** Synthesis of catechol-functionalized poly(ethylene oxide) block and random copolymers. **K.M. Mattson, A. Latimer, A. McGrath, N. Lynd, P. Lundberg, Z. Hudson, C.J. Hawker**

**11:40 POLY 231.** Synthesis, polymerization, and characterization of sulfonamide based bifunctional monomers. **B. Hall, L. Meyer, J. Munch, E. Fossum**

## Section E

Marriott Marquis San Diego Marina  
Balboa

### Excellence in Graduate Polymer Research

*Cosponsored by PRES, PROF, SOCED and YCC Financially supported by POLY IAB; Tosoh; Wiley*

H. Cheng, C. J. Landry-Coltrain, *Organizers*

C. J. Ellison, T. E. Long, *Organizers, Presiding*

**8:00 POLY 232.** Dynamic bonds in covalently crosslinked polymer networks for photo-activated strengthening and healing. **M.B. Gordon, J.M. French, N.J. Wagner, C.J. Kloxin**

**8:30 POLY 233.** Postpolymerization modification of liquid crystal alignment in covalent adaptable networks. **M.K. McBride, D. Liu, M. Hendriks, D. Broer, C. Bowman**

**9:00 POLY 234.** Thiol-trifluorovinyl ether (Thiol-TFVE) photochemistry: A new route to semifluorinated materials. **B.R. Donovan, J. Ballenas, D.L. Patton**

**9:30** Intermission.

**9:45 POLY 235.** Functionalized triptycene based poly(ether ether ketone) for ion exchange membranes. **L.C. Moh, J.B. Goods, T.M. Swager**

**10:15 POLY 236.** Development of polyimine-based dynamic covalent network: From malleable polymers to high-performance composites. **P.J. Taynton**

**10:45 POLY 237.** One-electron process in a gel polymer Li-O<sub>2</sub> battery. **C.V. Amanchukwu, H. Chang, Y. Shao-Horn, P.T. Hammond**

## Section F

Marriott Marquis San Diego Marina  
Presidio 2

### Responsive Nanostructures & Nanocomposites

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

D. Choi, P. Frank, *Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 238.** Withdrawn.

**8:25 POLY 239.** Transiently responsive protein-polymer conjugates via a grafting-from RAFT approach: For intracellular co-delivery of proteins and immune-modulators. **N. Vanparijs, B. De Geest**

**8:45 POLY 240.** Acid-cleavable acetal-linked paclitaxel-polymer conjugates via a drug-functionalized RAFT CTA approach. **B. Louage, B. De Geest**

**9:05 POLY 241.** Stacking clay-based and intumescent multilayer thin films to completely stop fire on highly flammable polyurethane foam. **K. Holder, M. Huff, M. Cosio, J.C. Grunlan**

**9:25 POLY 242.** Shape-control in self-assembly of bioreducible poly(ether)olides. **O. Schaefer, D. Huesmann, K. Klinker, M. Barz**

**9:45** Intermission.

**10:00 POLY 243.** *In Situ* formation of nanoparticles in polymer matrices using thermal and photothermal processing. **F. Zeng, J. Spicer**

**10:20 POLY 244.** Carbon nanotube-polymer composites for chemical warfare agent sensing. **J.F. Fennell, H. Hamaguchi, T.M. Swager**

**10:40 POLY 245.** Serendipitous discovery of an unlikely poly(arylene ether) switch and recent application to VOC sensing. **R. Campos, J.F. Reuther, D. Kovalev, N.R. Mammoottil, C. Merten, B.M. Novak**

**11:00 POLY 246.** Blending approach for the assembly of micellar nanoparticles. **D. Wright, J.P. Patterson, N.C. Gianneschi, C. Chassenieux, O. Colombani, R.K. O'Reilly**

**11:20 POLY 247.** Hybrid hydrogels of thermosensitive block copolymers and hairy nanoparticle. **B. Hu, R.A. Wright, D.M. Henn, S. Jiang, B. Zhao**

## Section G

Marriott Marquis San Diego Marina  
Solana

### Supramolecular Polymers: From Structure to Advanced Functionality

L. Montero, W. Weng, *Organizers*

J. Foster, J. B. Matson, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 248.** Bioinspired supramolecular polymers. **M.B. Baker, L. Albertazzi, C. Leenders, A. Palmans, E.W. Meijer**

**8:35 POLY 249.** Utilizing the steric congestion of brush polymers: From nucleic acid delivery to self-assembly. **K. Zhang, X. Lu, X. Tan, F. Jia**

**9:05 POLY 250.** Responsive polymers by supramolecular design: Self-healing materials and pressure sensitive chemistry. **S. Chen, P. Michael, D. Döhler, W.H. Binder**

**9:35** Intermission.

**9:50 POLY 251.** Functionalization of electrospun polycyclodextrin fibers with bioactive peptide molecules and their biological applications. **S. Hamsici**

**10:20 POLY 252.** Withdrawn.

**10:50 POLY 253.** Disassembly and immolation pathways of drug-based supramolecular polymers. P. Zhang, H. Cui, R. Lin

**11:20 POLY 254.** Morphological control of the release profile of H<sub>2</sub>S-releasing micelles. J. Foster, J.B. Matson

#### ACS Award in Industrial Chemistry: Symposium in honor of Ted C. Germroth

Sponsored by I&EC, Cosponsored by POLY

#### ACS Award for Creative Invention: Symposium in honor of Antonio Facchetti

Sponsored by PMSE, Cosponsored by POLY

#### Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Henry E. Bryndza

Sponsored by INOR, Cosponsored by ENVR, ORGN and POLY

#### Eli Pearce Memorial Symposium

Sponsored by IAC, Cosponsored by CHAS, POLY and SCC

## TUESDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom B

#### Applications of Polymer Surfaces & Interfaces

##### Membranes

Cosponsored by COLL and PMSE

S. T. Iacono, J. M. Mabry, A. Tuteja, *Organizers, Presiding*

S. M. Ramirez, *Presiding*

**1:00 POLY 255.** Microvascular materials for carbon capture and self-improvement: How do we make materials that make themselves better? A.P. Esser-Kahn, M. Kleiman, K. Brubaker, D.T. Nguyen

**1:30 POLY 256.** Reversible CO<sub>2</sub> capture from an amine functionalized polymer thin film. B. Barkakaty, J.F. Browning, B.S. Lokitz

**2:00 POLY 257.** Improved carbon dioxide separation performance in amidoximated polydimethylsiloxane-norbornene membranes. T. Hong, S. Chatterjee, S.M. Mahurin, D. Jiang, B.K. Long, J.W. Mays, A.P. Sokolov, T. Saito

**2:20 POLY 258.** Development and characterization of advanced gas separation membranes using vinyl-added polynorbornenes bearing CO<sub>2</sub>-philic functionalities. K.R. Gmernicki, E. Hong, T. Hong, T. Saito, B.K. Long

**2:40 POLY 259.** Polymer nanocomposite membrane for gas separation. Y. Huang, E. Buening, C. Bilchak, L. Wang, S. Kumar, B.C. Benicewicz

**3:00 POLY 260.** Ionically-crosslinked polymer and nanoplatelet multilayer films for gas separation. J.C. Grunlan, B.A. Wilhite

**3:30** Intermission.

**3:40 POLY 261.** Functionalization and surface characterization of sulfone polymers with partially fluorinated POSS chain-ends. S.E. Morgan, K.M. Knauer, A.R. Jennings, S.T. Iacono

**4:10 POLY 262.** Novel ligand functionalized membranes for monoclonal antibody purification. S. Colak Atan, A. Vail, J.K. Rasmussen, C. Bothof, G. Griesbraber, F. Sgolastra

**4:40 POLY 263.** Hygro-responsive membranes for high efficiency separation of miscible liquids. E.R. Post, G. Kwon, A.K. Kota, C. Li, J.T. Reams, J.M. Mabry, A. Tuteja

**5:00 POLY 264.** Superoleophobic-superhydrophilic surfaces via thiol-ene photopolymerization for efficient oil-water separations. L. Xiong, W. Guo, D.L. Patton

### Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

#### 13th International Symposium on Biorelated Polymers

##### Synthesis of Biorelated Polymers for Tissue Engineering & Therapeutics

R. Ottenbrite, *Organizer*

C. Scholz, *Organizer, Presiding*

J. Kressler, *Presiding*

**1:00** Introductory Remarks.

**1:05 POLY 265.** Materials design for novel nanotherapeutics based on control of gaseous molecules *in vivo*. Y. Nagasaki

**1:35 POLY 266.** Acid-triggered oxidative stress amplifying polymeric micelles: Applications in anticancer and antibacterial therapy. D. Lee, H. Park, E. Jung, D. Yoo

**2:05 POLY 267.** Poly(phosphoester)s: From adhesives to stealth polymers. F. Wurm, T. Wolf, G. Becker, M. Steinmann, H. Tee, A. Cankaya

**2:35** Intermission.

**2:50 POLY 268.** Highly porous polymers and hydrophobic-hydrophilic bicontinuous polymers for bio-related applications through emulsion templating. M.S. Silverstein

**3:20 POLY 269.** Osteomimetic graphene composite scaffolds for bone regeneration. S.A. Sydik, A. Arnold, B. Hold, Z. Wright

**3:50 POLY 270.** One-pot synthesis of poly(lactide)-based block copolymers for bone tissue engineering applications. P.P. Smith, A.L. Rightler, D. Price, S.G. Boyes

**4:10 POLY 271.** Highly tunable library of thermoresponsive, biodegradable polyesters based on N-substituted diols. J.P. Swanson, M.R. Martinez, L.R. Monteleone, F. Haso, P.J. Costanzo, T. Liu, A. Joy

### Section C

Marriott Marquis San Diego Marina  
Del Mar

#### Undergraduate Research in Polymer Science

##### Bio-inspired Polymers & Biomedical Applications

Financially supported by University of Southern Mississippi; POLY IAB; Sabic

J. Lott, S. E. Morgan, S. I. Nazarenko, *Organizers, Presiding*

**1:00 POLY 272.** Synthesis and characterization of NIPAM and acrylic acid-based polymer-lysozyme conjugates. L. Qiao, S.L. Goh

**1:20 POLY 273.** Synthetic design of block copolymer amphiphiles for nanomaterial dispersion. B. Alameda, S. Feist, H. Heintzmann, P.J. Costanzo

**1:40 POLY 274.** Functional, composite polythioether nanoparticles via thiol-alkyne photopolymerization in miniemulsion. S.E. Walley, D.N. Amato, D.V. Amato, J. Narayanan, B.R. Donovan, J.R. Douglas, A.S. Flynt, D.L. Patton

**2:00 POLY 275.** Mechanically tunable pululan-chitin nanocrystal scaffold for biological application. C. Sago, A. Maiorana, R.A. Gross

**2:20** Intermission.

**2:30 POLY 276.** Optimizing gene silencing in light-responsive siRNA polyplexes by varying polymer block lengths. V. Muir, C. Greco, M.O. Sullivan, T.H. Epps

**2:50 POLY 277.** Characterization of reagent pencils onto solvent-free deposition of reagents onto paper-based diagnostic device. C.H. Liu, H.T. Mitchell, I.C. Noxon, C.E. Immoos, N. Martinez, A.W. Martinez, P.J. Costanzo

**3:10 POLY 278.** Amino acid-modified norbornyl polymers as analogues to hydrogel-forming peptides. D. Crystal, A.P. Blum, A.S. Carlini, S. Sahu, F.J. Hidalgo, N.C. Gianneschi

**3:30 POLY 279.** Employment of cysteine and thiazolidine chemistry for novel polymer coupling and architectures. K.E. Eckhart, A.M. Ventura, A.J. Varni, C. DeHoe, P.J. Costanzo

**3:50** Intermission.

**4:00** Panel Discussion.

### Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

#### Click Reactions for Producing Advanced Materials

W. Kern, F. Wiesbrock, *Organizers*

G. N. Tew, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 POLY 280.** Photoredox catalysts: An efficient tool for click chemistry and polymer post-modification. C. Boyer

**1:35 POLY 281.** Multiplexed nanoarrays via 4D surface photochemistry. X. Liu, Y. Zheng, A. Braunschweig, Y. Ji

**1:55 POLY 282.** Click chemistry dye conjugate dendrimers containing controlled ratios of dye per particle: Synthesis, characterization, and biological evaluation. M.M. Banaszak Holl, C.A. Dougherty, S. Vaidyanathan, S.C. Dimaggio, J.M. Manono

**2:25** Intermission.

**2:45 POLY 283.** Thiol-Yne photo-click chemistry: Towards biocompatible and tough photopolymers for 3D printing. T. Griesser

**3:15 POLY 284.** Retro-Staudinger cycloaddition enabled by polymer mechanochemistry. M.J. Robb, J.S. Moore

**3:35 POLY 285.** Step-growth clickable nano/micro-particles. C. Wang, C. Bowman

**3:55 POLY 286.** Sufex on the surface: A flexible platform for postpolymerization modification of polymer brushes. J. Yatvin, K. Brooks, J.J. Locklin

**4:15 POLY 287.** From imaging to therapy: Polymeric nanoparticles for *in vivo* click chemistry. A. Birke, M. Barz

### Section E

Marriott Marquis San Diego Marina  
Balboa

#### Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC  
Financially supported by POLY IAB; Tosoh; Wiley

C. J. Ellison, T. E. Long, *Organizers*

H. Cheng, C. J. Landry-Coltrain, *Organizers, Presiding*

**1:00 POLY 288.** Poly(cyclohexylethylene)-block-poly(ethylene oxide) block polymers for metal oxide templating. M.W. Schulze, C. Sinturel, M.A. Hillmyer

**1:30 POLY 289.** Design and synthesis of nitrogen-doped hierarchical carbon for selective carbon capture and electrocatalysis. J. To, J. He, D. Ng, S. Siahrostami, K. Kim, A. Koh, F. Studt, J.K. Norskov, T.F. Jaramillo, J. Wilcox, Z. Bao

**2:00 POLY 290.** Optically reprogrammable buckling of nanocomposite polymer films. A.W. Hauser, A.A. Evans, D. Liu, K.C. Bryson, J. Na, D. Broer, R.C. Hayward

**2:30 POLY 291.** Probing the surface-localized hyperthermia of gold nanoparticles in a microwave field using polymeric thermometers. C.P. Kabb, R. Carmean, B.S. Sumerlin

### Section F

Marriott Marquis San Diego Marina  
Catalina

#### Anionic Polymerisation: Still Living After 60 Years

Cosponsored by PMSE and RUBB  
Financially supported by ExxonMobil; Kraton; Synthomer; Goodyear; Eastman Chemical

L. R. Hutchings, *Organizer*

J. W. Mays, *Organizer, Presiding*

S. Carloti, *Presiding*

**1:00** Introductory Remarks.

**1:05 POLY 292.** Polyhomologation: Another version of monomer activated anionic polymerization. N. Hadjichristidis, H. Zhang, Z. Zhang, N. Alkayal, D. Wang, Y. Gnanou

**1:35 POLY 293.** Living anionic polymerization of 1-adamantyl 4-vinylphenyl ketone. T. Ishizone

**2:05 POLY 294.** Synthesis of randomly branched polymers by anionic chain-transfer polymerisation. L.R. Hutchings

**2:25 POLY 295.** Synthesis and application benefits of 1,3-butadiene and divinylbenzene copolymers. C. Roeschlaub

**2:45** Intermission.

**3:05 POLY 296.** Precise characterization of polymers prepared by anionic polymerization. T. Chang

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**3:35 POLY 297.** New synthetic strategy for the synthesis of amphiphilic PDMS-PEO block copolymer and characterization of heterobifunctional PEO using normal phase-chromatography .  
G. Benzi, L.R. Hutchings

**3:55 POLY 298.** High conductivity durable anion conducting membranes.  
K. Misichronis, S. Foister, N. Kang, T. Zawodzinski, J.W. Mays

## Section G

Marriott Marquis San Diego Marina  
Solana

### Supramolecular Polymers: From Structure to Advanced Functionality

J. Foster, J. B. Matson, *Organizers*

L. Montero, W. Weng, *Organizers, Presiding*

#### 1:00 Introductory Remarks.

**1:05 POLY 299.** Supramolecular redox mediators for lithium-sulfur batteries. **B. Helms**, L. Gerber, P.D. Frischmann, S. Doris, F. Fan, Y. Chiang, X. Qu, A. Jain, K. Persson

**1:35 POLY 300.** Role of metal-ligand bond strength and exchange dynamics on the mechanical properties of self-healing metallopolymers. **D. Mozhdzhi, J. Neal**, S. Gringy, Y. Cordeau, S. Ayala, N. Holten-Anderson, Z. Guan

**2:05 POLY 301.** Highly branched and loop-rich polymer metal-organic-cage gels. **A.V. Zhukhovitskiy, M. Zhong**, E. Keeler, V.K. Michaelis, J.E. Sun, M.J. Hore, D.J. Pochan, R.G. Griffin, A.P. Willard, **J.A. Johnson**

#### 2:35 Intermission.

**2:50 POLY 302.** Halogen bond directed self-assembly of block copolymer complexes. **O.T. Ikkala, P. Metrangolo**, G.P. Resnati, R. Milani, N. Houbenon

**3:20 POLY 303.** Novel metal ligand containing block copolymers and their assembly.  
**G.N. Tew**

**3:50 POLY 304.** Living crystallization-driven self-assembly: A versatile, seeded growth approach to functional supramolecular materials. **I. Manners**

**4:20 POLY 305.** Synthesis and characterization of metallo-supramolecular nanocomposites. **A.M. Savage, F.L. Beyer**

### ACS Award for Creative Invention: Symposium in honor of Antonio Facchetti

*Sponsored by PMSE, Cosponsored by POLY*

## TUESDAY EVENING

### Section A

San Diego Convention Center  
Hall F

#### 13th International Symposium on Biorelated Polymers

R. Ottenbrite, C. Scholz, *Organizers*

#### 6:00 - 8:00

**POLY 306.** Printing of polymer hydrogel microparticles as drug delivery vehicles. **M.W. Lampley, M. Marin, B.R. Spears**, E. Harth

**POLY 307.** Crosslinked dendronized polyols as a general approach to brighter and more stable fluorophores. **Y. Li**, S.C. Zimmerman

**POLY 308.** Development of a light-mediated, cytocompatible controlled radical polymerization technique for cell surface engineering applications. **J. Niu, L. Dassau**, C.J. Hawker

**POLY 309.** Biodegradable polyesters from renewable resources. **M. Bilal, M. Eivazi**, A. Njau, J. Kressler

**POLY 310.** New amphiphilic polymers for peptide complexation. **O. Zholobko**, A. Kohut, S. Stafslien, L. VanderWal, I. Tarnavchik, A.S. Voronov

**POLY 311.** Trehalose polymers for stabilization of industrially important proteins. **J. Lee, J. Ko, Y. Liu, E. Lin, M. Messina, E. Bat**, P. Nauka, P. Wallace, F.E. Ruch, H.D. Maynard

**POLY 312.** Molecular design for dual modulation effect of amyloid protein aggregation. **Y. Song, L. Zhu, J.S. Moore**

**POLY 313.** H<sub>2</sub>O<sub>2</sub>-activatable and clot-targeting antithrombotic polymeric nanoparticles. **D. Lee, C. Kang, K. Kyun, J. Kim**

**POLY 314.** Targeting rate dependent selective imaging and inactivation of bacteria over mammalian cells by regioregular polythiophene with imidazolium solubilizing groups. **Y. Huang, H. Pappas, L. Zhang**, R. Cai, W. Tan, D.G. Whitten, K.S. Schanze

**POLY 315.** Nanofiber scaffolds as an ex-vivo method for stem cell growth. **S.N. Neal**

**POLY 316.** PHEMA hydrogels filled with nanogels of polyhexylacrylate (HA) core and polyethylene glycol (PEG) Shell: Preparation and Properties. **Y.D. Cerda**, A. Zizumbo, L. Ramos, A. Espinoza, A. Licea-Claverie

**POLY 317.** Pegylated cationic nanogels based on PDEAEM for drug delivery. **L. Manzanares, A. Licea-Claverie**

**POLY 318.** Investigating the unique structure and physical properties of spider prey wrap silk with electron microscopy and solid-state NMR. **D. Onofrei, T. Larson**, K. Potfay, B. Blass, J. Ayon, G.P. Holland

**POLY 319.** Controlled release of plant hormones for agricultural purposes. **M. Li**, M.A. Tshabalala, G. Buschle-Diller

### Section A

San Diego Convention Center  
Hall F

#### Anionic Polymerisation: Still Living After 60 Years

*Cosponsored by PMSE and RUBB*

L. R. Hutchings, J. W. Mays, *Organizers*

#### 6:00 - 8:00

**POLY 320.** Well-defined synthesis of miktoarm star polymers with a fullerene core. **X. Lu, A. Goodwin, J.W. Mays, N. Kang**

**POLY 321.** Withdrawn.

**POLY 322.** Revealing the initiation mechanism of aggregated sodium diphenylamide in anionic polymerization of isocyanates. **C. Chae, H. Seo, I. Bak, J. Lee**

**POLY 323.** Synthesis of well-defined poly(2-isopropenyl-2-oxazoline) via living anionic polymerization. **H. Feng, K. Hong**, J.W. Mays, N. Kang

**POLY 324.** Synthesis and TGIC characterization of H-shaped polymers: The monomer approach. **M. Oti, L.R. Hutchings**

**POLY 325.** Developing high temperature thermoplastic elastomers based on benzofulvene by living anionic polymerization in hydrocarbon solvent at room temperature. **W. Wang, N. Kang, J.W. Mays**

**POLY 326.** Synthesis and characterization of poly(dimethylbutadiene) copolymers. **R. Chinchilla-Pardos, L.R. Hutchings**

### Section A

San Diego Convention Center  
Hall F

#### Applications of Polymer Surfaces & Interfaces

*Cosponsored by COLL and PMSE*

S. T. Iacono, J. M. Mabry, A. Tuteja, *Organizers*

#### 6:00 - 8:00

**POLY 327.** Efficacy of phytochemical-based antimicrobial coatings. **W. Hui, Y. Li, J. Lee**, K. Yeung

**POLY 328.** Synthesis and applications of partially fluorinated organically modified silicas. **A.R. Jennings, A.J. Wilkins**, C.J. Thrasher, S.T. Iacono

**POLY 329.** Synthesis and characterization of conducting polymers containing polypeptide and ferrocene side chains as ethanol biosensors. **M. Kesik, H. Akbulut**, S. Soylemez, S. Cevher, G. Hizalan, Y. Arslan Udum, T. Endo, S. Yamada, A. Cirpan, Y. Yagci, L. Toppare

**POLY 330.** Neat and aqueous novel functional siloxane oligomers for adhesive and coating applications. **T.N. Biggs**

**POLY 331.** Polydimethylsiloxane/Polyaniline composite: Study and structural characterization of the elastomeric matrix obtained by gamma radiolysis and polycondensation route. **M. Melendez Zamudio**, A. Villegas, M. Rodrigo, J.A. Cervantes

**POLY 332.** Using highly branched silicone oils to tailor the properties of gels. **J. Morgan**, T. Chen, M.A. Brook

**POLY 333.** Rigid rod chain-growth polyaramid brushes: Improved synthesis, solubility, and potential applications. **F.C. Prehn**, S.G. Boyes

**POLY 334.** Synthesis of spread and set silicone boronic acid elastomers activated by contact with aqueous surfaces. **B.J. Macphail**, L. Dodge, M.A. Brook

**POLY 335.** Amphiphilic polymer-mediated surface modification and colloidal dispersion of nanoparticles. **P. Alexandridis**, A.M. Bodratti, M. Tsianou

**POLY 336.** Di-perylene bisimides as alternative acceptor molecules for polymer photovoltaics. **L. Moore**, M. Bhattacharya, Q. Wu, S.E. Morgan

### Section A

San Diego Convention Center  
Hall F

#### Click Reactions for Producing Advanced Materials

W. Kern, G. N. Tew, F. Wiesbrock, *Organizers*

#### 6:00 - 8:00

**POLY 337.** Withdrawn.

**POLY 338.** Self-assembly of the PEGylated rod-coil block copolymers derived from helical (R)- and (S)-triazolepolycarboindimides inspected by TMAFM and TEM. **O.V. Kulikov**, D. Sirwardane, G. McCandless, B.M. Novak

### Section A

San Diego Convention Center  
Hall F

#### Excellence in Graduate Polymer Research

*Cosponsored by PRES, PROF, SOCED and YCC Financially supported by POLY IAB; Tosoh; Wiley*

H. Cheng, C. J. Ellison, C. J. Landry-Coltrain, T. E. Long, *Organizers*

#### 6:00 - 8:00

**POLY 339.** Glass transition temperatures of amorphous linear aliphatic polyesters. **J. Shen**, Y. Caydamli, A. Gurarslan, A.E. Tonelli

**POLY 340.** Sorption and diffusion of organic vapors into PIM-1 and the effects of methanol conditioning. **M. Jue**, R.P. Lively

**POLY 341.** Design and synthesis of fluorescent conjugated polyelectrolytes for sensing fluoride ions. **W. Wu**, A. Chen, W.E. Bernier, W.E. Jones

**POLY 342.** Investigation of nitrobenzene-based redox-active polymers for non-aqueous redox flow batteries. **K.J. Cheng**, E. Chenard, E.B. Montoto, N. Gavvalapalli, R.D. Dmello, J. Hui, K.C. Smith, J. Rodriguez Lopez, J.S. Moore

**POLY 343.** Effect of branching on bis-MPA polymers: A comparative study of polymer architecture. **J.A. Giesen**, J.L. Marple, S.M. Grayson

**POLY 344.** Degradable ferulic acid based epoxy thermosets. **A. Maiorana**, A. Reano, R. Centore, F. Allais, R.A. Gross

**POLY 345.** Enhancing lactide polymerization control through the use of redox-active catalysts. **L. Brown**, J. Rhinehart, B.K. Long

**POLY 346.** Effect of electrostatic interactions on the response of zwitterionic glucose sensitive hydrogels designed for bio-process sensing. **T. Nguyen**, J.J. Magda, P. Tathireddy

**POLY 347.** Anti-cancer activity of H<sub>2</sub>S-releasing micelles. **J. Foster**, S. Schiffhauer, C. Finkielstein, J. Matson

### Section A

San Diego Convention Center  
Hall F

#### General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*

#### 6:00 - 8:00

**POLY 348.** Nanoporous cyclic brush polymers for selective carbon dioxide capture. **E. Leonhardt**, G. Sun, T. Williams, K.L. Wooley

**POLY 349.** Synthesis of fulvene containing polymers for use in light-harvesting material. **N.P. Godman**, S. Budy, A. Davidson, G.J. Balaich, D.W. Ball, S.T. Iacono

**POLY 350.** Highly ordered polymers for magneto-optical applications. **K.R. White**, T.M. Swager

**POLY 351.** Incorporation of different conjugated linkers into low band gap polymers based on 5,6-bis(octyloxy)-2,1,3-benzooxadiazole for tuning efficiency of organic photovoltaics. **S. Goker**, G. Hizalan, Y. Arslan Udum, L. Toppare

**POLY 352.** Coumarin-based fluorescent tag for art conservation epoxy visualization. **P.D. McFadden**, K. Frederick, L. Arguello, N. Odegaard, P. Vandiver, D.A. Loy

**POLY 353.** Comparison of the  $\pi$ -electron delocalization in 2-oxazolines and esters. **K.P. Luef**, M. Fimberger, R.C. Fischer, F. Stelzer, M. Kállay, F. Wiesbrock

- POLY 354.** Synthesis of PDPP2F-2E-T (polydifurodiketopyrrolopyrrole-diethynyl-hexylthiophenes) as low band gap polymers. **G.J. Malmanger, A.D. Morales, J.L. Duffy-Matzner, D.E. Weisshaar**
- POLY 355.** CO<sub>2</sub> capture by sulfur-bridged nanoporous covalent organic polymers. **M. Atas, M. Yavuz**
- POLY 356.** STORM Imaging of phase morphology of PS-*b*-PtBMA copolymer bio-interfacial thin films. **A. Leonardi, M. Kim, C.K. Ober**
- POLY 357.** Modification of macromolecular scaffolds for water purification using ring opening polymerization of biorenewable monomers. **A.M. Balija, P. Jennings, P. Janezcko, P. Feibusch**
- POLY 358.** Poly(arylene ether)s with ammonium groups located on pendent phenyl sulfonyl moieties for use as anionic exchange membranes. **T. Schumacher, E. Fossum, J. Yang**
- POLY 359.** Synthesis and characterization of novel cardo-containing copolyimide membranes for gas separation. **D.J. Kim, S. Han, S. Nam**
- POLY 360.** Synthesis of a new class of alternate ionic cyclocopolymers and their potential use as anticatalysts. **H.A. Al-Muallem, I.Y. Yaagoub, M.A. Mazumder, S.A. Ali**
- POLY 361.** Phase behavior of single component coacervates composed of random copolymers. **N. Dolinski, C.J. Hawker, J.H. Waite**
- POLY 362.** Multifunctional cancer-targeting strategy for encapsulating doxorubicin by folate-conjugated and quercetin-anchored pluronic mixed micelle systems. **Z. Feng, S. Hassanzadeh, T. Pettersson, M. Hakkaramian**
- POLY 363.** Novel salicylic acid-based chemically cross-linked pH sensitive hydrogels for biomedical applications. **B. Demirdirek, K.E. Uhrich**
- POLY 364.** Novel synthetic route towards incorporating photochromic spiropyrans into thiophene based semiconducting polymers. **D.S. Dissanayake, M.C. Stefan, M.C. Biewer**
- POLY 365.** Molecular weight dependence of domain spacing in novel liquid crystalline brush-like block copolymers. **L. Mahajan, D. Ndaya, P. Deshmukh, Y. Choo, M. Gopinadhan, C.O. Osuji, R. Kasi**
- POLY 366.** Enhancement of magnetic field on the ultrasonic degradation of polymer chains of spherical polyelectrolyte brushes. **X. Hou, Z. Yu, Y. Cang, Z. Shen, J. Deng, R. Zhang, X. Guo**
- POLY 367.** Six-arm star-shaped poly( $\epsilon$ -caprolactone)-*b*-poly(*n*-vinyl-caprolactam) micelles as nanocarriers of 5-fluorouracil. **G.D. Garcia Olais, N. Cortez Lemus**
- POLY 368.** Alkyleneedioxy containing PEEK polymers containing meta linkages. **J. Ohaeri, W.A. Feld**
- POLY 369.** Synthesis of functionalized PEEK analogues via "one-pot" reaction. **Z.B. Ewing, E. Fossum**
- POLY 370.** Phenylated PEEK containing pendant alkyl substituents. **M.D. Cerone, W.A. Feld**
- POLY 371.** Synthesis and characterization of sulfonated PEEK/polymeric nanoparticles composite membrane for fuel cell application. **S. Nam, D.J. Kim, C. Park**
- POLY 372.** GTP synthesis of the multifunctional polyacrylate and their analysis of functional group. **J. Lee**
- POLY 373.** Hyperbranched poly(*n*-(2-hydroxypropyl) methacrylamide) via RAFT self-condensing vinyl polymerization. **J.A. Alfurhood, H. Sun, P. Bachler, B.S. Sumerlin**
- POLY 374.** Evidence for in situ catalyst modification in atom transfer radical reactions with ruthenium benzylidene complexes. **J. Lee, J.M. Grandner, K. Engle, K.N. Houk, R.H. Grubbs**
- POLY 375.** Sterically-driven selectivity in ADMET polymerization of asymmetric  $\alpha,\omega$ -dienes for sequence-controlled polyolefins. **C. Reese, E.A. Hoff, J.D. Azoulay, D.L. Patton**
- POLY 376.** Synthesis and morphological phase behavior of ordered, micro-phase-separated, imidazolium-containing diblock copolymers made by ATRP. **Z. Shi, D. Wijayasekara, T.S. Bailey, D.L. Gin**
- POLY 377.** Synthesis and properties of polyimines containing 2,2,4,4-tetramethyl-1,3-cyclobutadiimine moiety. **Y. Lee, W. Lee, A. Ancill, J.J. Worman, B.J. Landi, C. Bae**
- POLY 378.** Novel copolymers of styrene with oxy ring-disubstituted butyl 2-cyano-3-phenyl-2-propenoates. **S.M. Rocus, G.B. Kharas, V. Elangovan, A. Kovaleva, S. Malik, O. Nwosu, A. Piche, L.A. Patel, S.J. Rosengarden**
- POLY 379.** Novel copolymers of styrene and fluoro ring-disubstituted butyl 2-cyano-3-phenyl-2-propenoates. **W.S. Schjervén, G.B. Kharas, U.A. Baray, S. Chan, M.T. Cole, A.F. Haddad, J.A. Lucente, K.J. Patterson, A. Raiko, K.N. Reget, C.A. Shamblen, E.M. Whitmore**
- POLY 380.** Thiol-acrylate hydrogels prepared via a new time-lapse polymerization method. **E. Jee, T. Bansagi, A. Taylor, J.A. Pojman**
- POLY 381.** Novel poly(chalcogenylene vinylene)s with systematically tunable physical and electronic properties through acyclic diene metathesis (ADMET). **Z. Zhang, Y. Qin**
- POLY 382.** Ruthenium catalyzed ring-opening metathesis polymerization of cyclic olefins. **A.R. Hill, M. Al-Hashimi, R. Tuba, H.S. Bazzi, R.H. Grubbs**
- POLY 383.** Comparison of the thermal properties of poly(arylene ether)s prepared from *N*, *N*-dialkyl-2,4-difluorobenzenesulfonamide and *N*, *N*-dialkyl-3,5-difluorobenzenesulfonamide. **J. Waweru, E. Fossum, S. Ujvary, J. van den Hoek**
- POLY 384.** Withdrawn.
- POLY 385.** Polybiphenylenes by cycloaddition co-polymerization of 1,2,4,5-tetrazines with 1,4-diethynylbenzene. **R.E. Bagge, D. Boday, D.A. Loy**
- POLY 386.** Linear poly(ethyleneimine) synthesis: Traditional and innovative approaches. **B. Zarin, B. Gordon III, L. Stratton**
- POLY 387.** Photochemical stability of Various RAFT agents and their uses in the polymerization of *N*-vinylpyrrolidone. **J. Cho, Y. Kwark**
- POLY 388.** General strategy for sequence-controlled polymerization using macrocyclic ROMP. **W. Gutekunst, C.J. Hawker**
- POLY 389.** Free-radical frontal polymerization properties of vinylic monomers in deep eutectic monomer mixtures. **K.F. Fazende, J.A. Pojman**
- POLY 390.** Synthesis of self-immolative coatings responsive to an aqueous amino acid solution. **B. Chou, K.J. Shea**
- POLY 391.** Sprinkle of salt to aid the synthesis of sodium polystyrene sulfonate via atom transfer radical polymerization. **P. Balding**

## Section A

San Diego Convention Center  
Hall F

### Industrial Research at the Interface of Inorganic Chemistry & Polymer Science

*Cosponsored by BMGT and INOR $\ddagger$*

N. S. Radu, L. Stratton, *Organizers*

6:00 - 8:00

**POLY 392.** Synthesis, characterization, and use of mesoporous polymer as hard template for the fabrication of spherical nickel oxide nanoparticles. **M.D. Alsubei, A. Bagabas, A.A. Elzatahry**

**POLY 393.** Construction of Versatile and Functional Nanostructures Derived from CO<sub>2</sub>-based Polycarbonates. **Y. Wang, D. Darenbourg**

## Section A

San Diego Convention Center  
Hall F

### Responsive Nanostructures & Nanocomposites

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

6:00 - 8:00

**POLY 394.** Carbon dots rooted agarose hydrogel hybrid platform for optical detection and separation of heavy metal ions. **N. Gogoi**

**POLY 395.** Synthesis and characterization of hard and soft nanocomposites derived from  $\beta$ -cyclodextrin ( $\beta$ -CD) and hyperbranched polyglycerol (HPG) templates. **J. Iocozzia, Z. Lin**

**POLY 396.** Redox responsive nanogels for hydrophilic delivery. **K. Raghupathi, S. Erron, W. Cui, J.A. Hardy, J. Mager, S. Thayumanavan**

**POLY 397.** Synthesis of stereospecific glycopolymer hydrogel networks for the determination of the effects of network architecture on water content and structure. **A. Fogel, S.E. Morgan**

**POLY 398.** Mesoporous polymers by selective swelling of block copolymers with different alcohols. **Y. Wang, N. Yan**

**POLY 399.** Bioinspired control of polymer self-assembly via ligand-metal ion interactions. **A. Knight, C.J. Hawker**

**POLY 400.** Synthesis of stereospecific glycopolymers as models to mimic amyloid- $\beta$  peptide/saccharide interactions. **P.K. Das, W. Guo, V. Rangachari, D.L. Patton, S.E. Morgan**

**POLY 401.** Synthesis and characterization of nanohydrogels prepared by gamma irradiation of thermosensitive micelles of poly(*N*-vinyl caprolactam)-*b*-poly(hexyl acrylate). **O. Ruiz, A. Licea, N. Cortez, E. Bucio**

**POLY 402.** Accelerated degradation of hydrogen peroxide sensitive polymeric nanoparticles by releasing of acid and reducing their local pH. **S. Lee, A. Stubelius, J. Olejniczak, A. Almutairi**

**POLY 403.** Highly sensitive activatable polymeric nanoparticles for magnetic resonance imaging diagnostic. **A. Foucault-Collet, M. Viger, N.J. Johnson, S. He, G. Collet, A. Almutairi**

**POLY 404.** Detecting inflammation *in vivo* using NIR activatable fluorescence imaging. **G. Collet, M. Viger, V. Nguyen Huu, J. Lux, M. Guma, A. Foucault-Collet, J. Olejniczak, S. Joshi-Barr, A. Garcia, B. Bartok, G.S. Firestein, A. Almutairi**

**POLY 405.** Raman investigations on nanocomposites of colloidal silver in block copolymers. **M. Chipara, E. Ibrahim, D.M. Chipara, J.A. Martinez**

## Section A

San Diego Convention Center  
Hall F

### Supramolecular Polymers: From Structure to Advanced Functionality

J. Foster, J. B. Matson, L. Montero, W. Weng, *Organizers*

6:00 - 8:00

**POLY 406.** Periodical mesoporous polymers from H-bonding-modulated block copolymer supramolecules. **Y. Wang, L. Guo**

**POLY 407.** Poly(glutamic acid)-based nanogels for drug delivery applications. **M. Gordon, S. Thayumanavan**

**POLY 408.** Synthesis of an amphiphilic Janus dendrimer and evaluation of its self-assembly process in water. **M. Elizondo-García, V. Márquez, I.D. Araya, M. Videá, F.D. González-Nilo, J.A. Valencia-Gallegos**

## Section A

San Diego Convention Center  
Hall F

### Sustainable Polymers, Processes & Applications

*Cosponsored by PMSE*

D. Boday, J. H. Wang, *Organizers*

6:00 - 8:00

**POLY 409.** Ethyl cellulose composite with dimer acid alkyl ester plasticizer derived from used vegetable oil. **S. Lee, J. Shin, Y. Kim**

**POLY 410.** Vanillin: A biobased crosslinker for melamine-formaldehyde coatings. **A. Rohly, D.C. Webster**

**POLY 411.** Moisture resistant indium complexes for ring opening polymerization of lactide. **T. Ebrahimi, D. Aluthge, S. Hatzikiriakos, P. Mehrkhodavandi**

**POLY 412.** Synthesis and functionalization of PLA-based systems. **C. Scherger, C. Wright, C.R. Pugh**

**POLY 413.** Renewable crosslinked elastomer derived from carvomenthene. **S. Lee, Y. Kim, J. Shin**

**POLY 414.** Development and evaluation of a physical-mechanical board based recycled polyethylene acacia wood farnesiana. **M. Solis**

**POLY 415.** Withdrawn.

**POLY 416.** Effects of exohelical functionalization on structure of water-soluble meta-poly(phenylene ethynylene) foldamers. **A. Booras, B. Abrams**

## Section A

San Diego Convention Center  
Hall F

Undergraduate Research  
in Polymer Science

Financially supported by University  
of Southern Mississippi; Sabc

J. Lott, S. E. Morgan, S. I. Nazarenko,  
Organizers

## 6:00 - 8:00

**POLY 417.** Online resources for the polymer education community. K. Aubrecht, E.B. Berda, K.A. Cavicchi, P.J. Costanzo, G.J. Gabriel, C. Goh, S.L. Goh, S.T. Iacono, S.E. Morgan, D.A. Savin

**POLY 418.** Stimuli responsive cyano-oligo(phenylene vinylenes). J. Davila, M. Woelner, J. Lott

**POLY 419.** Generation of layer-by-layer nanoparticle library to selectively target ovarian cancer. A. Shi, S. Correa, P.T. Hammond

**POLY 420.** UV-Initiated free-radical polymerization of acrylamide based glucose and galactose glycomonomers. S. Lewis, A. Fogel, S.E. Morgan

**POLY 421.** Study of vanillin-amine systems for potential uses in coatings. J.R. Bernier, A. Rohly, D.C. Webster

**POLY 422.** Incorporation of Diels-Alder chemistry into polymer matrices via an iminer approach. K.S. Barcus, E.D. Crenshaw, P.J. Costanzo

**POLY 423.** Synthesis and characterization of novel polyester polyols derived from bio-based succinic acid and various diols. C. Del Rosario, K.D. Ulrich, B. Thompson, W.D. Coggio, A. Schrock

**POLY 424.** Dynamics and location of doxyl-stearic acid spin probes in sulfonated poly(ether ether ketone) ionomer deduced from electron spin resonance studies. B. Hosea, M. Danilczuk, S. Schlick

**POLY 425.** Salts of natural plant acid as nontoxic flame retardants for polymeric materials. A. Dembski, B.A. Howell

**POLY 426.** Phosphorylated itaconic acid monomer for the preparation of nonmigrating flame retardants. V.R. Hill, B.A. Howell

**POLY 427.** Applications of impedance spectroscopy: Exploring the temperature dependence of ionic conductivity in novel oligo(ethylene oxide) brush homopolymers as solid electrolyte supports. C. Peterson, D.A. Waldow

**POLY 428.** Investigation of phase transition temperatures of oligo(ethylene oxide) grafted oxanorbornyl diblock copolymers for solid polymer electrolytes supports. D.A. Waldow, S.P. Modahl

**POLY 429.** Controlling nanoscale organization of thiophene-based conducting polymers with self-assembling peptides. T. Blatz, M. Fry, T.J. Albin, A. Murphy

**POLY 430.** Phosphorus flame retardants for polymeric materials from a renewable plant oil. G.W. Lienhart, B.A. Howell

**POLY 431.** Dioxalkylene PEEK polymers containing vanillin subunits. J. Herbort, N. Yahna, W.A. Feld

**POLY 432.** Synthesis and characterization of sulfobetaine containing copolymers. K. Mullen, M.A. Tapsak

**POLY 433.** Structurally controlled anionic polysoaps to serve as dispersants for hydrocarbon uptake in aqueous media: Investigating the structural contributions of hydrophobic content, and molecular weight. C.L. McCormick, P.D. Pickett, A. Ventura

**POLY 434.** Solid-state upconversion with CdSe nanocrystals and anthracene. G. Tablas, D. Simpson, X. Li, Z. Huang, J. Tamayo, M. Tang

**POLY 435.** Influence of dithiol length on the thermomechanical properties of oxidized thiol-ene polymers. A. Dyson, B. Gardner, A. Spiride, R. Reit, B.R. Lund, W. Voit

**POLY 436.** Localization and relaxation of singlet exciton formation in conjugated polymers under photoexcitation. C. Wang, L. Zhuang, R. Chen, S. Li, T.F. George

**POLY 437.** Withdrawn.

**POLY 438.** Metalized fluorosilicone aerogel thermites for highly energetic materials. A.J. Wilkins, A.R. Jennings, K. Proctor, S.T. Iacono

**POLY 439.** Solution processable dioxthiophene polymers as active materials in aqueous and organic supercapacitors. N. Kennard, A. Osterholm, J.F. Ponder, J.R. Reynolds

**POLY 440.** Sustainable copolymers with tailored thermal properties. M.D. Beam, D.K. Schneiderman, M.A. Hillmyer

**POLY 441.** Enz-RAFT polymerization in continuous flow. R. Pineda, A.C. Evans, S. Matsuda, A. Truong

## WEDNESDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom C

Applications of Polymer  
Surfaces & Interfaces

## New Techniques &amp; Characterization

Cosponsored by COLL and PMSE

S. T. Iacono, J. M. Mabry, A. Tuteja, *Organizers, Presiding*

**8:00 POLY 442.** Neutron reflectivity studies of polymer multilayers prepared by sequential spin coating. T.A. Seery, D. Schwärzle, O. Prucker, J. Rühle, M.D. Dadmun

**8:30 POLY 443.** Semifluorinated diblock copolymer under confinement: A neutron reflectivity study. U. Shtrestha, S.J. Clarson, D. Perahia

**9:00 POLY 444.** Unified approach for polymeric patterning via controlling the propagation of frontal photopolymerization waves. A. Vitale, M.G. Hennessy, O.K. Matar, J.T. Cabral

**9:20 POLY 445.** Thin surface-attached polymer networks for planar optronic system. M. Körner, A. Schuler, R. Rother, M. Henze, O. Prucker, C. Müller, J. Rühle

**9:50 POLY 446.** Reducing background noise in near-infrared medical imaging: Routes to activated fluorescing through surface modification of colloidal particles. M. Burdette, I. Bandera, S.H. Foulger

**10:20** Intermission.

**10:30 POLY 447.** Controlling cell adhesion on device surfaces by nanotopography. E. Liang, E. Mah, S. Wu, M. Dickson, M. Digman, A.F. Yee

**10:50 POLY 448.** Spatially selective nucleation and growth of water droplets on hierarchically patterned polymer surfaces. Y. Cho, T. Shim, S. Yang

**11:10 POLY 449.** Transparent and superamphiphobic surfaces from mushroom-like polymer micropillar array. S. Lee, Y. Rahmawan, S. Yang

**11:30 POLY 450.** Unique gradient nanostructure formation in photo-cured coatings via photo-driven controlled radical polymerization. T. Suga, K. Minamibayashi, H. Nishide

**12:00 POLY 451.** Characterization of solid-supported ultrathin films and molecular interactions using MP-SPR. N. Granqvist, A. Jokinen, J.W. Sadowski

## Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

13th International Symposium  
on Biorelated PolymersSynthesis of Biorelated Polymers for  
Tissue Engineering & Drug Delivery

R. Ottenbrite, C. Scholz, *Organizers*

A. E. Tonelli, F. Wurm, *Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 452.** Restructuring polymers via nano-confinement and subsequent release. A.E. Tonelli

**8:35 POLY 453.** Scaffolds of chitosan grafted onto poly(3-hydroxybutyrate). R. Olayo, M. Gonzalez-Torres, R. Rodriguez-Talavera, R.M. Toral-Morales, S. Vargas-Muñoz, J. Morales-Corona

**9:05 POLY 454.** Biodegradable trehalose glycopolymers for protein stabilization. E. Pelegri-O'Day, U. Lau, H.D. Maynard

**9:25 POLY 455.** Synthesis of bio-based copolymers via free radical polymerization of novel vinyl monomer from soybean oil. Z. Demchuk, I. Tarnavchyk, A. Popadyuk, A. Voronov

**9:45** Intermission.

**10:00 POLY 456.** Preparation of cubosomes using poly(glycerol adipate) grafted with oleic acid. M. Bilal, T. Naolou, J. Kressler

**10:30 POLY 457.** Synthesis of an injectable hydrogel platform for dual drug delivery using oxime click chemistry. K. Gilmore, D.B. Beezer, L.L. Kendrick, E. Harth

**10:50 POLY 458.** Designing visible light cured thiol-acrylate hydrogels for studying cell fate processes in 3D. J. Bragg, C. Lin, T. Lin

**11:10 POLY 459.** Towards a scalable, biomimetic antibacterial polymer surface. M. Dickson, E. Liang, N.I. Navarro, L.A. Rodriguez, A.F. Yee

**11:30 POLY 460.** Polymer-modulated bacteria behavior: Unifying bacteria aggregation and biofilm formation. L. Foster, H. Takahashi, S.I. Yusa, K. Kuroda

## Section C

Marriott Marquis San Diego Marina  
Del Mar

Responsive Nanostructures  
& Nanocomposites

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*  
P. Frank, *Presiding*

**8:00 POLY 461.** Unimolecular micelles based on arborescent polypeptides for sustained drug delivery. M. Aelsehli, M. Gauthier

**8:20 POLY 462.** Endowing nanoparticles with orthogonal functionalities via a core/shell/shell architecture. A. Bertin, A. Asaduajaman, K. Rurack

**8:40 POLY 463.** Biodegradable and injectable polymer-liposome hydrogel: A promising cell carrier. Y. Ma, X. Lu, Z. Chen

**9:00 POLY 464.** Aggregation-based polymer platforms for ratiometric fluorescence sensing and imaging. Y. Bao, R. Bai, M. Smet

**9:20** Intermission.

**9:35 POLY 465.** Stimulus-responsive nanoparticle for ablating drug-resistant tumors. J. Piao

**9:55 POLY 466.** Synthesis and characterization of extruded superparamagnetic Fe<sub>3</sub>O<sub>4</sub>-nanoparticle polyelectrolyte composites. J. Fu, J.B. Schlenoff, Q. Wang

**10:15 POLY 467.** Diatom drug composite for drug delivery. M. Thakkar, A. Raikar, S. Mitra

**10:35 POLY 468.** Synthesis of hierarchical ZnO nanorod/ PEDOT: PSS nanostructures for UV photodetection. Y. Ding, F. Zheng, Z. Zhu

## Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

Click Reactions for Producing  
Advanced Materials

W. Kern, G. N. Tew, *Organizers*

F. Wiesbrock, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 469.** CuAAC and thio-bromo-click-chemistry as tools to achieve responsiveness in polymer science. W.H. Binder

**8:35 POLY 470.** Synthesis of hyperbranched polymers following a chain-growth CuAAC click polymerization. H. Gao, Y. Shi, X. Cao

**8:55 POLY 471.** Withdrawn.

**9:15** Intermission.

**9:35 POLY 472.** New approaches for photoinduced CuAAC click reactions. Y. Yagci, G. Yilmaz, O. Taskin, S. Dadashi-Silab, M. Tasdelen

**10:05 POLY 473.** Kinetic effects and applications of copper, photoinitiator and intensity on the photo-induced Copper(II) Catalyzed Azide-Alkyne Cycloaddition (CuAAC) reaction. B. El-Zaatari, A. Shete, C.J. Kloxin

**10:25 POLY 474.** High glass transition thiol-click networks from maleimides. S. Parker, R. Reit, K. Yang, G. Ellison, B.R. Lund, H. Abitz, W. Voit

**10:45 POLY 475.** Thiolene addition across norbornene enables novel co-networks and multi-block copolymers. G.N. Tew

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## Section E

Marriott Marquis San Diego Marina  
Balboa

## Controlled Depolymerization

A. Almutairi, S. Liu, H. Xu, *Organizers, Presiding*

**8:00 POLY 476.** Poly(vinyl ether sulfone)s as acid-sensitive polymers for transient materials. **K.M. Hutchins**, H. Lopez Hernandez, S. White, N.R. Sottos, J.S. Moore

**8:15 POLY 477.** Self-immolative aromatizing polyester for next-generation lithography. **A. Lane**, K. Matsuzawa, R.A. Mesch, W. Wang, B. Cassidy, W. Joo, S.T. Phillips, C.G. Willson

**8:30 POLY 478.** ROS responsive Se/Te-containing polymers. **H. Xu**

9:05 Intermission.

**9:15 POLY 479.** Self-immolative molecular systems. **D. Shabat**

**9:50 POLY 480.** Hyperbranched self-immolative polymers (hSIPs) for programmed payload delivery and ultrasensitive detection. **S. Liu**, G. Liu

**10:25 POLY 481.** Cutting to the chase: Azo-containing polymeric materials. **Y.C. Simon**

## Section F

Marriott Marquis San Diego Marina  
Catalina

## Anionic Polymerisation: Still Living After 60 Years

*Cosponsored by PMSE and RUBB  
Financially supported by ExxonMobil; Kraton;  
Synthomer; Goodyear; Eastman Chemical*

L. R. Hutchings, J. W. Mays, *Organizers*

H. Frey, M. A. Hillmyer, *Presiding*

**8:00 POLY 482.** Well-defined block copolymers containing high dielectric constant blocks: Synthesis and application. **K. Hong**

**8:30 POLY 483.** Enzyme-mediated quasi-living polymerization: New "green" route to block copolymers. **I. Gitsov**, D. Scheibel, N.G. Vladimirov

**8:50 POLY 484.** Living anionic polymerization of activated aziridines. **F. Wurm**, E. Rieger

**9:10 POLY 485.** Living anionic polymerization of isocyanates. **C. Chae**, H. Seo, I. Bak, J. Lee

9:40 Intermission.

**10:00 POLY 486.** Sequence-determination and sequence-control in living anionic copolymerization of styrene and 1,1-diphenylethylene derivatives. **H. Ma**

**10:20 POLY 487.** Polybutadiene-block-poly(4-vinylpyridine) by living anionic polymerization as precursors to polyethylene-block-poly(4-vinylidimethylpiperidinium). **F. Liu**, D.M. Knauss

**10:40 POLY 488.** Flexible tubing development with K-Resin® SBC resins. **J.J. Zhou**

## Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**11:00 POLY 489.** Marrying anionic polymerization with other controlled polymerizations for architecturally complex block polymers. **M.A. Hillmyer**

## Section G

Marriott Marquis San Diego Marina  
Solana

## Supramolecular Polymers: From Structure to Advanced Functionality

J. Foster, J. B. Matson, *Organizers*

L. Montero, W. Weng, *Organizers, Presiding*

8:00 Introductory Remarks.

**8:05 POLY 490.** Supramolecular chemistry in skin-inspired electronic materials. **Z. Bao**

**8:35 POLY 491.** Dynamic biomolecular supramolecular polymers. **S.I. Stupp**

**9:05 POLY 492.** Supramolecular block copolymers from hydrogen bonding between highly immiscible segments. **L. Pitet**, E.J. Kramer, C.J. Hawker, E.W. Meijer

9:35 Intermission.

**9:50 POLY 493.** Designing new monomers for radical polymerization. **E. Pentzer**

**10:20 POLY 494.** Supramolecular polymer chemistry: Entanglements by design. **H.W. Gibson**, T. Price, D. Schoonover, A. Murugan, H.R. Wessels, F. Mazzini

**10:50 POLY 495.** Supramolecular polymers based on host-guest molecular recognition motifs. **F. Huang**, F. Wang, X. Yan, S. Dong, M. Zhang, Z. Zhang, J. Chen

**11:20 POLY 496.** Energy transfer relay upon panchromatic light absorption by two-dimensional porphyrin covalent arrays. **H. Choi**, J. Kang

**11:40 POLY 497.** Controlling polyplex properties by polymer microstructure. **P.S. Heller**, B. Weber, J. Zhou, D. Hobernik, M. Barz

## Computational Materials &amp; Nanoscience: Theory Meets Experiment

## Forum: Materials Genome &amp; Materials Informatics

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

## WEDNESDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom C

## Applications of Polymer Surfaces &amp; Interfaces

## Anti-fouling

*Cosponsored by COLL and PMSE*

S. T. Iacono, J. M. Mabry, A. Tuteja, *Organizers, Presiding*

**1:00 POLY 498.** Anti-fouling amphiphilic silicenes: Efficacy against marine biofouling. **M. Grunlan**, M. Hawkins, M.A. Ruffin, S. Stafslien, I. Linossier

**1:30 POLY 499.** Controlling surface composition and structure of antifouling coatings using functionalized siloxane block copolymers. **B. Wenning**, C. Pester, J.A. Finlay, N. Aldred, T. Clare, E.J. Kramer, C.K. Ober

**1:50 POLY 500.** Multilayered perfluorinated ionomeric reactive coating for abatement of organic pollutant. **M. Sansotera**, F. Persico, L. Magagnin, W. Navarri

**2:10 POLY 501.** Anti-fouling characteristics of superhydrophilic polyelectrolyte brushes. **A. Takahara**, Y. Higaki

**2:40 POLY 502.** Modification of blended polyethersulfone membranes by in-situ growth of zinc oxide nanostructures for prevention of biofouling during water treatment. **M.H. Al-Hinai**, P. Sathe, A.T. Al-Hinai, M.Z. Al-Abri, S. Dobretsov, J. Dutta

3:00 Intermission.

**3:10 POLY 503.** Partially hydrolyzed poly(2-oxazoline)s and poly(2-oxazine)s as additives for the preparation of self-disinfectant surfaces. **K.P. Luef**, M. Fimberger, **F. Wiesbrock**

**3:40 POLY 504.** Poly(ethylene) glycol modified amphiphilic siloxane polyurethane coatings and their performance as effective fouling release surfaces. **T. Galhenage**, D.C. Webster, A.M. Moreira, S. Stafslien, L. VanderWal, J.A. Finlay, S.C. Franco, T. Clare

**4:00 POLY 505.** Self-healing perfluoropolymer brushes as highly polymer-repellent coatings. **Z. Wang**, S. Pujari, M. Smulders, **H. Zuilhof**

**4:30 POLY 506.** Controlled release of phytochemical-based antimicrobial coating for sustained disinfection. **W. Hui**, Y. Li, J. Lee, K. Yeung

**5:00 POLY 507.** Dynamic contact angles (the Wilhelmy plate method) and zeta potentials: Uncommon methods for characterization of antimicrobial / cyto-compatible coatings. **K.J. Wynne**, C. Wang, D.L. Johnson, S. Nair

## Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

## 13th International Symposium on Biorelated Polymers

## Polymer-Nucleic Acid Interaction &amp; Drug Delivery

R. Ottenbrite, C. Scholz, *Organizers*

M. Barz, B. Klumperman, *Presiding*

1:00 Introductory Remarks.

**1:05 POLY 508.** Block copoly(ester)ides: Combining polypeptides with polypeptides. **M. Barz**

**1:35 POLY 509.** Synthesis and utilization of cationic and anionic PEGylated poly(amino acids) for gene and drug delivery. **D. Ulkoski**, C. Scholz

**1:55 POLY 510.** Polymer materials to fold and activate functional DNA and peptides. **A. Maruyama**

**2:25 POLY 511.** Endosomal escape and nuclear permeability triggered by membrane intercalation of linear poly(ethylenimine) drives gene expression. **M.M. Banaszak Holl**, S. Vaidyanathan, J. Chen

2:55 Intermission.

**3:10 POLY 512.** Cationic nanohydrogel particles as carriers for therapeutic oligonucleotide delivery. **L. Nuhn**, N. Leber, **R.W. Zentel**

**3:40 POLY 513.** Pegylated smart nanogels for drug delivery. **A. Licea-Claverie**, M.A. González-Ayón, A. Serrano-Medina, J.M. Cornejo-Bravo

## Section C

Marriott Marquis San Diego Marina  
Del Mar

## General Topics: New Synthesis &amp; Characterization of Polymers

D. Garcia, *Organizer*

A. Fogel, A. Snow, *Presiding*

**1:00 POLY 514.** Rapid photo-copolymerization of styrene and methacrylate derivatives. **Y. Yang**, A. Urbas, J. Sun

**1:20 POLY 515.** Diblock copolymer nanoparticles via RAFT aqueous emulsion polymerization of less activated monomers. **S.L. Canning**, S.J. Byard, P. Sassman, S.P. Armes

**1:40 POLY 516.** Polymerization of mono-, di- and trichloroethyl methacrylates: A study in chain transfer. **A. Snow**

**2:00 POLY 517.** Synthesis of well-defined, epoxide-containing styrenic polymers and their functionalization with alcohols. **D. McLeod**, N.V. Tsarevsky

**2:20 POLY 518.** Covalently cross-linked poly(*n*-butyl acrylate) networks prepared with a dual reversible addition fragmentation chain transfer/crosslinking agent. **J. Lee**, K.A. Cavicchi

**2:40 POLY 519.** Thermodynamic and kinetic syntheses of conjugated ladder polymers. **L. Fang**

**3:00 POLY 520.** Simple bench top approach to polymer brush nanostructures using visible light mediated metal-free atom transfer radical polymerization. **E. Discekici**, C. Pester, N.J. Treat, J. Lawrence, K.M. Mattson, B. Narupai, E. Toumayan, Y. Luo, P. Clark, J. Read De Alaniz, C.J. Hawker

**3:20 POLY 521.** Lewis acid-mediated stereospecific radical polymerization of acrylamides. **T. Fujita**, S. Yamago

**3:40 POLY 522.** How do spherical diblock copolymer nanoparticles grow during RAFT alcoholic dispersion polymerization? **E. Jones**, O. Mykhaylyk, M. Semsarilar, M. Boerakker, P. Wyman, S.P. Armes

**4:00 POLY 523.** Synthesis and characterization of graft thermoplastic elastomers polyisoprene-*g*-polystyrene (PI-*g*-PS) through anionic and emulsion polymerization. **H. Wang**, W. Wang, N. Kang, J.W. Mays

**4:20 POLY 524.** Ultrahigh molecular weight linear block copolymers: Rapid access by reversible-deactivation radical polymerization and self-assembly into large domain nanostructures. **J.D. Mapas**, J. Rzayev

**4:40 POLY 525.** Withdrawn.

## Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

## Click Reactions for Producing Advanced Materials

W. Kern, G. N. Tew, *Organizers*

F. Wiesbrock, *Organizer, Presiding*

1:00 Introductory Remarks.

**1:05 POLY 526.** Click chemistry tools for delivering cisplatin to cancer cells. **S. Dhar**

**1:35 POLY 527.** Engineering cell surfaces with synthetic polymers. **H.A. Klok**

**2:05 POLY 528.** Poly(lactic-co-glycolic acid)-based clickable polycondensation and blending of magneto-responsive colloidal polymers: Observation of mesoscopic phase separation. **J. Olejniczak**, A. Almutairi, V. Huu, S. Lee, M. Chan, G. Collet



- 2:25 POLY 529.** Bioorthogonal labeling of micellar nanoparticles. J. Michaelis, J.K. Kammeier, H. Wu, N.K. Devaraj, N.C. Gianneschi
- 2:45** Intermission.
- 3:05 POLY 530.** Diffusion-controlled interfacial bioorthogonal polymerization. X. Jia
- 3:35 POLY 531.** Ultra-tough aliphatic thiol-isocyanate elastomers achieved through thiol-click reactions. G. Ellison, X. Carrier, D.A. Zamorano, B.R. Lund, W. Voit
- 3:55 POLY 532.** Oxidation of thiol-ene networks for post-polymerization modification of thermomechanical properties. R. Reit, A. Dyson, B. Gardner, A. Spiride, B.R. Lund, W. Voit

## Section E

Marriott Marquis San Diego Marina  
Balboa

### Controlled Depolymerization

A. Almutairi, S. Liu, H. Xu, *Organizers, Presiding*

- 1:00 POLY 533.** Withdrawn.
- 1:15 POLY 534.** Light-triggered chemical amplification to accelerate degradation and release from polymeric particles. A. Almutairi
- 1:50 POLY 535.** Design, synthesis, and applications of new self-immolative and low ceiling temperature polymers. S.T. Phillips
- 2:25** Intermission.
- 2:35 POLY 536.** Self-immolative polyglyoxylates: Towards functional backbones and assemblies. E.R. Gillies, B. Fan, R. Yardley, J. Trant
- 3:10 POLY 537.** Polymer-drug conjugates capable of on-demand burst release via controlled depolymerization. K. Cai, Y. Zhang, J. Cheng
- 3:45 POLY 538.** Photodegradable and biodegradable alkoxyphenacyl polyesters. T. Li, G. Wang, K. Mishra, A. Joy

## Section F

Marriott Marquis San Diego Marina  
Catalina

### Anionic Polymerisation: Still Living After 60 Years

*Cosponsored by PMSE and RUBB  
Financially supported by ExxonMobil; Kraton; Synthomer; Goodyear; Eastman Chemical*

- L. R. Hutchings, J. W. Mays, *Organizers*
- T. Kitayama, I. Manners, *Presiding*
- 1:00 POLY 539.** Living polymerizations on different length scales. I. Manners
- 1:30 POLY 540.** Watching polymer chains grow by in-situ monitoring of living copolymerizations: From gradient assessment to one-step block copolymer synthesis. H. Frey, A.H. Müller, D. Leibig, E. Grune
- 2:00 POLY 541.** N-isopropyl-4-vinylbenzylamine: A novel initiator to build various polymer architecture through anionic polymerization. W. Lu, N. Kang, K. Hong, J.W. Mays
- 2:20 POLY 542.** Anionic polymerization: Versatile technique for end functionalized and branched polymers. N. Muhammad Sarih, L.R. Hutchings, F. Hamime, R.L. Thompson
- 2:40** Intermission.
- 3:00 POLY 543.** From retarded to activated anionic polymerization: A focus on magnesium and aluminum derivatives. S. Carlotti

- 3:30 POLY 544.** Novel and straightforward route to polycarbonates and its copolymers. D. Zhang, H. Zhang, Y. Alzahrany, N. Hadjichristidis, X. Feng, Y. Gnanou
- 3:50 POLY 545.** Anionic polymerization of BioFene (*trans*- $\beta$ -farnesene) and their physical properties. T. Yoo, T. Trnka, S.K. Henning, D.J. McPhee

## Section G

Marriott Marquis San Diego Marina  
Solana

### Supramolecular Polymers: From Structure to Advanced Functionality

J. B. Matson, L. Montero, *Organizers*

J. Foster, W. Weng, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05 POLY 546.** Synergy between aromatic gain and hydrogen-bonding in a supramolecular polymer. R. Kietlyka
- 1:35 POLY 547.** Synthesis and characterization of supramolecular self-healing polymers designed for application in lithium-ion batteries. J. Lopez, A. Pei, Z. Chen, Y. Cui, Z. Bao
- 1:55 POLY 548.** Nanoscale chemical and topological imaging of block copolymers with photo-induced force microscopy. D. Nowak, W. Morrison, S. Park, k. Schmidt, J.E. Frommer, D. Sanders
- 2:15 POLY 549.** Mechanical activation of mechanophore enhanced by strong hydrogen bonding interactions. Y. Chen, H. Zhang, X. Fang, Y. Lin, W. Weng
- 2:35** Intermission.
- 2:50 POLY 550.** Simplified tube models for entangled telechelic star polymers. D. Read, V. Boudara
- 3:10 POLY 551.** Withdrawn.
- 3:30 POLY 552.** Supramolecular triarylamine self-assemblies as functional nanomaterials. E. Moulin, N. Giuseppone
- 3:50 POLY 553.** Preparation of amylose supramolecular materials by vine-twining polymerization. J. Kadokawa

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Powering the Future: Novel Materials for Solar Cell Technologies

*Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY*

## WEDNESDAY EVENING

### Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom C

#### POLY/PMSE Plenary Lecture & Awards Reception

*Cosponsored by PMSE*

- M. Jeffries-El, C. Lipscomb, *Organizers*
- T. J. White, *Organizer, Presiding*
- 6:00 POLY 554.** Innovation in a mature field: The commercialization of olefin block copolymers. E. Carnahan

## THURSDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom C

#### Applications of Polymer Surfaces & Interfaces

##### Low Energy Surfaces & De-Icing

*Cosponsored by COLL and PMSE*

S. T. Iacono, J. M. Mabry, A. Tuteja, *Organizers, Presiding*

- 8:00 POLY 555.** Insights into surface structure and performance of fluorinated silicates from cohesive energy studies. A.J. Guenther, T.S. Haddad, K. Lamison, S.P. Kirby, R. Campos, J.R. Alston, J. Dossen, J.M. Mabry
- 8:30 POLY 556.** Anti-stick coatings using self-lubricating organogels (SLUGs). C. Urata, G. Dunderdale, M. England, A. Hozumi
- 8:50 POLY 557.** MQ silicones at interfaces. D.H. Flagg, T.J. McCarthy
- 9:10 POLY 558.** Smooth, all-solid, omniphobic surfaces. M. Boban, J.M. Mabry, A. Tuteja
- 9:30 POLY 559.** Ultralow wear fluoropolymer composites: Nanoscale functionality from microscale fillers. C.P. Junk, B.A. Krick, G.S. Blackman, A.A. Pitenis, K.L. Harris, W. Sawyer, S.C. Brown, H. Rosenfeld, D.J. Kasprzak, R.S. Johnson, C.D. Chan
- 10:00** Intermission.
- 10:10 POLY 560.** Elucidating the low surface energy of cubic fluoroPOSS compounds through the synthesis and surface characterization of fluoroPOSS cage mixtures. R. Campos, T.S. Haddad, B.M. Novak, J.M. Mabry
- 10:40 POLY 561.** Permanently grafted abrasion resistant nanocomposites for anti-icing applications. J. Gao, A.J. Martin, J. Yatvin, J.J. Locklin
- 11:00 POLY 562.** Designing durable ice-phobic surfaces. K. Golovin, S.P. Kobaku, D.H. Lee, E.T. DiLoreto, J.M. Mabry, A. Tuteja
- 11:20 POLY 563.** Scalable and durable polymeric ice-phobic and hydrate-phobic coatings. H. Sojoudi, H. A. Khanouki, M. Walsh, S. Shirazi, G. McKinley, K. Gleason
- 11:40 POLY 564.** Moving anti-ice coatings from the lab to the field: Key issues to overcome. J.P. Youngblood, J.A. Howarter, S. Kumar Raganathan, S. Sirupurapu

### Section B

Marriott Marquis San Diego Marina  
Torrey Pines 3

#### 13th International Symposium on Biorelated Polymers

##### Drug Delivery & Polymer-Physical Studies

- R. Ottenbrite, C. Scholz, *Organizers*
- D. J. Pochan, A. Voronov, *Presiding*
- 8:00** Introductory Remarks.
- 8:05 POLY 565.** Responsive polymer-mediated targeted delivery of curcumin to osteosarcoma cells. A.S. Voronov
- 8:35 POLY 566.** Engineering polymer hydrogel nanoparticles for lymph node targeted vaccine delivery. B. De Geest
- 9:05 POLY 567.** Biodegradable injectable polymer systems forming covalent hydrogel in response to temperature. Y. Ohya, Y. Yoshida, K. Kawahara, A. Kuzuya

- 9:35 POLY 568.** Synthesis and characterization of stable polypyrrole nanospheres. O. Zholobko, A.S. Voronov

**9:55** Intermission.

- 10:10 POLY 569.** Materials construction through peptide design and solution assembly. D.J. Pochan

- 10:40 POLY 570.** Effect of post-drawing on the macromolecular and functional properties of polymer nanofibers. D. Brennan, V.Z. Beachley

- 11:05 POLY 571.** Osmotic behavior of proteoglycan assemblies. F. Horkay, P.J. Basser

- 11:30 POLY 572.** Fast-scan DSC characterization of bulk bovine serum albumin. Z. Li, X. Hu, W. Hu

## Section C

Marriott Marquis San Diego Marina  
Del Mar

#### General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*

B. S. Lokitz, L. Moore, *Presiding*

- 8:00 POLY 573.** Thermally re-workable epoxy adhesives for use in artifact repair. P.D. McFadden, R.E. Bagge, E. Canosa, D.A. Loy, N. Odegaard, P. Vandiver
- 8:20 POLY 574.** Moldable plant biomass by cross-linking thermoset polymer and lignocellulose. S. Karumuri, S. Hizirolgu, A. Kalkan
- 8:40 POLY 575.** Lewis acidic silicone polymers: Creating stable, reversible elastomers. L. Zepeda-Velazquez, B. Macphail, M.A. Brook
- 9:00 POLY 576.** Development of organic charge transfer complexes for shock wave energy dissipation (SWED). Y. Ren, S. Lee, J. Christensen, W. Shaw, N. Plotnikov, T. Martinez, D.D. Dlott, J.S. Moore
- 9:20 POLY 577.** Facile synthesis of highly pH-responsive and water-soluble polyphosphonamidates. H. Wang, R. Li, J. Fan, L. Su, F. Zhang, K.L. Wooley
- 9:40 POLY 578.** Withdrawn.
- 10:00 POLY 579.** Enhancing the mechanical and electronic properties of poly(3-alkylthiophenes) through random copolymerization. S.A. Sydlík, Z. Smith, Z. Wright, A. Arnold
- 10:20 POLY 580.** Aza-Diels-Alder route to polyquinolines. M. Umerani, D.J. Dibble, A. Mazaheripour, Y.S. Park, J.W. Ziller, A.A. Gorodetsky

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- 10:40 POLY 581.** Hexaphenylbenzene and hexabenzocoronene-based porous polymer for selective adsorption of volatile organic compounds. A. Karunathilake, C. Thompson, R. Smaldone
- 11:00 POLY 582.** Cleavable side-chain promoted interesting chemistry. Z. Guo, L. Fang
- 11:20 POLY 583.** Novel functional conjugated polymers derived from a common set of enediene building blocks. Y. Qin
- 11:40 POLY 584.** Periodic conjugated polymers: The group 16 dance. C. Tsai, A. Fortney, Y. Qiu, T. Kowalewski, K.J. Noonan

## Section D

Marriott Marquis San Diego Marina  
Torrey Pines 1 & 2

### Click Reactions for Producing Advanced Materials

G. N. Tew, F. Wiesbrock, *Organizers*  
W. Kern, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 585.** Use of click chemistry to construct complex, yet well-defined architectures. S.M. Grayson

**8:35 POLY 586.** Utilizing click chemistry to assemble nanocellulose, polymers and proteins into bioactive nanocomposites. E. Marrow, K.A. DiVito, S. Walper, M.A. Daniele

**8:55 POLY 587.** Stimuli-responsive switchable networks: Click and un-click reaction of furanyl-functionalized (co)poly(2-oxazolines) with bis(maleimide). S. Schiller, F. Stelzer, F. Wiesbrock

**9:15 POLY 588.** Tetrazines as polydiene modifiers and blowing agents. R.E. Bagge, D. Boday, D.A. Loy

**9:35** Intermission.

**9:55 POLY 589.** Cyclic defects and elasticity in click hydrogels. K. Kawamoto, M. Zhong, R. Wang, B.D. Olsen, J.A. Johnson

**10:25 POLY 590.** Copoly(2-oxazoline)-based photoresists from renewable resources. K.P. Luef, C. Petit, B. Grassl, S. Reynaud, F. Wiesbrock

**10:55 POLY 591.** Click chemistry-mediated synthesis of polyester-stat-poly(2-oxazoline) drug reservoirs. K.P. Luef, C. Petit, B. Grassl, F. Stelzer, S. Reynaud, F. Wiesbrock

## Section E

Marriott Marquis San Diego Marina  
Balboa

### Supramolecular Polymers: From Structure to Advanced Functionality

J. Foster, W. Weng, *Organizers*

J. B. Matson, L. Montero, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 POLY 592.** Endgroup functionalization of poly(ethylene terephthalate) derivatives with ureidopyrimidinone. K.R. Houston, A.S. Jackson, R.W. Yost, H.S. Carman, V.S. Ashby

**8:25 POLY 593.** Withdrawn.

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

†Cooperative Cosponsorship

**8:45 POLY 594.** Induction of CD and CPL to non-chiral fluorescent dyes in chiral nanopocket created by L-glutamide-based helical nano-assemblies. Y. Okazaki, T. Goto, Y. Kuwahara, M. Takafuji, R. Oda, H. Ihara

**9:05 POLY 595.** Chemistry in the confined spaces of porous polymers. J. Byun, N.A. Dogan, H.A. Patel, D. Thirion, V. Rozynev, S. Subramanian, E. Ozdemir, C.T. Yavuz

**9:25 POLY 596.** Synthesis and characterization of ionically crosslinked polymer networks. K.A. Cavicchi, G. Deng, M. Yang

## Section F

Marriott Marquis San Diego Marina  
Catalina

### Anionic Polymerisation: Still Living After 60 Years

Cosponsored by PMSE and RUBB  
Financially supported by ExxonMobil; Kraton; Synthomer; Goodyear; Eastman Chemical

J. W. Mays, *Organizer*

L. R. Hutchings, *Organizer, Presiding*

J. He, *Presiding*

**8:00 POLY 597.** Extending the capability of living anionic polymerization: From architecture to microstructure of polymers. J. He

**8:30 POLY 598.** Multigraft copolymer superelastomers. K. Misichronis, W. Wang, A. Goodwin, N. Kang, J.W. Mays, T. Saito

**8:50 POLY 599.** Novel catechol-containing vinyl monomers for carbanionic Polymerization: *In Situ* monitoring of the formation of poly(styrene-co-vinyl catechol) copolymers by carbanionic living copolymerization. D. Leibig, H. Frey

**9:10 POLY 600.** Anionic polymerization of methacryloyl chloride. T. Kitayama, S. Nakano, T. Kitaura, Y. Kohsaka

**9:40** Intermission.

**10:00 POLY 601.** Kraton performance polymers: 50 years of experience with commercial scale anionic polymerization. M. Stöl

**10:20 POLY 602.** Thermoplastic elastomers with complex architecture by sequential addition. T. Huang, D. Wijayasekara, T.S. Bailey, D.M. Knauss

**10:40 POLY 603.** Generating complex self-assemblies from block polymers: Triply-periodic structures from anionic polymerization. T.H. Epps, M. Tureau

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: The Future of Spectroscopies: Quantum & Classical Fields; Theoretical Perspectives

Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY

## THURSDAY AFTERNOON

### Computational Materials & Nanoscience: Theory Meets Experiment

#### Forum: Exciting Aspects of Excitation Dynamics & Dissociation at the Nanoscale

Sponsored by MPPG, Cosponsored by COMP, ENFL, INOR, ORGN and POLY

## PMSE

### Division of Polymeric Materials Science and Engineering

A. Tsou, B. Olsen, C. Stafford, X. Jia and C. Soles, *Program Chairs*

#### OTHER SYMPOSIA OF INTEREST:

**Click Chemistry in Carbohydrate, Materials Science & Biomedicine: Symposium in Honor of Professor Sharpless's 75th Birthday** (see CARB, Wed, Thurs)

**New Horizons in Sustainable Materials** (see CELL, Sun, Mon)

**Proteins & Polymers Under Confinement** (see COLL, Sun)

**Frontier of the Interface of Materials & Biology: Protein Based Nanomaterials** (see COLL, Sun, Mon)

**Membrane Technology for Water-Energy Sustainability** (see ENVR, Wed, Thurs)

**Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials** (see PHYS, Mon, Tue, Wed, Thurs)

#### SOCIAL EVENTS:

**Social Hour, Tue**  
**Reception, Wed**

#### BUSINESS MEETINGS:

**Business Meeting, Mon**  
**Executive Committee, Sun**

## SUNDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Miramar Room

#### James V. Crivello Memorial Symposium

B. C. Benicewicz, G. E. Wnek, *Organizers*  
C. Y. Ryu, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 PMSE 1.** High-resolution patterning through application of Crivello salts. C.G. Willson

**8:35 PMSE 2.** Perspectives in polymers for electronics: From photopolymers to active materials. E. Reichmanis

**9:05 PMSE 3.** Adventures with onium salts: From photolithography and 3D optical data storage to photodynamic therapy. K.D. Belfield

**9:35** Intermission.

**9:50 PMSE 4.** Synthesis and photochemical crosslinking of cycloliner polycarbosilanes. L.V. Interrante, X. Liu, S.W. LeFevre, C.Y. Ryu

**10:20 PMSE 5.** Graft polymerization of P4VP on HIPE foams. J.G. Pribyl, R.B. Fletcher, T.C. Shehee, K. Taylor-Pashow, B.C. Benicewicz

**10:50 PMSE 6.** Influence of chirality on polymers: From optical switches to organic vapor sensors. B.M. Novak

### Section B

Marriott Marquis San Diego Marina  
Leucadia

#### Clay/Polymer Composites: Nanoclays & Other Natural Nanoparticles

##### Polymer-Clay Nanocomposites

Financially supported by I-Minerals, Inc.

E. Ruiz-Hitzky, A. Takahara, L. Zhang, *Organizers*

Y. M. Lvov, *Organizer, Presiding*

K. Ariga, *Presiding*

**8:00 PMSE 7.** The art of composite materials: From biomimetics to Kirigami. N. Kotov

**8:30 PMSE 8.** Unexpected application of clay-polymer nanocomposite science: The genesis of oil and gas in shale source rocks. H.J. Van Damme

**9:00 PMSE 9.** Polymer/clay nano-composite formation: Clay dispersion control via solid-state processing. T. Saito, M. Okamoto

**9:30 PMSE 10.** Clay nanobrick wall multilayer thin films: Processing and gas permeability and separation. J.C. Grunlan

**10:00** Intermission.

**10:10 PMSE 11.** Nanocomposite gels and soft nanocomposites with polymer-clay networks. K. Haraguchi

**10:40 PMSE 12.** Formation of exfoliated polymer/clay nanocomposites at melt state: Mechanism and practice. T. Tang, X. Wen

**11:10 PMSE 13.** Polymer/clay nanocomposites in the form of aerogels. D.A. Schiraldi

### Section C

Marriott Marquis San Diego Marina  
Palomar Room

#### Directed Polymer Assembly

C. Li, *Organizer*

M. Herrera-Alonso, *Organizer, Presiding*

**8:30 PMSE 14.** Crafting threads of diblock copolymer micelles via flow-enabled assembly. Z. Lin, B. Li

**8:50 PMSE 15.** Exotic nanoparticle construction and interparticle assembly with block copolymers in solution. D.J. Pochan

**9:10 PMSE 16.** Solution self-assembly of block copolymers in microfluidic devices: Polymeric drug delivery vehicles manufactured in the lab-on-chip. M.G. Moffitt, D. Sinton, A. Bains

**9:30 PMSE 17.** Solute-induced morphological transitions of molecular brush amphiphiles. M. Herrera-Alonso

**9:50** Intermission.

**10:05 PMSE 18.** Homoporous structures derived from amphiphilic block copolymers. Y. Wang

**10:25 PMSE 19.** Hierarchically structured supramolecular elastomers and metamaterials. H. Frauenrath

**10:45 PMSE 20.** Hierarchical structure and dynamics of oligo-fluorene functionalized block copolymers for thermoreversible gel applications. V. Prabhu, G. Wei, S. Venkataraman, Y. Yang, J.L. Hedrick

**11:05 PMSE 21.** Facile directed-assembly ordering of polymer nanoparticle films. A. Karim

## Section D

Marriott Marquis San Diego Marina  
Presidio 1

## Dynamic &amp; Tunable Biomaterials

**Patterned & Tunable Biomaterials**  
*Financially supported by Society for Biomaterials, Aldrich Materials Science, ACS Biomaterials Science & Engineering*

A. P. Dove, A. M. Kloxin, C. Magin, *Organizers*  
C. Jewell, J. K. Pokorski, *Presiding*

**8:30 PMSE 22.** Control of mesh size and modulus by kinetically dependent cross-linking in hydrogels. **M. Becker**

**9:00 PMSE 23.** Tunable scaffolds from novel, 3D-printable biomaterials. **M. Guvendiren, K. Dube, J. Molde, J. Kohn**

**9:20 PMSE 24.** Expansion microscopy: Nanoscopic characterization of polyacrylate polymers. **R. Gao, D. Oran, S.G. Rodrigues, E.S. Boyden**

**9:40 PMSE 25.** Mimicking collagenous tissues with dynamically controlled hydrogels through peptide self-assembly and light-mediated click chemistry. **C. Guo, A.M. Hilderbrand, A.M. Kloxin**

**10:00** Intermission.

**10:15 PMSE 26.** Tunable and dynamic biomaterials interfaces via controlled radical polymerization. **H.A. Klok**

**10:45 PMSE 27.** Photoreversible patterning of hydrogel biomaterials with site-specifically modified proteins. **C.A. DeForest**

**11:15 PMSE 28.** New advances in grafting ROMP polymers to proteins. **J.K. Pokorski**

## Section E

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

## Bioresponsive &amp; Biomimetic Synthetic Polymers &amp; Materials

D. Bong, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 PMSE 29.** Bifacial "polymer nucleic acid" for DNA and RNA nanoparticle loading, silencing delivery, and aptamer turn-on. **D. Bong**

**9:10 PMSE 30.** Discovery and use of heparin mimetic polymers in angiogenesis. **H.D. Maynard, S. Paluck, T.H. Nguyen**

**9:45** Intermission.

**9:55 PMSE 31.** Oxidative responsiveness of arylboronic acid-installed polycarbonate nanoparticles. **M. Herrera-Alonso**

**10:30 PMSE 32.** Seek, destroy, and heal: Enzyme-responsive nanoparticles as *in vivo*, targeted delivery systems. **N.C. Gianneschi, K.L. Christman**

**11:05 PMSE 33.** Art of falling apart: Controlling polymer degradation for health sciences. **A. Almutairi**

## Section F

Marriott Marquis San Diego Marina  
Presidio 2

## Flow-Induced Crystallization of Polymers

**Structure, Process & Properties**  
A. Doufas, S. Hatzikiriakos, *Organizers, Presiding*

**8:00 PMSE 34.** Flow-induced crystallization: From solutions to melts to process modeling. **A.J. McHugh**

**8:30 PMSE 35.** Probing shish-kebab precursor structures in model polyethylene blends under shear. **B.S. Hsiao**

**9:00 PMSE 36.** Probing polyethylene crystallization via simultaneous Raman spectroscopy and rheology. **A. Kotula, A.R. High Walker, K. Migler**

**9:30** Intermission.

**9:45 PMSE 37.** Real-time microstructural monitoring during the blown film extrusion of polyolefins. **G. Gururajan**

**10:15 PMSE 38.** Flow-induced crystallization behavior of linear polyolefins in uniaxial extension. **M. Sentmanat**

**10:45 PMSE 39.** Effect of flow and pressure on crystallization of LLDPE: An experimental study using *in-situ* x-ray. **E.M. Troisi, G. Portale, G. Peters**

### Biomass & Polymer Extrusion, Composite & Reaction Technologies: New Insights, Future Potential & Principles to Practice

*Sponsored by CELL, Cosponsored by PMSE and POLY*

#### Applications of Polymer Surfaces & Interfaces

#### New Processes & Surface Functionalization

*Sponsored by POLY, Cosponsored by COLL and PMSE*

#### Sustainable Polymers, Processes & Applications

*Sponsored by POLY, Cosponsored by PMSE*

## SUNDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
Miramar Room

## James V. Crivello Memorial Symposium

B. C. Benicewicz, C. Y. Ryu, G. E. Wnek, *Organizers*

J. A. Moore, *Presiding*

**1:00 PMSE 40.** Functional materials obtained by cationic photocuring. **S. Marco**

**1:30 PMSE 41.** Photopolymerized Cu(I)-catalyzed azide-alkyne-cycloaddition (CuAAC)-based networks. **A.D. Baranek, H. Song, A. Flores, P. Finnegan, M.K. McBride, C. Bowman**

**2:00 PMSE 42.** Functional materials via thiol-X photopolymerization in dispersed phase. **D.N. Amato, D.V. Amato, O. Mavrodi, S.E. Walley, J.R. Douglas, D. Mavrodi, D.L. Patton**

**2:30** Intermission.

**2:45 PMSE 43.** Photoinitiated polymerization of acrylate, methacrylate, and vinyl ether end-functional polyisobutylene macromonomers. **R. Tripathy, R. Faust, J. Crivello**

**3:15 PMSE 44.** Network structure and properties of sustainable epoxy and oxetane thermosets polymerized by cationic photoinitiator. **Z.T. Yang, L. Iordanov, B. Rupp, M. Patel, C. Bae, C.Y. Ryu**

**3:45 PMSE 45.** New application of onium salt-based, photoinitiated polymerization. **G.E. Wnek, A.Y. Walker**

**4:15** Concluding Remarks.

## Section B

Marriott Marquis San Diego Marina  
Leucadia

## Clay/Polymer Composites: Nanoclays &amp; Other Natural Nanoparticles

## Tubule Clay Nanocomposites

*Financially supported by I-Minerals, Inc.*

Y. M. Lvov, E. Ruiz-Hitzky, A. Takahara, L. Zhang, *Organizers*

P. Aranda, L. Zhang, *Presiding*

**1:00 PMSE 46.** Design and characterization of (organic material/halloysite nanotube) hybrids. **A. Takahara**

**1:30 PMSE 47.** Tailoring interface in elastomer/clay nanocomposites for improved reinforcing efficiency and lowered permeability. **B. Guo, L. Zhang**

**2:00 PMSE 48.** Enzyme encapsulation in clay nanotubes for nanoconfined biocatalysis. **Y.M. Lvov, J.R. Tully**

**2:30 PMSE 49.** Catalytic nanoarchitectonics with clay nanotube. **K. Ariga, H. Abe**

**3:00 PMSE 50.** Halloysite/surfactant hybrids as sustainable nanomaterials. **G. Lazzara, G. Cavallaro, S. Millioto, F. Parisi**

**3:30 PMSE 51.** Functionalization of halloysite nanotubes and their applications in surface-enhanced Raman scattering substrates, electrochemical sensors, and photocatalysts. **M. Du, H. Zhu, M. Zou, P. Wang**

**4:00 PMSE 52.** Halloysite as nano-chamber for metal-organic frameworks and other organic compounds. **J. Ko, B. Yoo, J. Ryu, D. Sohn**

## Section C

Marriott Marquis San Diego Marina  
Palomar Room

## Directed Polymer Assembly

M. Herrera-Alonso, *Organizer*

C. Li, *Organizer, Presiding*

**1:30 PMSE 53.** Precisely functionalized molecular nanoparticles are unique elements for macromolecular science: From "nanoatoms" to giant molecules. **S.Z. Cheng, M. Huang, K. Yue, Z. Lin, X. Feng, W. Zhang, W. Zhang**

**1:50 PMSE 54.** Self-assembly of poly(hydroxystyrene)-based block copolymers. **P. Gopalan, C. Kanimozhi, S. Larson, J. Choi**

**2:10 PMSE 55.** Directed, hierarchical self-assembly of multifunctional microgel. **J. Liang, F. Teng, M. Libera**

**2:30 PMSE 56.** Directing polymer assembly using liquid-liquid interface. **C. Li, W. Wang, H. Qi, S. Mei**

**2:50** Intermission.

**3:05 PMSE 57.** Computational insights on the orientation control of high- $\chi$  block copolymers using phase-selective, surface active additives. **K. Schmidt, A. Vora, G. Alva, A. Chunder, M. Tjo, T. Magbitang, N. Arellano, A. Bowers, K. Nguyen, E. Lofano, J. Cheng, J.W. Pitera, D.P. Sanders**

**3:25 PMSE 58.** Directed self-assembly of polycarbonate-containing high- $\chi$  block copolymers for sub 20-nm pitch patterning. **A. Vora, K. Schmidt, N. Arellano, T. Magbitang, A. Chunder, J. Cheng, D. Sanders**

**3:45 PMSE 59.** Solvent- and surfactant-mediated self-assembly of diblock polythiophene copolyelectrolytes for organic photovoltaic devices. **M. Chevrier, A. Thomas, S. Clement, R.C. Evans, J.E. Houston**

**4:05 PMSE 60.** Manipulating ordering and orientation in nanostructured thin films by combining substrate and solvent annealing effects. **T.H. Epps, M. Luo, C.K. Shelton**

## Section D

Marriott Marquis San Diego Marina  
Presidio 1

## Dynamic &amp; Tunable Biomaterials

## Responsive &amp; Structured Biomaterials

*Financially supported by Society for Biomaterials, Aldrich Materials Science, ACS Biomaterials Science & Engineering*

A. P. Dove, A. M. Kloxin, C. Magin, *Organizers*

C. A. DeForest, C. Guo, *Presiding*

**1:30 PMSE 61.** Thermoresponsive hydrogels as self-cleaning membranes for implanted glucose biosensors. **M. Grunlan, A.A. Abraham, A.K. Means, R. Fei, A.K. Locke, G.L. Cote**

**2:00 PMSE 62.** Programming intelligent protein biomaterials. **J.K. Montclare**

**2:20 PMSE 63.** Controlled release of dexamethasone loaded in core-shell SF/PEO. **M.H. El-Newehy, W. Chen, D. Li, A. El-Shanshoury, H. El-Hamshary, S. Al-Deyab, X. Mo**

**2:40 PMSE 64.** Antibacterial aerogels from cellulose nanofibrils. **J. Henschen, J. Illergård, P. Larsson, M.K. Ek, L. Wågberg**

**3:00** Intermission.

**3:15 PMSE 65.** Unimolecular-molecular brush nanoparticles as solute stabilizers. **M. Herrera-Alonso**

**3:45 PMSE 66.** Rational vaccine design using self-assembled polyionic immune signals. **Y. Chiu, P. Zhang, C. Jewell**

**4:15 PMSE 67.** Structure-based design of dendritic peptide bolaamphiphiles for siRNA delivery. **Z. Guan, M. Johnson, H. Zeng, N. Oldenhuys**

**4:35 PMSE 68.** Design and construction of coherently dynamic, auxetic two-dimensional protein crystals. **Y. Suzuki, G. Cardone, D. Restrepo, P. Zavattieri, T.S. Baker, F.A. Tezcan**

## Section E

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

## Bioresponsive &amp; Biomimetic Synthetic Polymers &amp; Materials

D. Bong, *Organizer*

K. Ahn, *Presiding*

**1:00 PMSE 69.** Enhanced wet-adhesion inspired by interfacial mussel foot proteins. **K. Ahn**

**1:35 PMSE 70.** Modular 'lego-like' polyes-ters with 'peptide-like' pendant functional groups. **Y. Xu, J.P. Swanson, Q. Liu, A. Joy**

**2:10 PMSE 71.** Lung-specific gene delivery using biodegradable polypeptides. **J. Wang**

**2:45** Intermission.

**2:55 PMSE 72.** Multifunctional polypeptide(oid)s: Adjusting particle morphology and function to biomedical applications. **M. Barz**

**3:15 PMSE 73.** Phosphorylated poly(ester-urea)-based biomimetic, degradable tissue adhesives. **V. Bhagat, J. Zhou, M. Becker**

**3:35 PMSE 74.** Enzyme-regulated topology of a cyclic peptide brush polymer for tuning assembly. **Z. Wang, N.C. Gianneschi**

**3:55 PMSE 75.** Conjugated polymer nanoparticles for improved, peptide-mediated drug delivery. **M. Twomey, M. An, J. Moon**

**4:15 PMSE 76.** Synthetic polypeptides with well-defined microstructures. **C. Lavilla, A. Heise**

## Section F

Marriott Marquis San Diego Marina  
Presidio 2

### Flow-Induced Crystallization of Polymers

#### Structure, Process & Properties

A. Doufas, S. Hatzikiakos, *Organizers, Presiding*

**1:00 PMSE 77.** Design of polypropylene resins for fabrication of low-density, closed-cell strand foams. **R.L. Sammler**

**1:30 PMSE 78.** Polymer-carbon nanotube composites: Enhancing structure-property relationships. **E.L. Heeley, D. Hughes, E. Crabb, M. Kershaw, O. Shebanova, T. McNally**

**2:00 PMSE 79.** Ultra-high molecular weight polyethylene/boron nitride nanotube for heat-transfer applications. **N. Tajaddod, T. Luo, M. Minus**

**2:30** Intermission.

**2:45 PMSE 80.** Strain-induced crystallization in elastomers of propylene-ethylene copolymers. **A.J. Norman, J.R. Hagadorn, A.H. Tsou, Y. Sun**

**3:15 PMSE 81.** Strain-induced crystallization studies of poly(trimethylene terephthalate). **N. Vasanthan**

**3:45 PMSE 82.** Direct observation of crystallization during shear flow with various molecular weight polymers. **G. Matsuba, Y. Ohkawa**

**4:15 PMSE 83.** Relationship between poor physical property of recycled polymer and its molded history. **S. Yao, A. Tominaga, N. Takenaka, R. Nakano, H. Sekiguchi, E. Takatori**

### Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINP, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

### Applications of Polymer Surfaces & Interfaces

#### New Processes & Surface Functionalization

Sponsored by POLY, Cosponsored by COLL and PMSE

### Biomass & Polymer Extrusion, Composite & Reaction Technologies: New Insights, Future Potential & Principles to Practice

Sponsored by CELL, Cosponsored by PMSE and POLY

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

### Sustainable Polymers, Processes & Applications

Sponsored by POLY, Cosponsored by PMSE

## SUNDAY EVENING

### My Comments to the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINP, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## MONDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom C

### ACS Award in Applied Polymer Science: Symposium in honor of Thomas P. Russell

Cosponsored by POLY

C. J. Hawker, K. L. Wooley, *Organizers, Presiding*

**8:00 PMSE 84.** Large area flexible biomimetic surfaces. **Y. Li, J. John, K.W. Kolewe, J.D. Schifman, K.R. Carter**

**8:30 PMSE 85.** Applying Russell's rules. **C.G. Willson**

**9:00 PMSE 86.** Polymer chemistry of graphenes: Synthesis, processing, applications. **K. Muellen**

**9:30 PMSE 87.** All-acrylic and tunable upper service temperature superelastomers synthesized using the grafting-through approach. **J.W. Mays, A. Goodwin, W. Wang, N. Kang**

**10:00 PMSE 88.** Functional polymers for nanomaterials and devices. **T. Emrick**

**10:30 PMSE 89.** DNA-functionalized anisotropic particle assembly. **M. Olvera De La Cruz, M. Girard, J. Millan**

**11:00 PMSE 90.** Design amphiphilic peptide-polymer conjugates toward modular nanocarrier. **T. Xu**

### Section B

Marriott Marquis San Diego Marina  
Leucadia

### Clay/Polymer Composites: Nanoclays & Other Natural Nanoparticles

#### Fibrous & Tubule Nanoclay Composites

Financially supported by I-Minerals, Inc.

Y. M. Lvov, E. Ruiz-Hitzky, L. Zhang, *Organizers*

A. Takahara, *Organizer, Presiding*

J. C. Grunlan, *Presiding*

**8:00 PMSE 91.** Clay-based nanocomposites for supported graphene production. **E. Ruiz-Hitzky, A. Gomez-Aviles, C. Ruiz-Garcia, F.M. Fernandes, M. Darder, P. Aranda**

**8:30 PMSE 92.** Preparation of halloysite/alginate aerogel beads by freeze-drying for dye removal. **Y. Zhao, G. Liu, B. Zhang**

**9:00 PMSE 93.** Halloysite clay nanotubes as novel carriers for polyphenols delivery. **C. Dionisi, N. Hanafy, V. Vergaro, Y.M. Lvov, S. Leporatti**

**9:30 PMSE 94.** Fabrication of enzyme-activated, intracellular drug-delivery nanocontainers using polymer-capped halloysite nanotubes. **R. Fakhru'llin**

**10:00** Intermission.

**10:10 PMSE 95.** Clay-biopolymer nanocomposites for environmental remediation. **P. Aranda, M. Darder, A.C. Alcantara, Y. Koriche, E. Padilla-Ortega, N. Jovic-Jovicic, E. Ruiz-Hitzky**

**10:40 PMSE 96.** Tunable, controlled release of molecular species from halloysite nanotubes. **D. Elumalai, J.R. Tully, Y.M. Lvov, P.A. Derosa**

**11:10 PMSE 97.** Sepiolite-based bionanocomposites as nucleic acids nanocarriers for applications in biotechnology. **F.A. Castro Smirnov, O. Piétrement, P. Aranda, J. Ayache, B.S. Lopez, E. Ruiz-Hitzky**

### Section C

Marriott Marquis San Diego Marina  
Mission Hills

### Directed Polymer Assembly

M. Herrera-Alonso, C. Li, *Organizers*

P. Gao, W. Huang, *Presiding*

**8:30 PMSE 98.** Template synthesis of nanomaterials by ink-jet printing. **P. Gao, A. Hunter, W.A. Phillip**

**8:50 PMSE 99.** Withdrawn.

**9:05 PMSE 100.** Tin-containing block copolymers for the direct pattern transfer of sub-10 nm features. **M. Maher, K. Mori, S. Sirard, E. Gurer, C. Bates, A. Dinholi, G. Blachut, C.J. Ellison, C.G. Willson**

**9:20 PMSE 101.** Probing the structure evolution and kinetics of block-copolymer ordering *in-situ* under dynamic zone annealing using grazing incidence SAXS. **S. Samant, J.W. Strzalka, G. Singh, A. Karim**

**9:35 PMSE 102.** Temperature-induced self-assembly of thermosensitive, diblock copolymer, brush-grafted silica nanoparticles. **R. Wright, B. Hu, D. Henn, B. Zhao**

**9:50** Intermission.

**10:05 PMSE 103.** Enhanced block copolymer phase separation using click chemistry and ionic junctions. **Y. Luo, C.J. Hawker, D. Montarnal, N.J. Treat, G.H. Fredrickson, P.D. Hustad**

**10:25 PMSE 104.** Polymer-directed assembly of conjugated organic shish-kebabs: Orthogonal ambipolar semiconductors for single active layer logic gates. **W. Huang, J. Markwart, A. Briseño, R.C. Hayward**

**10:45 PMSE 105.** Directed self-assembly of silicon-containing block copolymers with a hybrid chemo-/grapho- epitaxial flow. **G. Blachut, S. Sirard, M. Maher, Y. Asano, Y. Someya, A. Lane, W. Durand, R. Gronheid, D. Hymes, C.J. Ellison, C.G. Willson**

**11:00 PMSE 106.** Withdrawn.

**11:15 PMSE 107.** Thermochromic supramolecular self-assemblies. **T. Yuan, L. Fang, M.A. Olson**

### Section D

Marriott Marquis San Diego Marina  
Point Loma

### ACS Award for Creative Invention: Symposium in honor of Antonio Facchetti

Cosponsored by POLY

A. L. Briseno, T. J. Marks, *Organizers*

N. Stingelin, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 PMSE 108.** Interface science of soft matter and hybrid photovoltaics. **T.J. Marks**

**8:30 PMSE 109.** New polymerization methods for plastic electronics. **M. Leclerc**

**8:55 PMSE 110.** Semiconducting polymers and small molecules for transistors and solar cells. **I. McCulloch**

**9:20 PMSE 111.** Use of polymeric semiconductors in flexible sensors. **A.C. Arias, Y. Khan, C. Lochner, A. Pierre, F. Pavinatto**

**9:45** Intermission.

**10:15 PMSE 112.** Development of high-performance, printed, integrated circuits with ambipolar conjugated polymers. **Y. Noh**

**10:40 PMSE 113.** Relating molecular structure to solid-state order and device performance in small-molecule organic semiconductors. **J.E. Anthony**

**11:05 PMSE 114.** Design and development of functional organic small molecules and polymers for optoelectronics. **H. Usta, G. Demirel, A. Facchetti, M. Muccini**

**11:25 PMSE 115.** Heavily n-dopable  $\pi$ -conjugated redox polymers for ultrafast energy storage. **Y. Yao**

### Section E

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

### Bioresponsive & Biomimetic Synthetic Polymers & Materials

D. Bong, *Organizer*

A. J. Luthi, *Presiding*

**8:30 PMSE 116.** Enzyme-responsive polymeric micelles as targeted therapeutic delivery vehicles. **A.J. Luthi, L. Adamiak, S. Beck-Pancer, S. Nguyen, J. Kammeyer, K.L. Christman, N.C. Gianneschi**

**8:50 PMSE 117.** Promotion of cell survival and migration using FGF-2 mimetic peptide amphiphile nanoribbons. **C. Rubert-Perez, Z. Alvarez-Pinto, S. Stupp**

**9:10 PMSE 118.** Acid-degradable, mannoseylated nanogels for dendritic cell targeting. **R. De Coen, L. Nuhn, B. De Geest**

**9:30 PMSE 119.** Redox-degradable biocompatible hyperbranched polyglycerols: Synthesis, copolymerization kinetics, degradation, and biocompatibility. **J. Lee, B.S. Kim, S. Son**

**9:50** Intermission.

**10:00 PMSE 120.** Self-transfecting micellar siRNA. **A. Rolloff, D.A. Nelles, G.W. Yeo, N.C. Gianneschi**

**10:20 PMSE 121.** Synthesis of polymer hydrogel nanoparticles as heat protectants for IgG. **B. Chou, R.J. Dalal, K.J. Shea**

**10:40 PMSE 122.** Biomimetic vaccine nanogels for cell-uptake-triggered immune activation. **L. Nuhn, N. Vanparijs, B. De Geest**

**11:00 PMSE 123.** Hydrogel surface functionalization via size-exclusion diffusivity. **J.M. Grolman, X. Lu, J.S. Moore**

**11:20 PMSE 124.** ROMP polymer amphiphiles: Tuning structure and function towards impactful biological interactions. **S. Barnhill, A. Rush, N.C. Gianneschi**

### Section F

Marriott Marquis San Diego Marina  
Presidio 1

### Flow-Induced Crystallization of Polymers

#### Modeling

A. Doufas, S. Hatzikiakos, *Organizers, Presiding*

**8:30 PMSE 125.** Flow-induced crystallization of isotactic polypropylene: Modeling formation of multiple crystal phases and morphologies. **G. Peters, P. Roozemond**

**9:00 PMSE 126.** Polymer melt crystallization: A molecular dynamics study. S. Hatzikiriakos, V. Triandafilidi, J. Rottler

**9:30 PMSE 127.** Molecular simulation of flow-enhanced nucleation in alkane melts. D. Nicholson, G.C. Rutledge

## Section G

Marriott Marquis San Diego Marina  
Presidio 2

### Dynamic & Tunable Biomaterials

#### Dynamic Hydrogel-Based Biomaterials for Biological Applications

*Financially supported by Society for Biomaterials, Aldrich Materials Science, ACS Biomaterials Science & Engineering*

A. P. Dove, A. M. Kloxin, C. Magin, *Organizers*

A. Engler, K. A. Kilian, *Presiding*

**8:30 PMSE 128.** Synthesis of dynamic stem cell niches using bioorthogonal photo-click chemistries. M.A. Azagarsamy, K. Kyburz, H. Ma, K.S. Anseth

**9:00 PMSE 129.** Injectable hyaluronic hydrogel functionalized with rod-like nanoparticles for cartilage tissue engineering. P. Maturavongsadit, J. Luckanagul, B. Xiangdong, Q. Wang

**9:20 PMSE 130.** Tunable elastic poly(ester urea)s for tendon-bone repair in rotator cuff applications. E. Childers, M. Becker

**9:40 PMSE 131.** High-throughput screening of cell contact guidance on directional nanotopographic gradients. Q. Zhou, P. Kühn, T. van Kooten, P. van Rijn

**10:00** Intermission.

**10:15 PMSE 132.** Hyaluronic acid-based dynamic and permissive hydrogels for tissue repair and regeneration. X. Jia

**10:45 PMSE 133.** Catechol-bearing networks: From underwater adhesives to electrochemical storage devices. C. Bettinger

**11:15 PMSE 134.** Reflectin as a material for neural stem cell growth. R. Kautz, L. Phan, J. Arulmoli, I. Kim, D. Le, M. Shenk, M. Pathak, L. Flanagan, F. Tombola, A.A. Gorodetsky

#### Frederic Stanley Kipping Award in Silicon Chemistry: Symposium in honor of Michael A. Brook

*Sponsored by POLY, Cosponsored by PMSE*

#### WCC 2016 Rising Stars Awards Symposium

*Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE*

#### Sustainable Polymers, Processes & Applications

*Sponsored by POLY, Cosponsored by PMSE*

## MONDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom C

#### ACS Award in Applied Polymer Science: Symposium in honor of Thomas P. Russell

*Cosponsored by POLY*

C. J. Hawker, K. L. Wooley, *Organizers, Presiding*

**1:00 PMSE 135.** Coupling molecular recognition and viscoelastic behavior in engineered protein hydrogels. D.A. Tirrell, L. Dooling

**1:30 PMSE 136.** Ambiguous surfaces: Antifouling and fouling release coatings based on self-assembly. B. Wenning, D. Calabrese, C.K. Ober

**2:00 PMSE 137.** Densely grafted copolymers by ATRP. K. Matyjaszewski

**2:30 PMSE 138.** Influence of macromolecular architecture on the physical properties of thin polymer films. P.F. Green

**3:00 PMSE 139.** Applications of polymers for control of fluid flow. D. Weitz

**3:30 PMSE 140.** Some surprises and research opportunities from deep imaging of polymers and colloids. S. Granick

**4:00 PMSE 141. Award Address (ACS)** Award in Applied Polymer Science sponsored by Eastman Chemical Company). Structuring liquids. T.P. Russell

### Section B

Marriott Marquis San Diego Marina  
Leucadia

#### Clay/Polymer Composites: Nanoclays & Other Natural Nanoparticles

##### Clay-Polymer Nanocomposites

*Financially supported by I-Minerals, Inc.*

Y. M. Lvov, A. Takahara, L. Zhang, *Organizers*

E. Ruiz-Hitzky, *Organizer, Presiding*

B. Guo, *Presiding*

**1:00 PMSE 142.** Industrialization and engineering application of clay/rubber nanocomposites. X. Wu, Y. Wang, Y. Lu, Y. Wu, L. Zhang

**1:30 PMSE 143.** Clay-organic self-assembly for nanomedicine. J. Choy

**2:00 PMSE 144.** Edge charge neutralization of montmorillonite clay: Improved gas barrier in multilayer nanobrick wall thin films with better clay coverage. Y. Song, D. Hagen, K. Falke, J.C. Grunlan

**2:30 PMSE 145.** Parallelism of nonlinear rheological behavior manifesting in filled elastomers. S. Li, Y. Mi, X. Wang

**3:00 PMSE 146.** Laponite nanodisks modified with folic acid via a PEG spacer as a platform for anticancer drug loading, release, and chemotherapy of tumors. X. Shi, Y. Wu, K. Li, R. Guo, L. Kong, M. Shen, Q. Zhao

**3:30 PMSE 147.** Intrinsic properties of materials containing natural nanofibers and nanosheets having a realistic geometry. J.F. Douglas

**4:00 PMSE 148.** Developing polymer-clay composite sorbents for the removal of emerging organic pollutants from water. Y. Mishael

### Section C

Marriott Marquis San Diego Marina  
Mission Hills

#### Hybrid Polymers & Nanocomposites

*Financially supported by Chinese Chemical Society (CCS)-Polymer Division (PD)*

Z. Li, Q. Lin, *Organizers*

D. Wang, *Organizer, Presiding*

**1:00** Introductory Remarks by PMSE Representative.

**1:05** Introductory Remarks by CCS Representative.

**1:10 PMSE 149.** Janus nanocomposites towards interfaces manipulation. Z. Yang

**1:40 PMSE 150.** Single-component, hybrid nanocomposites: Materials for print passives and photonics. R. Vaia, J. Che, C.A. Grabowski, Y. Jiao, M. Hsiao, L.F. Drummy

**2:10 PMSE 151.** Hybridization of carbon nanomaterials and their polymer nanocomposites. T. Liu

**2:40** Intermission.

**3:10 PMSE 152.** Chain dynamics in polymer nanocomposites. K.I. Winey

**3:40 PMSE 153.** Polymer/graphene functional nanocomposites. Z. Yu

**4:10 PMSE 154.** F-catalytic rearrangements of silsesquioxanes (SQs) and analogs: New cage sizes and unusual reactive properties. R.M. Laine, J.C. Fugral, M. Bahrami, H. Hashemi, J. Kieffer, X. Mao, T.G. Goodson

### Section D

Marriott Marquis San Diego Marina  
Point Loma

#### ACS Award for Creative Invention: Symposium in honor of Antonio Facchetti

*Cosponsored by POLY*

T. J. Marks, N. Stingelin, *Organizers*

A. L. Briseno, *Organizer, Presiding*

**1:00 PMSE 155.** Post-polymerization modification of conjugated polymers. M.J. Heeney

**1:25 PMSE 156.** Precise synthesis of semi-conducting polymers. C. Luscombe

**1:50 PMSE 157.** Electron-deficient thienocenes for opto/electronic applications. K. Takimiya, M. Nakano, I. Osaka

**2:15 PMSE 158.** Nonbonding "conformational locks" for constructing highly planar  $\pi$ -conjugated systems. A. Facchetti, T.J. Marks, H. Huang, T. Dong, P. Ye

**2:40** Intermission.

**3:10 PMSE 159.** Design and synthesis of organic semiconductor. S.R. Marder, J. Zhang, A. Rojas, T. Parker, S. Blakey, Q. Shi, C. Scott

**3:35 PMSE 160.** Coordination-based molecular assemblies as highly efficient electrochromic materials. M. Lahav, N. Eloom-Dov, S. Shankar, M.E. Van Der Boom

**4:00 PMSE 161.** Nanostructured organosilicon luminophores as a molecular "lego" for engineering of highly efficient light-emitting materials. S. Ponomarenko, N. Surin, O. Borshechev, M. Skorotetsky, S. Pisarev, T. Starikova, A. Tereschenko, E. Svidchenko, Y. Luponosov, Y. Fedorov

**4:25 PMSE 162.** Latent hydrogen bond: A versatile tool enabling the facile preparation of performing optic and optoelectronic organic devices. L. Beverina, M. Sassi, D. Galliani, F. Bruni, A. Scaccabarozzi, M. Campione, R. Ruffo, U. Giovannella, S. Luzzati, F. Meinardi, N. Stingelin, S. Brovelli

### Section E

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

#### Bioresponsive & Biomimetic Synthetic Polymers & Materials

D. Bong, *Organizer*

J. Ma, *Presiding*

**1:00 PMSE 163.** Polycatechol nanoparticle MRI contrast agents. Y. Li, Y. Huang, N.C. Gianneschi

**1:20 PMSE 164.** Salt-responsive polyzwitterionic surface regeneration with switchable fouling/antifouling and friction/lubrication properties. H. Chen, J. Yang, S. Xiao, R. Hu, M. Zhang, B. Ren, F. Yang, J. Ma, B. Jiang, J. Zheng

**1:40 PMSE 165.** Avian-inspired, synthetic melanin nanostructures via self-oxidation polymerization of dopamine. N. Zang, Y. Li, X. Ming, X. Yue, M. Shawkey, A.N. Dhinojwala, N.C. Gianneschi

**2:00 PMSE 166.** Programmable interactions between micellar nanoparticles and human serum albumin. X. Yue, J.K. Kammerer, Z. Wang, Y. Li, N.C. Gianneschi

**2:20** Intermission.

**2:30 PMSE 167.** Development of novel polysaccharide hydrocolloid composite: Influence of physicochemical properties on biochemical activity. J. Ma, O. Ahmad, J. Landolina, J. Lee, W. Luo

**2:50 PMSE 168.** Glycocalyx-mimetic interfaces with tunable protein and particulate adsorption characteristics. R. Kumar, K. Cheng, J. Prisyby, K. Liu, J. Lahann

**3:10 PMSE 169.** Mechanics and structure of strain-stiffening biomimetic hydrogels. M. Jaspers, A.E. Rowan, P. Kowar

**3:30 PMSE 170.** Selective detection of phase transitions in model biological membranes using novel, conjugated polyelectrolyte probes. J.E. Houston, R. Evans, M. Kraft, U. Scherf, A. Terry

### Section F

Marriott Marquis San Diego Marina  
Presidio 1

#### Dynamic & Tunable Biomaterials

##### Dynamic Modulation of Biomaterial Properties

*Financially supported by Society for Biomaterials, Aldrich Materials Science, ACS Biomaterials Science & Engineering*

A. P. Dove, A. M. Kloxin, C. Magin, *Organizers*  
C. Bettinger, J. S. Forsythe, *Presiding*

**1:30 PMSE 171.** Dynamically stiffening hydrogels promote malignant transformation and mechanical signaling. A. Engler

**2:00 PMSE 172.** Bulky urea bond for the design of dynamic and hydrolysable biopolymers. H. Ying, K. Cai, J. Cheng

**2:20 PMSE 173.** Self-healing hydrogels based on inclusion complexation of natural compounds. Y. Jia, J.X. Zhu

**2:40 PMSE 174.** Tuning stiffness of hydrogels by reversible host-guest interactions. H. Shih, C. Lin

**3:00** Intermission.

**3:15 PMSE 175.** Dynamic control of stem cell activity in composite hydrogels using permanent magnets. A. Abdeen, J. Lee, K.A. Kilian

**3:45 PMSE 176.** Light-responsive hydrogels for cell patterning and 3D culture. J.S. Forsythe, V. Truong, K. Tsang, Y. Shi

**4:15 PMSE 177.** Direct-gradient photolithography of photodegradable hydrogels with patterned stiffness control with sub-micron resolution. S. Norris, P. Tseng, A.M. Kasko

### Section G

Marriott Marquis San Diego Marina  
Presidio 2

#### General Papers/New Concepts in Polymeric Materials

##### Biological & Biomedical Polymers

C. L. Soles, *Organizer*

M. Jorfi, *Presiding*

**1:00 PMSE 178.** Evolution of cancer-targeting peptides from hydrogel materials. S.H. Medina, S. Miller, J. Schneider

- 1:20 PMSE 179.** Strain stiffening and negative normal stress in alginate gels. **S. Kundu**, S. Hashemnejad
- 1:40 PMSE 180.** Synthetic control of molecular-to-macroscopic collagen assembly and structural mimicry. **D. Aishanjiang**, E.C. Green, H. Li
- 2:00 PMSE 181.** Crosslinked, polymer-stabilized, low-boiling-point perfluorocarbons for clinical, acoustic-triggered ultrasound imaging. **Y. Huang**, N.C. Gianneschi
- 2:20 PMSE 182.** Cross-linkable polypeptide(s) for reversible polyplex stabilization. **P.S. Heller**, M. Barz
- 2:40** Intermission.
- 3:00 PMSE 183.** Protective role of synthetic immunostimulatory glycans in a *Toxoplasma gondii* mice challenge model. **S.H. Eassa**, T.J. Lynch, L. Soderberg
- 3:20 PMSE 184.** Simulation-guided design of block ionomer microstructure: Enhancing the performance of peptoplexes as non-viral transfection agents. **B. Weber**, J. Zhou, P.S. Heller, F. Schmidt, **M. Barz**
- 3:40 PMSE 185.** Novel, carbamate-based poly(olefin-sulfone)s as smart materials for drug delivery. **K. Kumar**, E.J. Castañón, A.P. Goodwin
- 4:00 PMSE 186.** Radiation-grafting of 2-MBA onto polypropylene films for drug delivery. **H. Magana**, K. Palomino, J.M. Cornejo-Bravo, C. Alvarez-Lorenzo, A. Concheiro, E. Zavala-Lagunes, E. Bucio
- 4:20 PMSE 187.** Electron donating group effect on antioxidant activity of polyphenol-based antioxidant dendrimers. **C.Y. Lee**
- 4:40 PMSE 188.** Shape-changing, photo-degradable hydrogels as 3D cell culture environments. **E. Kápylä**, S. Delgado, A.M. Kasko

#### WCC 2016 Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE

#### Applications of Polymer Surfaces & Interfaces

#### Composites, Brushes & Medical Devices

Sponsored by POLY, Cosponsored by COLL and PMSE

#### Sustainable Polymers, Processes & Applications

Sponsored by POLY, Cosponsored by PMSE

#### Undergraduate Research Posters

#### Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

Technical program information known at press time. The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## MONDAY EVENING

### Section A

San Diego Convention Center Hall D/E

#### Sci-Mix

C. L. Soles, *Organizer*

#### 8:00 - 10:00

278-280, 284, 287, 296, 300, 306, 310, 313, 315-316, 319, 326-327, 330, 333-334, 337-338, 344-345, 351-352, 358, 360, 363-364, 369-370, 375, 378-379, 384, 386, 390-391, 393, 395-397, 401, 403-404, 407, 409, 415, 419, 427, 430, 434, 437-439, 445, 447-449, 451,455. See subsequent listings.

#### Potpourri of Polymer Projects: Take a Byte out of the NGSS

Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB

## TUESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

#### Cooperative Research Award: Symposium in honor of Brian Benicewicz & Gordon Calundann

S. C. Jana, *Organizer*

C. Tang, *Organizer, Presiding*

E. Mutoro, *Presiding*

**8:00 PMSE 189.** Functional polymeric materials: A journey learning from BB. **C. Tang**

**8:30 PMSE 190.** Nylon filtration membranes. **L. Xiao**

**9:00 PMSE 191.** Development and commercialization of portable fuel cell systems based on polybenzimidazole membranes. **R. Chen**

**9:30 PMSE 192.** Electrode side of high-temperature membrane electrode assemblies. **E.S. De Castro**, Y. Tsou

**10:00** Intermission.

**10:20 PMSE 193.** PBI-based membranes for hydrogen separation. **E. Mutoro**, G. Bechtloff, S. Bräuninger, B.C. Benicewicz

**10:50 PMSE 194.** Academic-industrial cooperation: History, pathway, and accomplishments. **B.C. Benicewicz**, **G. Calundann**

**11:20 PMSE 195.** Perspectives on PBI membranes and effective teams. **G. Calundann**, **B.C. Benicewicz**

### Section B

Marriott Marquis San Diego Marina  
Leucadia

#### Clay/Polymer Composites: Nanoclays & Other Natural Nanoparticles

#### Polymer-Clay Nanocomposites

Financially supported by I-Minerals, Inc.

**Y. M. Lvov**, E. Ruiz-Hitzky, A. Takahara, L. Zhang, *Organizers*

**R. Fakhrullin**, G. Lazzara, *Presiding*

**8:30 PMSE 196.** Clay-assisted, synergistic dispersion of carbon nanomaterials in polymer composites. **T. Liu**

**9:00 PMSE 197.** Polymer-organoclay nanocomposites prepared by microwave-assisted, surface-initiated polymerization from thiol-functionalized organoclays. **T. Schuyler**, M. Coeurdray, K. Mbow, I.L. Lagadic

**9:30 PMSE 198.** Flameretardancy study of corrugated cardboard for using cardboard beds. **Y. Mochizuki**, Y. Mizutani, M. Okoshi, H. Hamada

**10:00 PMSE 199.** Polymer nanolaminates and the consequences of intercalation. **E. Dunkerley**, **D.F. Schmidt**

**10:30 PMSE 200.** Elastomeric bioepoxy/clay nanocomposites. **A. Rigail-Cedeno**, **D.F. Schmidt**, M.I. Chavez Yagual, G.A. Vera Pauta

### Section C

Marriott Marquis San Diego Marina  
Rancho Santa Fe 1 & 2

#### Hybrid Polymers & Nanocomposites

Financially supported by Chinese Chemical Society (CCS)-Polymer Division (PD)

**Q. Lin**, D. Wang, *Organizers*

**Z. Li**, *Organizer, Presiding*

**8:00 PMSE 201.** Inorganic block copolymers for nanopatterning. **C.G. Willson**

**8:30 PMSE 202.** Block copolymer/inorganic nanoparticles hybrid aggregates with well-ordered structures. **K. Wang**, W. Li, **J. Zhu**

**9:00 PMSE 203.** Si-containing polymers as an enabling materials platform for nano-electronic manufacturing. **Q. Lin**

**9:30** Intermission.

**10:00 PMSE 204.** Preparation and functionalization of graphene nanosheets by solid-state shear milling technique and application of the graphene-based nanocomposites in lithium-ion battery. **C. Zhang**, X. Liu, C. Liu, H. Wen

**10:30 PMSE 205.** Block copolymer-directed hybrid materials: Experiments, theory, and applications. **U.B. Wiesner**

**11:00 PMSE 206.** Polymerization of inorganic nanoparticles: Chiroptical plasmonic polyanomers. **K. Liu**

**11:30** Concluding Remarks.

### Section D

Marriott Marquis San Diego Marina  
Point Loma

#### ACS Award for Creative Invention: Symposium in honor of Antonio Facchetti

Cosponsored by POLY

**A. L. Briseno**, T. J. Marks, N. Stingelin, *Organizers*

**A. Facchetti**, *Presiding*

**8:00 PMSE 207.** Control of crystal morphology in organic electronic applications. **A.L. Briseno**

**8:25 PMSE 208.** Solution processing as a tool for understanding morphology control and achieving high performance with organic semiconductors and conductors. **Z. Bao**

**8:50 PMSE 209.** Synthesis and application of n- and p-type semiconducting polymers for chemical sensors and thermoelectrics. **H.E. Katz**, K. Besar, R. Ireland, X. Zhao, D. Madan

**9:15 PMSE 210.** Indirect crystallization of small-molecule organic semiconductors: A pathway to high performance with consistency. **A. Amassian**

**9:40** Intermission.

**10:10 PMSE 211.** Nanoporous-crystalline polymers. **G. Guerra**, P. Rizzo, C. Daniel, V. Venditto, M. Accoella

**10:35 PMSE 212.** Boosting the speed of printed and direct-written polymer transistors. **M. Caironi**

**11:00 PMSE 213.** Organic semiconductors: The effect of small modifications on device performance. **R. Ponce Ortiz**, J. Seura, J.T. Lopez Navarrete, A. Facchetti, T.J. Marks

**11:20 PMSE 214.** Design, synthesis, and applications of high-performance polymer semiconductors in organic electronics. **X. Guo**

### Section E

Marriott Marquis San Diego Marina  
San Diego Ballroom C

#### Polymer-Related Energy Conversion & Storage

**Z. Lin**, S. C. Rasmussen, *Organizers*

**M. C. Stefan**, *Organizer, Presiding*

**8:00 PMSE 215.** Electron-deficient triazole units to construct conjugated polymers for solar cells: From chemistry to devices. **W. Li**, L. Yan, **W. You**

**8:30 PMSE 216.** All-conjugated block copolymer additives and compatibilizers for organic photovoltaics. **J.W. Mok**, **D. Kipp**, H. An, V. Ganesan, J.L. Lutkenhaus, **R. Verduzco**

**9:00 PMSE 217.** Design, synthesis, and properties of 3D molecules for organic photovoltaic applications. **S.R. Marder**, **K. Ziabrev**, X. Ba, Y. Fan, S. Zhang, J. Zhang, M. Said, S. Barlow, T. Parker, A. Amassian, R. Wolfe, J.R. Reynolds, Q. Shi, S. Blakey

**9:30 PMSE 218.** Benzodithiophene and benzodifuran organic semiconductors for organic photovoltaics. **M.C. Stefan**, J. Du, R. Gunawardhana, P. Huang, M.C. Biewer

**10:00** Intermission.

**10:15 PMSE 219.** Polymer design for lithium-ion battery electrodes. **Z. Bao**

**10:45 PMSE 220.** Role of oligomeric additives on P3HT/PCBM domain interfaces and photovoltaic performance. **Z. Seibers**, T. Le, E. Gomez, J. Carrillo, M. Kilbey

**11:05 PMSE 221.** Ternary blend polymer fullerene solar cells. **B.C. Thompson**

### Section F

Marriott Marquis San Diego Marina  
Catalina

#### Polyethylene

#### Catalysis

Cosponsored by WCC

Financially supported by ExxonMobil Chemical Company

**D. Thurman**, A. Winesett, *Organizers*

**G. E. Alliger**, *Organizer, Presiding*

**8:30 PMSE 222.** Homogeneous models for heterogeneous chromium-based ethylene polymerization catalysts. **K.H. Theopold**

**9:00 PMSE 223.** Functional precision polyolefins via ADMET. **K.B. Wagener**, **P. Bachler**, T.W. Gaines

**9:30 PMSE 224.** Design of new ruthenium-based catalysts for ethylene insertion polymerization. **Z. Guan**

**10:00** Intermission.

**10:15 PMSE 225.** Expanding the range of poly(ethylene-co- $\alpha$ -olefin) materials via dynamic two-state living copolymerization. **L.R. Sita**

**10:45 PMSE 226.** Pi stacking effects in electronically unsymmetrical Pd catalysts for ethylene/polar-monomer copolymerization. R.F. Jordan

**11:15 PMSE 227.** Controlled synthesis of simple hydrocarbon polymers from C1 carbon sources: Living polymerization of ylides. K.J. Shea

## Applications of Polymer Surfaces & Interfaces

### Energy Conversion

Sponsored by POLY, Cosponsored by COLL and PMSE

### Sustainable Polymers, Processes & Applications

Sponsored by POLY, Cosponsored by PMSE

## TUESDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

### Computation & Cheminformatics in Polymers Research

#### Molecular Dynamics & Mechanics

Financially supported by ExxonMobil Chemical, ExxonMobil Research & Engineering

G. Carri, G. Rodriguez, S. Tallury, *Organizers*  
J. D. Moore, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 PMSE 228.** Screening nucleating agents for polymer crystallization by molecular simulation. A.J. Bourque, R. Locker, G.C. Rutledge

**1:35 PMSE 229.** Molecular features that modulate mesoscale, biomolecular phenomena revealed through multiscale simulation. G.A. Voth

**2:05 PMSE 230.** Molecular modeling of crosslinking reactions in high-temperature bismaleimide resins: Matrimid-5292. V. Varshney, M.S. Radue, J. Baur, A.K. Roy, G. Odgaard

**2:35** Intermission.

**2:50 PMSE 231.** MD simulations of crystal and rotator phase melting in oligomeric IPP. S. Milner, Q. Chen

**3:20 PMSE 232.** High-throughput prediction of physical properties using atomistic simulation for thermoset polymers. J. Sanders, J. Gavartin, D. Giesen, T. Mustard, S. Kwak, M. Halls

**3:50 PMSE 233.** Prediction of surface and pH-specific binding of polymers and biomacromolecules to metal and oxide nanostructures using computational models. H. Heinz

### Section B

Marriott Marquis San Diego Marina  
Presidio 2

### General Papers/New Concepts in Polymeric Materials

#### Polymer Membranes, Barriers & Transport Media

C. L. Soles, *Organizer, Presiding*

**1:00 PMSE 234.** Polymer dynamics, free volume, and transport in cross-linked polymer networks. C.L. Soles, B. Friberg

**1:20 PMSE 235.** Structure and rheology of waterborne paints thickened by hydrophobically-ethoxylated urethane (HEUR) rheology modifiers. A.I. Nakatani, V. Ginzburg, A. van Dyk, T. Chatterjee, K. Beshah, F. Yuan, S. Wang, R.G. Larson

**1:40 PMSE 236.** Indentation methods to quantify bimodal polyethylene interfaces. A. Forster, D.L. Hunston, S.J. Watson

**2:00 PMSE 237.** Responsive, highly porous, hydrogel copolymers from emulsion templating. M. Ovidia, M.S. Silverstein

**2:20 PMSE 238.** Effect of free volume redistribution on the diffusivity of solvent in poly(vinyl alcohol). A. Noorjahan, P.Y. Choi

**2:40** Intermission.

**3:00 PMSE 239.** Ultrathin CVD-deposited metal-organic covalent network for gas separation. M. Wang, N. Boscher, K. Gleason

**3:20 PMSE 240.** Understanding structure-property relationships of anion-exchange membrane fuel cells. S.P. Ertem, T. Tsai, M.M. Donahue, W. Zhang, S. Seifert, Y. Liu, A.M. Maes, A.M. Herring, E.B. Coughlin

**3:40 PMSE 241.** Role of additive and free volume on the gas-barrier properties of poly(ethylene terephthalate). S. Zekriadehani, M. Coleman, S.A. Jabarin

**4:00 PMSE 242.** Implementing surface-free energy analyses to predict inhibition of biofilm growth on UV-curable coatings. E.B. Henry, A. Mahmood, T.B. Cavitt

### Section C

Marriott Marquis San Diego Marina  
Rancho Santa Fe 1 & 2

### Hybrid Polymers & Nanocomposites

#### Hybrid Polymers

Financially supported by Chinese Chemical Society (CCS)-Polymer Division (PD)

Z. Li, Q. Lin, D. Wang, *Organizers*

R. B. Grubbs, *Presiding*

**1:00 PMSE 243.** Magnetic plastics and gels from hybrid cobalt-block copolymer materials. R.B. Grubbs, B. Jiang

**1:20 PMSE 244.** Spatial distribution of guest in low-dimensional nanospace materials. M. Ogawa

**1:40 PMSE 245.** Hybrid, amorphous nanoparticles composed of calcium phosphate and a cationic polymer. N. Taheri Qazvini, M. Sadati, M.V. Tirrell, J.J. De Pablo

**2:00 PMSE 246.** Wetttable/non-wetttable surfaces using FOSM-DMA-FOSM triblock copolymers. N. Salunke, A. Karim, R.A. Weiss

**2:20 PMSE 247.** Electrical modulation of plasmonic properties for gold nanorod-electroactive polymer nano-hybrids. P.A. Ledin, J. Jeon, J. Geldmeier, J.F. Ponder, M.A. Mahmoud, M.A. El-Sayed, J.R. Reynolds, V.V. Tsukruk

**2:40** Intermission.

**3:00 PMSE 248.** Withdrawn.

**3:20 PMSE 249.** Infiltration, imidization, and cross-linking of polyimides in molecular-scale confinement. J.J. Forstvedt, S.G. Isaacson, R.H. Dauskardt

**3:40 PMSE 250.** Structure-property relationship of poly(1,3,5-hexahydro-1,3,5-triazine) materials modified by reactive blending. M. Fevre, R.J. Wojtecki, J.M. Garcia, J.L. Hedrick

**4:00 PMSE 251.** Modular integration of upconversion nanocrystal and folate-targeted dendrimer for near-infrared imaging and light-triggered drug release. P.T. Wong, D. Chen, S. Tang, S. Yanik, M. Payne, J. Mukherjee, A. Coulter, K. Tang, K. Tao, K. Sun, S. Choi

### Section D

Marriott Marquis San Diego Marina  
Point Loma

### ACS Award for Creative Invention: Symposium in honor of Antonio Facchetti

Cosponsored by POLY

A. L. Briseno, N. Stingelin, *Organizers*

T. J. Marks, *Organizer, Presiding*

**1:00 PMSE 252.** Polymer-SWNT hybrids: Toward high-performance field effect transistors. M. Loi

**1:25 PMSE 253.** Micro- and nanocrystals of organic semiconductors. W. Hu

**1:50 PMSE 254.** Materials and structures for OLET technology. M. Muccini

**2:15 PMSE 255.** Novel oxo-amininate Mo and W precursors for atomic layer deposition. M. Delferro, P.C. Stair, T.J. Marks, A.R. Moutat

**2:40** Intermission.

**3:10 PMSE 256.** Understanding voltage loss in organic bulk heterojunction solar cells. T.T. Nguyen

**3:35 PMSE 257.** Structure-property relationships of a record-breaking n-type semiconducting polymer: N2200. A. Salleo

**4:00 PMSE 258.** Printed electronics and photonics: Future challenges and opportunities provided by multicomponent systems. N. Stingelin

**4:25 PMSE 259. Award Address (ACS Award for Creative Invention sponsored by Corporation Associates).** Materials chemistry and process engineering for flexible opto-electronics. A. Facchetti

### Section E

Marriott Marquis San Diego Marina  
San Diego Ballroom C

### Polymer-Related Energy Conversion & Storage

Z. Lin, S. C. Rasmussen, M. C. Stefan, *Organizers*

M. Kilbey, *Presiding*

**1:00 PMSE 260.** Organic-inorganic nanocomposites via placing monodisperse nanocrystals in direct and permanent contact with polymer toward energy conversion and storage. Z. Lin

**1:30 PMSE 261.** Rational material design, interface, and device engineering for high-performance polymer and perovskite solar cells. A.K. Jen

**2:00 PMSE 262.** Influence of the functionalized side chains of polythiophene diblock copolymers: CdSe nanoparticle (NP) bulk heterojunction solar cells. M.C. Stefan, C. Bulumulla, J. Du, K. Washington, C. Mills, M.C. Biewer

**2:20 PMSE 263.** Plasmonic transition via interparticle coupling of Au@Ag core-shell nanostructures sheathed in double hydrophilic block copolymer for high-performance polymer solar cell. E. Seo, S. Ko, S. Min, J. Lee, J. Kim, B.S. Kim

**2:40 PMSE 264.** Non-conjugated flexible linkers: A new approach to master blend morphology in all-polymer solar cells. B.C. Schroeder, Y. Zhou, Y. Chiu, X. Gu, Z. Bao

**3:00** Intermission.

**3:10 PMSE 265.** Withdrawn.

**3:30 PMSE 266.** Exploring more electron-deficient monomers in catalyst-transfer polycondensation. K.J. Noonan

**4:00 PMSE 267.** Conjugated polymers for photovoltaics and energy storage. J.R. Reynolds

**4:30 PMSE 268.** Application of ambipolar units to nontraditional donor-acceptor polymers: A potential new paradigm for the design of low-band gap materials. T. Anderson, M.E. Mulholland, M.R. Delgado, R. Schwiderski, S.C. Rasmussen

### Section F

Marriott Marquis San Diego Marina  
Catalina

### Polyethylene

#### Crystallization

Cosponsored by WCC  
Financially supported by ExxonMobil Chemical Company

G. E. Alliger, A. Winesett, *Organizers*

D. Thurman, *Organizer, Presiding*

**1:30 PMSE 269.** Molecular alignment of LLDPE during cold drawing: An *in-situ* tensile-SANS study. C. Lopez-Barron, Y. Zeng, J. Schaefer, A. Eberle, F.S. Bates, T.P. Lodge

**2:00 PMSE 270.** Characterization of the primary and secondary crystallization kinetics of a linear, low-density polyethylene in quiescent and flow conditions. G. Peters

**2:30 PMSE 271.** Melt memory of crystallization and melt structure of random ethylene copolymers. R.G. Alamo, X. Chen, A. Mamun, M. Ren

**3:00** Intermission.

**3:15 PMSE 272.** Withdrawn.

**3:45 PMSE 273.** Why do lamellae rotate? Polyethylene crystallinity evolution under the stretch. S. Yakovlev

**4:15 PMSE 274.** Interplay of macromolecular architecture and flow in polymer crystallization. J.A. Kornfield

### Applications of Polymer Surfaces & Interfaces

#### Membranes

Sponsored by POLY, Cosponsored by COLL and PMSE

#### Anionic Polymerisation: Still Living After 60 Years

Sponsored by POLY, Cosponsored by PMSE and RUBB

## TUESDAY EVENING

### Section A

San Diego Convention Center  
Hall F

#### Joint PMSE/POLY Poster Session

C. L. Soles, *Organizer*

**6:00 - 8:00**

### General Papers/New Concepts in Polymeric Materials.

- PMSE 275.** Effect of PLGA molecular weight on the drug incorporation and release profile by synthesized magnetite/PLGA nanoparticle via double emulsion. **Y. Tan, M. Nithitanakul**
- PMSE 276.** Larger aspect-ratio clay nanoplatelets for improved flame barrier on polyurethane foam. **P. Advincula, A. Cain, J.C. Grunlan**
- PMSE 277.** PEI-cored star copolymers: Electrochemical crosslinking and nanoparticle stabilizers. **A. Advincula, P. Cao, R.C. Advincula**
- PMSE 278.** Deformation of clay-filled epoxy nanocomposites. **S. Ahuja**
- PMSE 279.** Simple approach for surface immobilization of poly(N-isopropylacrylamide) using organosilane networks. **A. Alghunaim**
- PMSE 280.** Device physics of the organic alloying effect in high-efficiency ternary blend polymer/fullerene bulk-heterojunction solar cells. **T. Aubry, B.J. Schwartz**
- PMSE 281.** Novel patterning of Au thin films on PMMA via microcontact and inkjet printing of halogenated solvents followed by selective polishing. **B.H. Augustine, W.C. Hughes, K.T. Krist, H. Hu, G. Rich, S. Colbert, W. Stahl**
- PMSE 282.** Hyperbranched phosphonic acid polymers via RAFT-SCVP. **P.R. Bachler, K.B. Wagener, B.S. Sumerlin**
- PMSE 283.** Towards multi-modal imaging nanoparticles via tunable ion-pairing nanoprecipitation. **L. Behar, N. Pinkerton, S. Chassaing, J. Marty**
- PMSE 284.** 3D printing of porous materials for catalytic applications. **V. Blaszczak, S. Manzano, I.I. Slowing, W.T. Grubbs**
- PMSE 285.** Controlled contamination as a disruptive effect on hydrogen-bonded liquid crystals: 1,8-Bis-(4-pyridyloxy) octane. **E. Bornowski, M.D. Heltne, E.A. John, K.N. Wiegell**
- PMSE 286.** Effects of inert fillers on frontal polymerization temperature and velocity in acrylate composites. **S. Bynum, K. Blackburn, J. Guidry, J.A. Pojman**
- PMSE 287.** Enzyme-responsive polymeric nanomaterials for paclitaxel delivery to tumor tissue. **C.E. Callmann, N.C. Gianneschi**
- PMSE 288.** Controlled contamination as a disruptive effect on hydrogen-bonded liquid crystals: Intentional stoichiometric imbalance in assembled chain structures. **J. Carli, K.N. Wiegell**
- PMSE 289.** Synthesis of simple metallocene polyethers. **C.E. Carrher, M.R. Roner, L. Reckleben, K.M. Black, J. Frank, R. Crichton**
- PMSE 290.** Graphite matrix for MALDI MS for metal-containing polymers derived from 3-amino-1,2,3-triazole, 6-aminopenicillanic acid, and salicylic acid. **C.E. Carrher, R. Crichton, D. Patel, M. Lynch, M.R. Roner**
- PMSE 291.** Deep-eutectic solvents as delivery vehicles in the non-aqueous synthesis of functional macroporous poly(HIPe)s CNT nanocomposites. **A. Carranza, M. Perez-Garcia, K. Song, G. Jeha, Z. Diao, R. Jin, A. Soltero-Martinez, M. Terrones, J.A. Pojman, J.D. Mota-Morales**
- PMSE 292.** Nitrogen-enriched, nanoporous carbon derived from polybenzoxazine for CO<sub>2</sub> gas adsorption. **T. Chaisuwat, N. Manmuanpom, S. Wongkasemjit**
- PMSE 293.** Novel and high-strength, hybrid, double-network hydrogels based on carboxymethylcellulose. **Q. Chen, H. Chen, X. Yan, D. Wei, B. Jiang, L. Zhu, J. Yang, L. Huang, J. Zheng**
- PMSE 294.** Development of flexible polymer nanocomposite for trace. **C. Chen, S. Ganguli, A.K. Roy, J. Foley**
- PMSE 295.** Nanostructured polymer lithography for electronic applications. **A.J. Christy, J.D. Harris, D. Estrada**
- PMSE 296.** Self-assembly of stable radical block copolymers for charge transport studies. **A. Cintora, A. Moehle, C. Liedel, G. Fuchs, C.K. Ober**
- PMSE 297.** Controlling crack patterns and ultra-high aspect ratio ribbons in polydimethylsiloxane thin films. **S. Conjurske, K. Jiao, P. Kohli**
- PMSE 298.** Nanoparticle polymer synthesis and testing affinity with IgG. **R.J. Dalal, B. Chou, K.J. Shea**
- PMSE 299.** Nanoscale mosaic polymer brushes synthesized from block-copolymer supramolecular assembly. **O. Davydovich, E. Chu, P.B. Moore, A. Sidorenko**
- PMSE 300.** Flame-retardant aerogels for foam applications. **T. Deans, L. Jefferson, D.A. Schiraldi**
- PMSE 301.** Lignin-modified poly(amide-imide) aerogel materials. **K. DeGracia, D.A. Schiraldi**
- PMSE 302.** Self-folding photodegradable hydrogels: From planar sheets to 3D structures. **S. Delgado, E. Käpylä, A.M. Kasko**
- PMSE 303.** Soybean-based polymer surfactants for personal care application. **Z. Demchuk, A. Popadyuk, I. Tarnavchik, S. Samanta, B.J. Chisholm, A. Voronov**
- PMSE 304.** Salicylic acid-based, pH-sensitive hydrogels as potential oral insulin delivery system. **B. Demirdirek, K.E. Uhrich**
- PMSE 305.** Fused pyrrolo[3,2-d:4,5-d']bisthi-azole-based *n*-type copolymers. **S. Dey, S.Y. Al Qaradawi, H.S. Bazzi, M.J. Heeney, M. Al-Hashimi**
- PMSE 306.** Withdrawn.
- PMSE 307.** Post-polymerization modification of reactive, azlactone-functionalized block copolymers: Rapid synthesis of polymeric amphiphiles for the assembly of drug delivery vehicles. **S. Eini, Q. Anex-Ries, A. Carroll, M.E. Buck**
- PMSE 308.** Montmorillonite-ionene nanocomposite as drug delivery system for diclofenac. **H. El-Hamshary, M.H. El-Newehy, S. Al-Deyab, M. Moydeen**
- PMSE 309.** Electrospun nickel/nitrogen-doped carbon nanofibers as non-precious and effective anode for direct methanol fuel cells. **M.H. El-Newehy, B. Thamer, N. Barakat, M. Abdelkareem, S. Al-Deyab, H. Kim**
- PMSE 310.** Silicone-hydrogel bandage lenses used in conjunction with pharmaceutical eye drops: An uptake and release study. **N. Erdal, K. Adolffson, M. Hakkarainen**
- PMSE 311.** Construction of solid-state nanoreactor for the synthesis and characterization of large-scale metallic nanoparticles. **A. Ethridge, D. Finley, M.L. Curry**
- PMSE 312.** Focus-variable, large-deformable, and plano-convex microlens based on non-ionic poly(vinyl chloride)/dibutyl adipate gels. **J. Lee, J. Jang, J. Bae, S. Kim, B. Nam**
- PMSE 313.** Sulfur-limonene polysulfide: A material synthesized entirely from industrial byproducts and its use in removing toxic metals from water and soil. **A. Evans, M. Crockett, M. Worthington, I. Albuquerque, A. Slattery, C. Gibson, D. Lewis, J. Campbell, G. Bernardes, J. Chalker**
- PMSE 314.** Hyperbranched ethylene oligomers by  $\kappa^2$ -(N,O)-salicylaldiminato Ni(II) complexes: DFT investigation of role of remote substituents. **L. Falivene, L. Cavallo, L. Caporaso**
- PMSE 315.** Azobenzene surfactant: Light-induced, local hydrodynamic flow at the liquid-solid interface. **D. Feldmann, N. Lomadze, S.A. Santer**
- PMSE 316.** Structure-property-function relationships of biodegradable nylon 4, elucidated by computational chemistry and NMR experiments. **Y. Fukuda, Y. Sasanuma**
- PMSE 317.** Lysozyme immobilization on silicone rubber modified with EGDMA/GMA graft started by radiation and free radicals. **G. Rojas-Flores, E. Bucio**
- PMSE 318.** Analysis and characterization of thiol-acrylate polymers for use as biomaterials. **L.A. Garber, J.A. Pojman, D. Hayes**
- PMSE 319.** Tuning protein folding for molecular interfacial reinforcement of biopolymeric nanocomposites. **Y. Yin, K. Hu, A.M. Grant, Y. Zhang, V.V. Tsukruk**
- PMSE 320.** Inclusion behavior between cyclodextrin and poly(ethylene glycol). **K. Huang, L. Li, X. Guo**
- PMSE 321.** High-selective removal of methylene blue from organic solution using spherical polyelectrolyte brushes. **Z. Yu, X. Hou, Y. Cang, J. Deng, Z. Shen, R. Zhang, X. Guo**
- PMSE 322.** Rheology and adhesion of poly(methacrylic acid)/laponite nanocomposite hydrogels. **M. Wang, M. Shen, J. Wang, K. Chen, L. Li, X. Guo**
- PMSE 323.** Synthesis and characterization of thermosensitive biomaterials based on chitosan. **Y. Wang, J. Wang, L. Li, X. Guo**
- PMSE 324.** Temperature triggered poly(N-isopropylacrylamide-co-acrylic acid) hydrogel adhesive. **X. Guo, A. Smith, M. Wang**
- PMSE 325.** Effects of surface modification of silica nanoparticles on the mechanical properties of UV-curable silica/polyurethane acrylate nanocomposites. **K. Ha, B. Seo, H. Kim, S. Park, S. Kim**
- PMSE 326.** Metal coordination complexes in mechanically responsive systems. **K. Hall, K.J. Franz**
- PMSE 327.** Chain motions and secondary relaxations of fullerene-containing nanocomposites as investigated by broadband dielectric spectroscopy. **H.M. Ahmed, A.D. Windham, M.K. Hassan, M.M. Al-Ejji, N.H. Al-Qahtani, K.A. Mauritz, J. Buchanan**
- PMSE 328.** Cyclopenta-fused, polycyclic, aromatic hydrocarbon-based conjugated polymers. **M.P. Hautzinger, S.R. Bheemreddy, K.N. Plunkett**
- PMSE 329.** Amide chemistry towards novel, high-performance organic semiconductors. **B. He, T. Chen, L. Klivansky, Y. Liu**
- PMSE 330.** Capture the triplets, Pt-containing conjugated polymers and small molecules. **W. He, Y. Qin**
- PMSE 331.** Controlled contamination as a disruptive effect on hydrogen bonded liquid crystals: 1,10-Bis-(4-pyridyloxy) decane. **M.D. Heltne, E.A. John, E. Bornowski, K.N. Wiegell**
- PMSE 332.** pH dependence of thermally induced sol-gel transitions of aqueous solutions of tertiary amine-containing thermosensitive ABA triblock copolymers. **D.M. Henn, R. Wright, J.W. Woodcock, B. Hu, B. Zhao**
- PMSE 333.** Post-polymerization modification of an engineering polymer to optimize for use in gas separation membranes. **L.J. Hill, V. Kusuma, A. Marti, D. Hopkinson, H.B. Nulwala**
- PMSE 334.** Layer-by-layer assembly of hexagonal boron nitride for flame-retardant polyurethane foam. **K. Holder, L. Huff, S. Ruiz, E. Brown, P. Advincula, J.C. Grunlan**
- PMSE 335.** Intravenously administered, high-temperature nanoparticles halt bleeding and improve survival after trauma. **M. Holland, M. Lashof-Sullivan, R. Groynom, A. Shoffstall, E.B. Lavik**
- PMSE 336.** Producing collagen-fibrin matrices to investigate tendon engineering strategies. **D. Holland, L. Trichet, M. Picaut, O. Ronsin, M. Bonnin, G. Mosser, D. Duprez, T. Baumberger, T. Coradin**
- PMSE 337.** Withdrawn.
- PMSE 338.** Structure analysis of butt fusion weld zone of HDPE pipe by using high-resolution x-ray scattering. **H. Song, M. Kang, S. Choi**
- PMSE 339.** Strain-induced crystallization of natural rubber as studied by utilizing strain jumping device. **H. Song, M. Kang, G. Kwag**
- PMSE 340.** Degradation of self-immolative polymers in response to hydrogen peroxide. **P. Hsu, J. Olejniczak, A. Almutairi**
- PMSE 341.** Adapting silsesquiazane precursor to prepare polyimide/silica nanohybrid films. **T. Huh, S. Park, Y. Kwart**
- PMSE 342.** Di(1-benzothieno)[3,2-b:2',3'-d]pyrrole-based conjugated polymers for improving open-circuit voltage in organic photovoltaic cells. **I. Jung, J. Kim, S. Nam, C. Lee, D. Hwang, S. Yoon**
- PMSE 343.** Preparation of polycarbonate/poly(methyl methacrylate-co-phenyl methacrylate) blends and their miscibility and physical properties. **D. Seong, O. Kim, S. Hwang**
- PMSE 344.** Responsive plasmonic behavior of electrically tunable gold nanocube@ polyaniline core/shell nanostructures. **J. Jeon, P.A. Ledin, J. Geldmeier, J.F. Ponder, M.A. Mahmoud, M.A. El-Sayed, J.R. Reynolds, V.V. Tsukruk**
- PMSE 345.** Composite microparticles of halloysite clay nanotubes bound by calcium carbonate. **Y. Jin, R.B. Yendluri, B. Chen, J. Wang, Y.M. Lvov**
- PMSE 346.** Polyelectrolyte complex composite with graphitic benzoxazine for flexible capacitor electrodes. **P. Jitwatcharakul, T. Chaisuwat, S.T. Dumas**
- PMSE 347.** Controlled contamination as a disruptive effect on hydrogen-bonded liquid crystals: 1,6-Bis-(4-pyridyloxy) hexane. **E.A. John, E. Bornowski, M.D. Heltne, K.N. Wiegell**
- PMSE 348.** Biobased composites from thermoplastic polyurethane elastomer and cross-linked acrylated-epoxidized soybean oil. **L. Jong, Z. Liu**
- PMSE 349.** Temperature dependency of Pernambuco wood hardness. **D. Katahira, S. Tun**
- PMSE 350.** Flexible strings with patterns of hydrophobicity. **M. Keckley, A. Bosshardt, Y. Rubin, J. Zehner, C. Fukushima, M. Mulligan, B. Sanii**



- PMSE 351.** Ultrafast spectroscopic study of donor-acceptor light-harvesting organic conjugated polymers. **B. Keller**, A.M. McLean, B. Kim, T.G. Goodson, J. Kim
- PMSE 352.** Synthesis and characterization of poly(alkoxy selenophene): A novel conjugated polymer with narrow band gap. **D. Khambhati**, S. Selvaraju, T.L. Nelson
- PMSE 353.** Controlling morphology of polybenzoxazine-derived, nanoporous carbon monoliths through facile sol-gel synthesis. **R. Khwanrit**, U. Thubsuang, S. Wongkasemjit, T. Chaisuwan
- PMSE 354.** Investigation of non-phthalate plasticized poly(vinyl chloride) (PVC)/montmorillonite (MMT) nanocomposites. **S. Kim**, C. Park, S. Park
- PMSE 355.** Synthesis and characterization of cardanol-based epoxy/amine systems. **E. Kinaci**, E. Can, J.J. La Scala, G.R. Palmese
- PMSE 356.** Compose polycarbonate and multiwall carbon nanotube grafted with poly methyl methacrylate. **S. Kim**, K. Park, L. Choi, C. Kim
- PMSE 357.** Synthesis of CMC-graft-poly(itaconic acid) by inverse suspension polymerization as biodegradable superabsorbent polymers. **S. Ko**, R. Park, Y. Kwark
- PMSE 358.** Chitosan-functionalized, porous, antibacterial, and antifouling polyolefin membranes designed from PE/PEO blends. **P.S. Mural**, G. Madras, S. Bose
- PMSE 359.** Insulator materials for gas-electric motors. **M. Lebron-Colon**, J.B. Hurst, D. Santiago-Dejesus, C. Hung, J. Hamel
- PMSE 360.** Fabrication and characterization of pH-sensitive thiol-ene PEG-carboxymethylcellulose hydrogel for drug release and macrophage encapsulation. **S. Lee**, M. Kim, C. Ki
- PMSE 361.** Preparation and properties of flame-retardant copolyamide66. **Y. Li**, K. Liu, R. Xiao
- PMSE 362.** Clay, aerogel-supported palladium nanoparticles as catalysts. **Y. Lian**, D.A. Schiraldi
- PMSE 363.** Conformational studies of OPV oligomers: Torsional barriers to planarization in crystal structure. **J. Lin**, Y. Jin, S.A. Lopez, N. Druckerman, S.E. Wheeler, K.N. Houk
- PMSE 364.** Oligo poly(ethylene glycol) fumarate expandable cages for vertebral body replacement. **X. Liu**, A. Paulsen, H. Giambini, J. Guo, A.L. Miller II, P. Lin, M.J. Yaszemski, L. Lu
- PMSE 365.** Laponite® and Laponite®-PEO hydrogels with enhanced elasticity in phosphate-buffered saline. **X. Liu**, S. Bhatia
- PMSE 366.** Self-immolative nucleic acid-drug conjugate as a dual-action therapeutic agent. **X. Tan**, **J. Logan**, K. Zhang
- PMSE 367.** Pyridine-grafted diblock copolymer and transferrin core-shell nanoparticle for targeted drug delivery. **L. Lu**
- PMSE 368.** Polyurethane hydrogel foams as multifunctional wound contact-dressing materials. **J. Lundin**, G. Daniels, B. Streifel, S.L. Giles, J.H. Wynne
- PMSE 369.** Enhanced flame retardancy of latex coating doped with clay nanotubes. **A. Joshi**, M. Storms, V. Mazurenko, **Y.M. Lvov**
- PMSE 370.** Characterizing the nanoscale properties of cyclic block copolymers in thin films. **B. Lwoya**
- PMSE 371.** Facile synthesis of porous graphene/polyaniline composites for supercapacitors. **C. Ma**, Y. Feng, J. Shen, D. Zhang, Y. Yu, Y. Liu, Y. Min
- PMSE 372.** Backbone-dependent, self-assembly behaviors of phenylene-based, cationic conjugated polymers. **P. Manandhar**, T. Vokata, J. Moon
- PMSE 373.** *In situ* determination of polymer diffusion in nanocomposites. **H. Martin**, M.D. Dadmun, S. Satija, G. Yuan
- PMSE 374.** Development of benzoxazine-based composites for electrically conductive adhesives (ECAs) applications. **K. Matkaran**, U. Thubsuang, S. Wongkasemjit, T. Chaisuwan
- PMSE 375.** Injectable hyaluronic-based hydrogels as biomimic scaffold for cartilage tissue engineering. **P. Maturavongsadit**, J. Luckanagul, B. Xiangdong, Q. Wang
- PMSE 376.** Synthesis and photo-initiated cationic polymerization of kick-started oxetanes. **A. Meehan**, Z.T. Yang, C. Bae, C.Y. Ryu
- PMSE 377.** Preparation of hybrid materials based on mesoporous silica nanoparticles and polyacrylamide. **H.I. Melendez**, E.R. Ibarra-Vallejo, G. Castruita-de Leon, B.A. Puente-Urbina, S.P. Garcia
- PMSE 378.** Study on the effect of modification site on the trehalose polymers on protein stabilization. **M. Messina**, J. Ko, N. Boehnke, E. Pelegri-O'Day, J. Strouse, H.D. Maynard
- PMSE 379.** Oil spill remediation through halloysite Pickering emulsification with enhanced bacterial decomposition. **R. Minullina**, A. Panchal, Y.M. Lvov
- PMSE 380.** Study on a new additive to enhance the glass transition temperature of poly(methyl methacrylate). **A. Miyagawa**, S. Nobukawa, M. Yamaguchi
- PMSE 381.** Flameretardancy of carbon fiber-reinforced plastics composites. **Y. Mochizuki**, M.S. Aly-Hassan, M. Okoshi, H. Hamada
- PMSE 382.** Dynamics of strongly confined, grafted polymer chains. **J. Murphy**, W.R. Lenart, Y. Wei, M.J. Hore
- PMSE 383.** Physical property prediction of epoxy-based thermoset polymers using automated high-throughput atomistic simulations. **T.J. Mustard**, J. Sanders, J. Gavartin, D. Giesen, S. Kwak, T. Hughes, M. Halls
- PMSE 384.** Pursuit of a broad-spectrum antivenin for venomous serpents. **J. O'Brien**, K.J. Shea
- PMSE 385.** Functionalization of Jeffamine derivatives as gelling agents for oils. **M.C. Paderes**, J. HermosoLimon, C. James, A. Mai, M. Dolatkhani, E. Fratini, S. Fernandez-Prieto, J. Smets, W.M. De Borggraeve
- PMSE 386.** Synthesis and electronic applications of novel conjugated polymers based on thienylenevinylene and thiophene-phenylene-thiophene. **D. Patra**, H.S. Bazzi, L. Fang, M. Al-Hashimi
- PMSE 387.** Novel copolymers thermo and pH-sensitive of poly(N-vinylcaprolactam-co-4vinylpyridine) onto silicone rubber for drug delivery. **V.H. Pino**, C. Alvarez-Lorenzo, A. Concheiro, E. Bucio
- PMSE 388.** Efficient, greener synthesis and characterization of poly-L-ornithine polymers for drug-delivery applications. **E. Ponnusamy**
- PMSE 389.** Condition monitoring and characterization of deformations in EPDM seals used in nuclear power plants. **P. Pourmand**, M.S. Hedenqvist, U.W. Gedde
- PMSE 390.** Engineering ion-containing block copolymers as next-generation water purification membranes. **F. Romero**, H. Hong, M. Green
- PMSE 391.** Determination of tracer diffusion coefficients of soft nanoparticles in a polymer matrix using neutron reflectivity. **S. Rostom**, A. Imel, J.W. Mays, M.D. Dadmun
- PMSE 392.** One-step synthesis of highly porous silicon nitride and silicon carbide from polymer-crosslinked silica aerogels. **M.A. Saeed**, P.M. Rewatkar, S. Donthula, C. Sotiriou-Leventis, N. Leventis
- PMSE 393.** Multiscale, hierarchical, nanoporous aerogels based on  $\beta$ -cyclodextrin for CO<sub>2</sub> sequestration. **P.M. Rewatkar**, **M.A. Saeed**, S. Donthula, H. Majedi Far, N. Leventis, C. Sotiriou-Leventis
- PMSE 394.** Withdrawn.
- PMSE 395.** Novel, polymeric sulfothetins zwitterions. **C.F. Santa**, T. Enrick
- PMSE 396.** Beating the heat: Fast scanning melts silk, beta-sheet crystals. **C. Schick**, E. Zhuravlev, P. Cebe
- PMSE 397.** Optically controlled shape of soft nano-objects. **S. Schimka**, S.A. Santer, L. Hartmann, N. Mujic-Ninnemann, D. Bléger, M. Wehle, R. Lipowsky, M. Santer
- PMSE 398.** Uncompromised mechanical performance in melt-blended copolyester nanocomposites. **H. Jafferji**, O. Keane, J. Moeller, J. Song, E. Reynaud, **D.F. Schmidt**
- PMSE 399.** Radical scavenging efficiencies of silane-grafted carbon nanotubes and their effects on crosslinking reactions of vinyl ester/styrene resins. **Y. Shieh**, W. Wang, M. Hsieh
- PMSE 400.** Synthesis and controlled-release properties of thermoresponsive halloysite/poly(n-isopropylacrylamide) particles. **J. Shin**, S. Kim, H. Kim, D. Sohn
- PMSE 401.** Functionalized nanofiber scaffolds for nerve regeneration. **E. Silantyeva**, J. Carpenter, R. Willits, M. Becker
- PMSE 402.** Influence of rubber latex as an impact modifier in wood composites. **N. Siripornamart**
- PMSE 403.** Directed self-assemblies of diblock copolymers for ordered inorganic nanostructures. **S. Kim**, C. Lee, B. Sohn
- PMSE 404.** High oxygen and moisture barrier of oriented polypropylene film with multilayer thin-film nanocoatings. **Y. Song**, P. Tzeng, J.C. Grunlan
- PMSE 405.** Structure and properties of a high-temperature polymer containing boron and silicon. **N. Song**, L. Ni
- PMSE 406.** Silicon photonic microring resonators for chemical agent transport. **A. Stanton**, K. Miller, P.V. Braun, R. Bailey
- PMSE 407.** Nature-inspired solar cell materials. **H. Su**, H. Bronstein, T.J. Marks, H.S. Bazzi, D.G. Seapy, M. Al-Hashimi
- PMSE 408.** Designing benzoxazine-based carbon towards highly conductive graphene-like material. **W. Sukpomchaikul**, B. Kasapabutr, S. Wongkasemjit, T. Chaisuwan
- PMSE 409.** Permeation barrier properties of multilayered polymer films for flexible organic devices. **M. Sun**, S. Zhu, C. Zhang, M. Herbert, D.A. Schiraldi, E. Baer
- PMSE 410.** Electrically induced selectivity of functional poly-*p*-xylylenes deposition. **H. Sun**, C. Wu, H. Chen
- PMSE 411.** Polymer-nanoparticle composite thin-films for photon upconversion. **J. Tamayo**
- PMSE 412.** Controlled-surface radical graft polymerization of poly(ethylene terephthalate) fibers. **M. Tamizifar**, G. Sun
- PMSE 413.** Optimization of wasted tire ground rubber/wood flour toward the high mechanical properties in polypropylene composite. **R. Thongthanom**, H. Manuspiya
- PMSE 414.** Nano-engineered eggshell toughened poly(lactic acid)/aliphatic-aromatic copolyester flexible polymer blend. **V.K. Rangari**, **B.J. Tiimob**, S. Jeelani
- PMSE 415.** Triptycene-containing polymers as surfactant additives for organic photovoltaic devices. **T.N. Truong**, **A. Maurano**, **V. Bulovic**, **T.M. Swager**
- PMSE 416.** Preparation and characterization of poly(S/DVB)/HIPE filled with nanocrystalline cellulose from water hyacinth. **T. Tulaphol**, P. Sapsithong, M. Nithitanakul
- PMSE 417.** Thiol-acrylate materials for microfluidic applications. **M.P. Tullier**, B. Roberts, A.T. Melvin, J.A. Pojman
- PMSE 418.** Enzyme stabilization by adsorption on and into clay nanotubes. **J.R. Tully**, R.B. Yendliuri, Y.M. Lvov
- PMSE 419.** Gas barrier properties of phosphate glass/barrier polymer films. **R. Tyler**, S. Lee, J. Maia, D.A. Schiraldi
- PMSE 420.** Synthesis, characterization, and water uptake studies of model coating binders for corrosion protection applications. **J.H. Vergara**, J. Sadler, J.J. La Scala, G. Palmese
- PMSE 421.** Selective oxidation of alcohols using photoactive VO@-C<sub>60</sub>. **S. Verma**, N.R. Baig, M. Nadagouda, R.S. Varma
- PMSE 422.** Polymeric ladderane constructed in solid state. **Z. Wang**
- PMSE 423.** Biobased poly(furfuryl alcohol)/clay composite aerogel prepared by a freeze-drying method. **T. Wang**, D.A. Schiraldi
- PMSE 424.** Effect of swelling in the tailoring of homoporous membranes by soaking block copolymer/homopolymer blends in selective solvents. **Y. Wang**, M. Wei
- PMSE 425.** Significant enhancement of crystallization kinetics of poly(lactide) in its immiscible blends through an interfacial effect from comb-like, grafted side chains. **Y. Zhang**, **Z. Wang**
- PMSE 426.** Stereocomplex crystallite-assisted, shear-induced crystallization kinetics at a high temperature for asymmetric biodegradable PLLA/PDLA blends. **J. Bai**, **Z. Wang**
- PMSE 427.** pH-dependent hysteretic pore size of nanoporous block polymer membranes lined by polyacrylic acid brushes. **J.L. Weidman**, R. Mulvanna, Y. Zhang, B.W. Boudouris, W.A. Phillip
- PMSE 428.** Bacterial cellulose/chitosan-loaded turmeric extract for use as antibacterial wound dressing. **S. Wichai**, P. Ekabutr, P. Pavasant, P. Supaphol
- PMSE 429.** PVP-alginate-chitosan, hydrogel-pad-loaded turmeric extract for potential wound dressing. **S. Wongkittithavorn**, P. Ekabutr, P. Pavasant, P. Supaphol
- PMSE 430.** Enzyme-directed assembly of nanoparticles with biodegradable and biocompatible polymers. **D. Wright**, J.P. Patterson, A.S. Carlini, N.C. Gianneschi
- PMSE 431.** Application of pseudo surface reaction nonequilibrium solution-diffusion model in pervaporation mass transfer analysis. **Y. Xia**, T. Wang, X. Zhan, L. Yu, **J. Li**
- PMSE 432.** Hairy nanoparticles prepared via anionic polymerization. **W. Xiong**, X. Wang
- PMSE 433.** Short, electrospun carbon nanofiber-reinforced polyimide composites and their dielectric, mechanical, and thermal properties. **W. Xu**, X. Wang, T. Yang, C. Zhang, Y. Ding, H. Hou
- PMSE 434.** Hybrid double-network hydrogels with strong mechanical and antifouling properties. **H. Chen**, **F. Yang**, Q. Chen, R. Hu, M. Zhang, J. Ma, B. Ren, B. Jiang, J. Zheng

PMSE 435. Withdrawn.

PMSE 436. Controlled release of camptothecin from halloysite nanotubes coated with block-copolymers of polylysine with polyethylene glycol. R.B. Yendluri, R. Minullina, G. Parekh, U. Kansakar, Y.M. Lvov, M. DeCoster

PMSE 437. FTIR spectroscopic analysis of the crystallization of precision halogen-substituted polyethylenes. X. Zhang, L. Santonja, K. Wagener, E. Boz, R.G. Alamo

PMSE 438. Desymmetrized vertex design for the synthesis of covalent organic frameworks (COFs) with heterogeneous pore structure. Y. Zhu, W. Zhang

PMSE 439. Experimental test of Tammann's nuclei development approach in crystallization of macromolecules. E. Zhuravlev, R. Androsch, J.W. Schmelzer, A.S. Abyzov, V. Fokin, C. Schick

PMSE 440. Biodegradable multienzyme: Poly(acrylic acid) nanoconjugates for applications in catalysis under non-physiological conditions. O.V. Zore, C.V. Kumar, R. Kasi

PMSE 441. Control of the unique nanostructures formed by emulsification-induced assembly of semicrystalline polymer amphiphiles. S. Jin, I. Kim, J. Ryu, E. Lee

PMSE 442. Molecular bilayer rectifiers made by diazonium reduction: Fabrication and characteristics. A. Bayat, R.L. McCreery

PMSE 443. First-principles study of carbyne structural stability. C. Holmes, K. Kwon, S. Jang, K. Kim

#### Directed Polymer Assembly.

PMSE 444. Synthesis and self-assembly properties of alternated multi-block copolymers for third-generation organic photovoltaic. A. Gasperini, K.A. Svula

PMSE 445. Polyolefin-*b*-polymethacrylate copolymers: Synthesis, characterization, and application as viscosity modifiers. Y. Yang, A.H. Tsou, M.N. Webster, D.J. Crowther, J.M. Soulagés

PMSE 446. Efficiently controllable hybrid micelle of poly(3-adeninehexylthiophene)/[6,6]-phenyl-C61-butyric acid methyl ester for a flexible metal-insulator-semiconductor device. Y. Lin, R. Singh, F. Ko, C. Cheng

PMSE 447. Investigating the effect of water as a co-solvent in an alcoholic RAFT PISA formulation. E. Jones, M. Semsarilar, P. Wyman, M. Boerakker, S.P. Armes

PMSE 448. Multi-compartmental polymeric microcapsules with dual-carrier and programmable release capabilities. W. Xu, V.V. Tsukruk

#### Clay/Polymer Composites: Nanoclays & Other Natural Particles.

PMSE 449. Sandwich organization induced by large inorganic  $K_2Nb_2O_{17}$  nanosheets of non-ionic surfactant liquid crystalline phases. R. Guégan, N. Miyamoto

PMSE 450. Sb intercalated, layered double hydroxides-poly(vinyl chloride) nanocomposites: Preparation, characterization, and thermal stability. S. Liu, X. Chen, K. Yan, Y. Zhang, Y. Ye, P. Zhang

PMSE 451. Probeless exfoliation of TMDs: A scalable approach. A. Jawaid, R. Vaia

PMSE 452. Effect of unsaturated fatty acids as oxygen scavengers in polyethylene terephthalate (PET). M.A. Miranda, M. Coleman, S.A. Jabarin

PMSE 453. Cold and melt crystallization studies of poly(trimethylene terephthalate) nanocomposite. N. Vasanthan, L. Smith, A. Krishnama

PMSE 454. Flameretardancy study of PVA use for cardboard beds. Y. Mochizuki, Y. Mizutani, M. Okoshi, H. Hamada

#### Hybrid Polymers And Nanocomposites.

PMSE 455. Promoting selective CNT-polymer interaction in hybrid polymer/CNT buckypapers (hPBPs) through phase separation mechanisms. H. Li, M. Minus

#### Anionic Polymerisation: Still Living After 60 Years

Sponsored by POLY, Cosponsored by PMSE and RUBB

#### Applications of Polymer Surfaces & Interfaces

Sponsored by POLY, Cosponsored by COLL and PMSE

#### Sustainable Polymers, Processes & Applications

Sponsored by POLY, Cosponsored by PMSE

## WEDNESDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

#### Computation & Cheminformatics in Polymers Research

##### Multiscale Methods

Financially supported by ExxonMobil Chemical, ExxonMobil Research & Engineering

J. D. Moore, G. Rodriguez, S. Tallury, *Organizers*  
G. Carri, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 PMSE 456. High-throughput characterization of polymer-polymer interactions out-of-equilibrium. A. Alexander-Katz

9:05 PMSE 457. Modeling structure and rheology of waterborne paints thickened by hydrophobically-ethoxylated urethane (HEUR) rheology modifiers: From molecular to coarse-grained description. F. Yuan, V. Ginzburg, A. van Dyk, T. Chatterjee, A.I. Nakatani, S. Yu, S. Wang, R.G. Larson

9:35 PMSE 458. Guidance for the design of pervaporation membranes from molecular simulations and experiments. F. Khabaz, S. Mani, R. Godbole, R. Hedden, R. Khare

10:05 Intermission.

10:20 PMSE 459. Functional soft-matter design through guided molecular ordering. B. Sumpster, R. Kumar, I. Ivanov

10:50 PMSE 460. Synergistic efforts of computational modeling and experimentation towards material design. T. Chantawansri, C.B. Rinderspacher, T.W. Sirk, J. Andzelm, J. Lenhart

11:20 PMSE 461. Development of an integrated, computational data environment to support multiscale modeling of soft materials for the materials genome initiative. F.R. Phelan, T.W. Rosch, C. Jeong, B. Moroz, S.S. Youssef

### Section B

Marriott Marquis San Diego Marina  
Presidio 2

#### General Papers/New Concepts in Polymeric Materials

##### Polymer Nanostructures

C. L. Soles, *Organizer*

D. Wang, *Presiding*

8:00 PMSE 462. Nucleation and mechanical enhancement in polyethylene-graphene nanocomposites. A.J. Bourque, R. Locker, M. Vadlamudi, A.H. Tsou

8:20 PMSE 463. Directionally controlled actuation of soft robotic lifters, accordions, and valves using chained iron micro-particles. M.M. Schmauch, S.R. Mishra, O.D. Velev, J.B. Tracy

8:40 PMSE 464. Poly(alkyl methacrylates)-grafted silica nanoparticles in linear low-density polyethylene nanocomposites. M.M. Khani, E. Mumpower, D. Woo, B.C. Benicewicz

9:00 PMSE 465. Mechanism and application of selective hydrogen-deuterium exchange reaction for saturated polyolefins. Y. Zeng, C.R. Lopez-Barron, S. Kang, A. Eberle, F.S. Bates, T.P. Lodge

9:20 PMSE 466. Combinatorial libraries of alloy nanoparticles individually synthesized through scanning probe spray gradients. J.L. Hedrick, K. Brown, P. Chen, M.C. Tapia, L. Moreau, C.A. Mirkin

9:40 Intermission.

10:00 PMSE 467. Robust strategy for crafting hollow metal telluride nanocrystals via precise molecular design. Y. He, X. Pang, Z. Lin

10:20 PMSE 468. Efficient, colorimetric, wide-range temperature sensor based on fluorescent, block-copolymer, functionalized graphene oxide. J. Lee, H. Yang, C. Park, H. Cho, B. Kim

10:40 PMSE 469. Helically wrapped poly(methyl methacrylate) on carbon nanotubes and its application for energy storage and mechanical properties. A. Bakhtiyari Davjani, H.C. Liu, H. Chang, S. Kumar

11:00 PMSE 470. Synthetic control of the structure of nanogel star polymers: Insights from simulation and experiment. A. Carr, W.C. Swope, V.A. Pionova, J.E. Rice, R.D. Miller

11:20 PMSE 471. Magnetic resonance imaging using responsive, targeted, shaped polymeric nanostructures. C.L. LeGuyader, M.E. Hahn, L. Randolph, N.C. Gianneschi

11:40 PMSE 472. Surface immobilization of thermo-responsive polymers by simply entrapping them in an aminopropyl-triethoxysilane network. A. Alghunaim, B.M. Zhang Newby

### Section C

Marriott Marquis San Diego Marina  
Rancho Santa Fe 1 & 2

#### Hybrid Polymers & Nanocomposites

##### Nanocomposites

Financially supported by Chinese Chemical Society (CCS)-Polymer Division (PD)

Z. Li, Q. Lin, D. Wang, *Organizers*

M. Shofner, *Presiding*

8:00 PMSE 473. Rheological behavior and water-based shear processing of cellulose nanocrystal/poly(vinyl alcohol) composites. M. Shofner, C. Meree, J.C. Meredith, G.T. Schueneman

8:20 PMSE 474. Tough, low flammability polymer aerogels incorporating inorganic nanoparticles. H. Sun, D.A. Schiraldi

8:40 PMSE 475. Tunable, thermal, and mechanical properties of polycarbonate composites for transient materials. K. Camera, C.K. Ober

9:00 PMSE 476. Enhanced ethylene/ethane separation and mitigated plasticization in polymer membranes incorporating metal-organic framework nanocrystals. J. Bachman, Z.P. Smith, T. Li, T. Xu, J.R. Long

9:20 PMSE 477. Layered polymer-zeolitic imidazolate framework composites fabricated using sacrificial, metal-oxide, nanocrystal precursors. S. Meckler, C. Li, W. Queen, T.E. Williams, J.R. Long, R. Buonsanti, D.J. Milliron, B. Helms

9:40 Intermission.

10:00 PMSE 478. Quantitatively comparison of binding affinity of poly(dopamine-co-N-isopropylacrylamide) and poly(nitrodopamine-co-N-isopropylacrylamide) to  $Fe_3O_4$  nanoparticles. S. Qiu, S. Jin, N. Yang

10:20 PMSE 479. Molecular dynamics simulations of interfacial interactions between elastomers and polyimides in flexible and stretchable electronic devices. R. Bhowmik, J. Deneault, M.J. Dalton, R.J. Berry, M.F. Durstock, B.J. Leever

10:40 PMSE 480. Corrosion protection of aluminum alloy via graphene-polymer nanocomposite coatings. S. De, J. Lutkenhaus

11:00 PMSE 481. Directed self-assembly of amphiphilic polymer-grafted silica nanoparticles. Y. Zheng, B.C. Benicewicz

### Section D

Marriott Marquis San Diego Marina  
Presidio 1

#### General Papers/New Concepts in Polymeric Materials

##### Crystallization & Polymer Fundamentals

C. L. Soles, *Organizer*

C. R. Snyder, *Presiding*

8:00 PMSE 482. Role of co-units in polymer crystallization and melting: New insights from fast scanning calorimetry on poly(ethylene-co-octene). C. Schick, E. Zhuravlev, M. Vadlamudi, A. Lestiger

8:20 PMSE 483. Crystalline supramolecular interaction between polyethylene and side chain crystalline polymer. S. Yao, R. Nakano, H. Sekiguchi, F. Yamasaki, H. Obuchi

8:40 PMSE 484. From crystal structure of nucleating agent to molecular mechanics computation of epitaxial growth of  $\beta$ -iPP. D. Wang

9:00 PMSE 485. Not all long chain branching in polyethylene is created equal. Y. Yu

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at:  
[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**9:20 PMSE 486.** Crystallization of polyethylene at large undercooling: Isothermal and non-isothermal study. E. Zhuravlev, M. Vadlamudi, C. Schick

**9:40** Intermission.

**10:00 PMSE 487.** Long-term stability of UHMM polyethylene fibers. A. Forster, A. Forster, J. Chin, N. Pautler, M. Riley, D. Jenket, Z. Tsinas, K. Kang, M. Al-Sheikhly

**10:20 PMSE 488.** On the conformational changes of isolated, short poly(ethylene) chains in water. A. Noorjahan, P.Y. Choi

**10:40 PMSE 489.** Flame retardation of polyethylene with low toxicity, bio-based additives. D.A. Schiraldi, T. Deans

**11:00 PMSE 490.** Property prediction of polymer systems through connectivity altering Monte Carlo moves: A comparison of Monte Carlo and molecular dynamics simulations. A. Bick, L. Subramanian

**11:20 PMSE 491.** Degradation mechanisms in unidirectional UHMPE soft ballistic inserts. Z. Tsinas, D. Jenket, A. Forster, M. Al-Sheikhly

**11:40 PMSE 492.** Performance evaluation of thermal aging methods for polymeric systems. Y. Balogun

## Section E

Marriott Marquis San Diego Marina  
Point Loma

### Polymer-Related Energy Conversion & Storage

Z. Lin, S. C. Rasmussen, M. C. Stefan, *Organizers*

K. J. Noonan, *Presiding*

**8:00 PMSE 493.** New electroactive polymers and nanomaterials. T.M. Swager

**8:30 PMSE 494.** Block copolymer-based composition and morphology control in nanostructured hybrids for energy conversion and storage. U.B. Wiesner

**9:00 PMSE 495.** Charge-transfer mechanism on a polymer thin-films electrode from polythiophenes bearing pendant nitroxide radicals. F. Li, Y. Zhang, S. Kwon, J. Lutkenhaus

**9:20 PMSE 496.** Conductive and thermoelectric materials based on PEDOT. J. Simonato, A. Carella, N. Massonnet, M. Gueye, E. Yvenou, R. Demadrille, A. De Geyer, J. Faure-Vincent

**9:40 PMSE 497.** Supramolecular polymers as high-performance binders for silicon anodes in lithium-ion batteries. A. Coskun

**10:00** Intermission.

**10:10 PMSE 498.** Cobaltocenium-containing polymer membranes for alkaline anion-exchange membrane fuel cells. H. Yuan, T. Tsai, E.B. Coughlin

**10:30 PMSE 499.** High-surface area carbon nanofiber supercapacitor electrodes derived from an *in-situ* porogen-containing terpolymer: P(AN-VIM-IA). J.P. Ferraris, N.C. Abeykoon, S. Mahmood

**11:00 PMSE 500.** Effects of crosslinking in a supramolecular binder on cycling stability of silicon microparticle anodes. J. Lopez, Z. Chen, C. Wang, S. Andrews, Y. Cui, Z. Bao

**11:20 PMSE 501.** Flexible, composite polymer/inorganic membranes for battery applications. R.D. Miller, K. Nguyen, S. Kitajima, H. Kim, E. Jung, L.E. Thompson, J.C. Scott, K. Virani, D.S. Bethune, W.W. Wilcke, M.L. Reich, M. Schneider, M. Kunze, W. Schmidbauer, N.B. Aetukuri

**11:40 PMSE 502.** Multi-cation side chain anion-exchange membranes. L. Zhu, J. Pan, M. Hickner

## Section F

Marriott Marquis San Diego Marina  
Santa Rosa

### Polyethylene

#### Fracture & Mechanical Properties

*Cosponsored by WCC  
Financially supported by ExxonMobil  
Chemical Company*

G. E. Alliger, D. Thurman, *Organizers*  
A. Winesett, *Organizer, Presiding*

**8:00 PMSE 503.** Melt fracture and wall slip of polyethylenes: Molecular effects. S. Hatzikiriakos

**8:30 PMSE 504.** Understanding blown film structure-property relationships for metallocene linear low-density polyethylenes. A.I. Norman, S. Perkins, A. Winesett, G. Gururajan

**9:00 PMSE 505.** Probing molecular mechanisms underlying failure in semicrystalline polymers. C.R. Snyder

**9:30 PMSE 506.** Relationships between polyethylene architecture and mechanical properties. A. Kannan, D.G. Bucknall, A. Eberle, T. Shaffer, A.I. Norman, S. Weigand

**10:00** Intermission.

**10:15 PMSE 507.** Assessing the molecular weight and topology effects on post-yield tensile tests for slow crack-growth resistance in polyethylene resins. P. DesLauriers, M.J. Lamborn, C. Dominguez, R.A. Garcia

**10:45 PMSE 508.** Assessment of strength, toughness, and lifetime of PE pressure pipes based on testing of the material thermomechanical properties. A. Chudnovsky

**11:15 PMSE 509.** Thermo-mechanical properties of short-chain branched semicrystalline polyethylene. V. Kumar, R. Locker, G.C. Rutledge

#### Applications of Polymer Surfaces & Interfaces

#### New Techniques & Characterization

*Sponsored by POLY, Cosponsored  
by COLL and PMSE*

#### Anionic Polymerisation: Still Living After 60 Years

*Sponsored by POLY, Cosponsored  
by PMSE and RUBB*

## WEDNESDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

#### Computation & Cheminformatics in Polymers Research

#### Cheminformatics & Data Driven Methods

*Financially supported by ExxonMobil Chemical,  
ExxonMobil Research & Engineering*

G. Carri, J. D. Moore, S. Tallury, *Organizers*

G. Rodriguez, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 PMSE 510.** Accelerating the discovery of novel polymers with computation and information. J.W. Pitera, A.C. Carr, G.O. Jones, W.C. Swope, J.E. Rice

**1:35 PMSE 511.** Rational computation-guided design of polymer dielectrics. R. Ramprasad

**2:05 PMSE 512.** Computational and data-driven discovery of novel, high-refractive index polymers. M. Faiz Atzal, S. Ganesh, J. Hachmann

**2:35** Intermission.

**2:50 PMSE 513.** Materials genome initiative: NIST, data, and open science. J. Warren

**3:20 PMSE 514.** Designing polymeric superplasticizers for cement using machine learning. N. Washburn, C. Gupta, M. Sverdløve, B. Graham, B. Decost, E. Holm

**3:50 PMSE 515.** Novel nanoporous materials: *In silico* design. C.M. Colina

**4:20 PMSE 516.** Predictive methods for dense polymer networks: Combating bias with bio-based structures. A.J. Guenther, B.G. Harvey, M.D. Ford, J. Reams, J.M. Mabry

### Section B

Marriott Marquis San Diego Marina  
Presidio 2

#### General Papers/New Concepts in Polymeric Materials

#### Electronic & Semiconducting Polymers

C. L. Soles, *Organizer*

L. J. Richter, *Presiding*

**1:00 PMSE 517.** Entrapment of metal complexes into PEDOT via vapor-phase complexation. S. Acharya, L. Spiccia, C.A. Ohlin, B. Winther-Jensen

**1:20 PMSE 518.** Towards intrinsically stretchable and healable semiconducting polymers. S. Rondeau-Gagne, J. Oh, Y. Chiu, Z. Bao

**1:40 PMSE 519.** Isolation of pristine electronics-grade, semiconducting carbon nanotubes by switching the rigidity of the wrapping polymer backbone. Y. Joo, G. Brady, M. Shea, M.B. Oviedo, C. Kanimozhi, S. Schmitt, B. Wong, M. Arnold, P. Gopalan

**2:00 PMSE 520.** Patternable conjugated polymers with latent hydrogen-bonding on the main chain. Y. Zhu

**2:20 PMSE 521.** Additive-free, high-performance, all-polymer solar cells based on naphthalene diimide-based polymer acceptor with high-electron mobility. J. Choi, K. Kim, H. Yu, C. Lee, H. Kang, I. Song, Y. Kim, J. Oh, B. Kim

**2:40** Intermission.

**3:00 PMSE 522.** Impact of polystyrene oligomer side-chain on n-type polymer semiconducting properties for organic field-effect transistor. T. Kurosawa, Y. Chiu, Y. Zhou, X. Gu, Z. Bao

**3:20 PMSE 523.** Synthesis of polybenzoquinolines as graphene nanoribbon precursors. D.J. Dibble, Y.S. Park, A. Mazaheripour, M.J. Umerani, A.A. Gorodetsky

**3:40 PMSE 524.** Towards controlled synthesis of conjugated polymers with functional side chains: An investigation of catalyst-transfer polycondensation for n-type materials. Y. Qiu, J.C. Worch, T. Kowalewski, K.J. Noonan

**4:00 PMSE 525.** Protein-based protonic transistors. D.D. Ordinario, L. Phan, T. Nguyen, J. Jocson, A.A. Gorodetsky

**4:20 PMSE 526.** Chemical design of intrinsically stretchable and flexible organic polymer semiconductors. F. Lissel, Z. Bao

### Section C

Marriott Marquis San Diego Marina  
Rancho Santa Fe 1 & 2

#### Hybrid Polymers & Nanocomposites

#### Electronics & Clean Energy Applications

*Financially supported by Chinese Chemical  
Society (CCS)-Polymer Division (PD)*

Z. Li, Q. Lin, *Organizers*

D. Wang, *Organizer, Presiding*

**1:00 PMSE 527.** Self-healing polymer gate insulator as high-capacitance gate dielectrics. Y. Kim, J. Ko, Y. Kim

**1:20 PMSE 528.** Aramid nanofibers/graphene layer-by-layer electrodes for structural energy and power. S. Kwon, J. Lutkenhaus

**1:40 PMSE 529.** Conjugated polymer-CdSe quantum dot core/shell composite nanofibers for organic solar cells. Y. Qin

**2:00 PMSE 530.** Withdrawn.

**2:20 PMSE 531.** Nanogapped plasmonic nanoparticles: Towards tailored nanogap engineering. J. Zhou, H. Duan

**2:40** Intermission.

**3:00 PMSE 532.** Porous materials consisting of metal ion and polyelectrolyte complex for gas sensor application. Y. Tsuge, S. Shiratori

**3:20 PMSE 533.** Dramatically increased photoluminescence quantum yields in polyfluorene-di-ureasil organic-inorganic hybrid composites. R.C. Evans, N. Willis-Fox, A. Marques, J. Art, U. Scherf, L. Carlos, H. Burrows

**3:40 PMSE 534.** Preparation and characterization of nanocomposite, polymer dielectric networks containing covalently linked fullerenes. A.D. Windham, H.M. Ahmed, M.K. Hassan, K.A. Mauritz, J. Buchanan

**4:00 PMSE 535.** Withdrawn.

### Section D

Marriott Marquis San Diego Marina  
Presidio 1

#### General Papers/New Concepts in Polymeric Materials

#### Advances in Polymer Synthesis

C. L. Soles, *Organizer*

M. A. Quadir, *Presiding*

**1:00 PMSE 536.** New models to explain the stereoselectivity of propene polymerization by group 4 metal catalysts. G. Talarico, C. De Rosa, R. Di Girolamo

**1:20 PMSE 537.** Surface crowdedness effect on heterogeneous mechanochemistry. J. Li, B. Hu, K. Yang, B. Zhao, J.S. Moore

**1:40 PMSE 538.** High-energy explosives with novel binder optimizations guided by JMP. E. Cooke, B. Wingerd, E. Beckel, P. Anderson, A. Paraskos

**2:00 PMSE 539.** Mechanochemistry for soft, active materials and devices. G.R. Gossweiler, T. Kouznetsova, Q. Wang, X. Zhao, S. Craig

**2:20 PMSE 540.** Effects of the organometallic coupling agent on the adhesion of the ground rubber particle/VE composite. B. Fathi, S. Elkoun, M. Robert

**2:40** Intermission.

**3:00 PMSE 541.** Nanoporous polyurea from triisocyanates reacting with mineral acids. M.A. Saeed, S. Donthula, H. Majedi Far, P.M. Rewatkar, C. Sotiriou-Leventis, N. Leventis

**3:20 PMSE 542.** Cure-on-demand polymerizations using the urease-catalyzed hydrolysis of urea to trigger thiol-acrylate polymerization. **J.A. Pojman, E. Jee, A. Taylor, J. Nelson**

**3:40 PMSE 543.** 4D nanomanufacturing using flow through photochemical polymerizations. **A.B. Braunschweig, X. Liu, Y. Zheng**

**4:00 PMSE 544.** Low temperature imidization of poly(amic ester) by organic and inorganic salts. **A. Dick, E. Maines, J. Schwartz, W.K. Bell, P.A. Kohl, C.G. Willson**

**4:20 PMSE 545.** Excellent performance and uses of HNBR-specialty rubber prepared effectively by Zhan catalysts. **Z.J. Zhan, W. Ren**

**4:40 PMSE 546.** Determining the material development trajectory during photopolymerization. **S. Sarkar, P.J. Baker, E. Chan, S. Lin-Gibson, M.Y. Chiang**

## Section E

Marriott Marquis San Diego Marina  
Point Loma

### Polymer-Related Energy Conversion & Storage

Z. Lin, S. C. Rasmussen, M. C. Stefan, *Organizers*

N. Washburn, *Presiding*

**1:00 PMSE 547.** Design and synthesis of pi-conjugated materials for electrochemical energy storage. **D.S. Seferos**

**1:30 PMSE 548.** F-substituted polymers for high-efficiency, bulk-heterojunction solar cells. **P. Beaujuge**

**1:50 PMSE 549.** Tuning the degree of intermixing in sequentially-processed polymer/fullerene photovoltaics: The role of swelling by solvent additives. **M.T. Fontana, J.C. Aguirre, S.A. Hawks, G. Zhang, P. Yee, H. Kang, R. Huber, L. Schelas, Z. Fan, S.H. Tolbert, B.J. Schwartz**

**2:10 PMSE 550.** Bottom-up approaches for precisely nanostructuring hybrid organic/inorganic multi-component composites for organic photovoltaics. **Y. Qin**

**2:30 PMSE 551.** Water-absorbable, polymer-coated phase change material for thermal energy storage. **T. Do, U. Choi**

**2:50** Intermission.

**3:05 PMSE 552.** Nanoscale polymers as solid-state electrolytes and dielectrics in next-generation 3D architectures for batteries and capacitors. **J.W. Long, J.M. Wallace, M.B. Sassin, D.R. Rolison**

**3:25 PMSE 553.** On the nature of polymer/fullerene intermolecular interactions and their impact on the performance of organic solar cells. **J.E. Bredas**

**3:55 PMSE 554.** Fabricating of high-performance functional graphene fiber with diamine covalent for micro-capacitive energy storage. **T. Fan, C. Zhao, Z. Xiao, R. Gao, D. Zhang, X. Liu, Y. Liu, H. Meng, Y. Min**

**4:15 PMSE 555.** Synthesis and characterization of single-ion conducting polymers for lithium-ion batteries. **M.A. Morris, T.H. Epps**

**4:35 PMSE 556.** Improved dielectric properties of polystyrene-block-poly(methylmethacrylate copolymer-poly(vinylidene fluoride) blend films: The role of ordered morphology of block copolymer. **A.V. Bunha, C.A. Grabowski, M. Hsiao, M.J. Dalton, M.F. Durstock**

## Section F

Marriott Marquis San Diego Marina  
Santa Rosa

### Polyethylene

#### Characterization & Reaction Engineering

*Cosponsored by WCC  
Financially supported by ExxonMobil  
Chemical Company*

D. Thurman, A. Winesett, *Organizers*

G. E. Alliger, *Organizer, Presiding*

**1:30 PMSE 557.** Recent advances and challenges in characterizing the microstructure of polyolefins. **R. Cong, W. deGroot**

**2:00 PMSE 558.** Bimodal comb block polyolefins by serial reactors. **A.H. Tsou, C.R. Lopez-Barron, P. Jiang, D.J. Crowther**

**2:30 PMSE 559.** Advanced scanning probe microscopy (SPM) methods to probe structure and rheological properties of polyethylene. **D. Yablon**

**3:00** Intermission.

**3:15 PMSE 560.** Observing the deformation of polyethylene lamellae by AFM. **N. Mullin, M.P. Weir, J.K. Hobbs, R.C. Savage**

**3:45 PMSE 561.** Polyethylene: Predictions from reactor to rheology. **D. Read, C. Das**

**4:15 PMSE 562.** Impact of polyolefin characterization techniques on polyolefin reaction engineering. **J.B. Soares**

#### Applications of Polymer Surfaces & Interfaces

##### Anti-fouling

*Sponsored by POLY, Cosponsored by COLL and PMSE*

##### Anionic Polymerisation: Still Living After 60 Years

*Sponsored by POLY, Cosponsored by PMSE and RUBB*

## WEDNESDAY EVENING

### POLY/PMSE Plenary Lecture & Awards Reception

*Sponsored by POLY, Cosponsored by PMSE*

## THURSDAY MORNING

### Section A

Marriott Marquis San Diego Marina  
Rancho Santa Fe 3

#### Computation & Cheminformatics in Polymers Research

##### Theory & Simulation

*Financially supported by ExxonMobil Chemical, ExxonMobil Research & Engineering*

J. D. Moore, G. Rodriguez, S. Tallury, *Organizers*

G. Carri, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 PMSE 563.** Polymer rheology predictions from first-principles. **J. Schieber**

**8:35 PMSE 564.** Evolution of polymer morphology during annealing: Insight gained from modeling. **J. Weinhold**

**9:05 PMSE 565.** Structural evolution during directed assembly of polymeric materials. **J.J. De Pablo**

**9:35** Intermission.

**9:50 PMSE 566.** Systematic and simulation-free coarse graining of multi-component polymeric systems. **D. Yang, Q. Wang**

**10:20 PMSE 567.** Insight into phase behavior, microstructure, and interfacial behavior of complex fluids. **L. Wang, A. Haghmoradi, A. Bansal, K.R. Cox, W.G. Chapman**

**10:50 PMSE 568.** Progress in fully fluctuating field theoretic simulations of polymers. **K.T. Delaney, G.H. Fredrickson**

### Section B

Marriott Marquis San Diego Marina  
Presidio 2

#### General Papers/New Concepts in Polymeric Materials

##### Advances in Polymer Synthesis

C. L. Soles, *Organizer*

S. V. Orski, *Presiding*

**8:00 PMSE 569.** Design and mechanics of double-network elastomers. **T. Limpanichpakdee, J. Rieger, L. Bouteiller, C. Creton**

**8:20 PMSE 570.** Cross-linking polyethylene by thermal rearrangement. **N. Mitchell, B.K. Long**

**8:40 PMSE 571.** 3D-printed macroporous materials. **J. Ferrer, A. Bismarck, A. Menner**

**9:00 PMSE 572.** Synthesis of cyanate-ester functional benzoxazine and its polymer properties. **S. Ohashi, H. Ishida**

**9:20 PMSE 573.** Buried volume analysis for propene polymerization catalysis promoted by group 4 metals: A tool for molecular mass prediction. **L. Falivene, L. Cavallo, G. Talarico**

**9:40** Intermission.

**10:00 PMSE 574.** Using simulation to explore nanoscale network heterogeneity in gel-forming polymer systems. **A. Willard**

**10:20 PMSE 575.** New materials using tetrazines as monomers, or polymer modifiers and blowing agents. **D.A. Loy, R.E. Bagge, D. Boday**

**10:40 PMSE 576.** Base-catalyzed hydrolysis of industrially relevant copolyester model compounds. **E. Yildirim, C. Cleven, H. Cheema, A. Detwiler, A. El Shafei, M.A. Pasquinielli**

**11:00 PMSE 577.** Polymer photodegradation: Autocatalytic under sunlight. **S. Karumuri, A. Kalkan**

**11:20 PMSE 578.** Furan-based renewable amine hardeners for thermosetting epoxy. **S.K. Yadav, J.J. La Scala, J. Sadler, G. Palmese**

### Section C

Marriott Marquis San Diego Marina  
Rancho Santa Fe 1 & 2

#### Hybrid Polymers & Nanocomposites Biomedical Applications

*Financially supported by Chinese Chemical Society (CCS)-Polymer Division (PD)*

Q. Lin, D. Wang, *Organizers*

Z. Li, *Organizer, Presiding*

**8:00 PMSE 579.** Design and production of functional thin-film backpacks for cell-based therapies. **R. Polak, R.M. Lim, R.E. Cohen, M.F. Rubner**

**8:20 PMSE 580.** Optimizing magnetic heating and elucidating local nanoparticle temperature profiles for application in an agar gel-based tumor model. **R. Shah, A. Dombrowsky, A. Paulson, M. Johnson, D.E. Nikles, C.S. Brazel**

**8:40 PMSE 581.** Modulating properties of chemically crosslinked PEG hydrogels via physical entrapment of silk fibroin. **J. Bragg, H. Kweon, Y. Jo, K. Lee, C. Lin**

**9:00 PMSE 582.** Potential of injectable and thermosensitive chitosan-carbon nanotube hydrogels for sustained delivery of methotrexate. **L. Saeednia, L. Yao, R. Asmatulu**

**9:20 PMSE 583.** Robust and tunable inorganic nanostructures from PEO-b-PHA structure-directing agent. **H.N. Lokupitiya, M. Stefiik**

**9:40** Intermission.

**10:00 PMSE 584.** Crystallization kinetics and morphology development in polymer: Silicon and carbon nanotube blends. **E.L. Heeley, D. Hughes, Y. Elaziz, E. Crabb, P.G. Taylor, T. McNally**

**10:20 PMSE 585.** Silk fibroin secondary structure on various graphene oxide substrates. **A.M. Grant, K. Hu, S. Young, Y.G. Yingling, V.V. Tsukruk**

**10:40 PMSE 586.** Phase behavior of polymer-grafted nanoparticles. **K. Mongcopa, R. Krishnamoorti**

**11:00 PMSE 587.** Improved carbon nanotube yarns through crosslinking. **X. Lu, N. Hiremth, M.C. Evora, N. Kang, K. Hong, G.S. Bhat, J.W. Mays**

### Section D

Marriott Marquis San Diego Marina  
Presidio 1

#### General Papers/New Concepts in Polymeric Materials

##### Polymer Surfaces & Interfaces

C. L. Soles, *Organizer*

J. L. Hedrick, *Presiding*

**8:30 PMSE 588.** Utilizing heterogeneous network formation to tune surface roughness: A method to control coating wettability. **C. Szczepanski, T. Darmanin, F. Guittard**

**8:50 PMSE 589.** Dip-pen nanodisplacement lithography: A versatile tool for constructing patterned 3D polymer surfaces. **Z. Zheng**

**9:10 PMSE 590.** Nonsolvent-induced phase separation synthesis of biomimetic PVDF microspheres for superhydrophobic coatings. **L. Berryman, L. Brockway, H. Taylor**

**9:30** Intermission.

**9:30 PMSE 591.** Photoinduced adhesion of polymer films to glass surfaces. **S. Mostafavi, F. Tong, C.J. Bardeen**

**9:50 PMSE 592.** UV-curable materials design using predictive surface-free energy analyses. **A. Mahmood, E.B. Henry, T.B. Cavitt**

**10:10 PMSE 593.** Utilizing chloroform post-treatment to improve the adhesion of Au thin films onto PMMA. **K. Krist, H. Hu, B.H. Augustine, W.C. Hughes**

**10:30 PMSE 594.** Development and assessment of surfactant force fields for studies of micellization with dissipative particle dynamics. **W.C. Swope, M. Johnston, R. Anderson, D. Bray, P. Warren, M. Noro**

## Section E

Marriott Marquis San Diego Marina  
Point Loma

### Polymer-Related Energy Conversion & Storage

Z. Lin, S. C. Rasmussen, *Organizers*

M. C. Stefan, *Organizer, Presiding*

**8:00 PMSE 595.** Unusual aggregation behavior and morphological control in bottlebrush-type copolymers based on poly(3-hexylthiophene)s. **M. Kilbey, S. Ahn**

**8:30 PMSE 596.** Redox-active macromolecular structures for energy storage in non-aqueous redox-flow batteries. **N. Gavvalapalli, E.B. Montoto, J. Hui, M. Burgess, K. Hernandez-Burgos, N. Sekerak, K.J. Cheng, E. Chenard, J.S. Moore, J. Rodriguez Lopez**

**8:50 PMSE 597.** Withdrawn.

**9:10 PMSE 598.** Optoelectronic properties of a DBFA-type block copolymer. **S.S. Sun, M. Hasib, T.H. Nguyen**

**9:30** Intermission.

**9:45 PMSE 599.** Conducting polymer binders for improving the cycling stability of aqueous sodium-ion anodes in stationary power storage. **N. Washburn, N. Sansone, A. Mohamed, J. Whitacre**

**10:15 PMSE 600.** Organometallics polymers as asymmetric pseudocapacitors: Molecular tuning of redox-electrodes for enhanced energy storage and controlled water chemistry. **X. Su, J. Elbert, T.F. Jamison, T. Hatton**

**10:35 PMSE 601.** Computational screening of polymers for water-splitting photocatalysis. **P. Guiglion, M. Zwijnenburg**

**10:55 PMSE 602.** Proof-of-concept investigations using environmentally responsive polymers as capping material for aluminum nanoparticles. **W. Zeng, P.A. Jelliss, S.W. Buckner**

## Section F

Marriott Marquis San Diego Marina  
Leucadia

### General Papers/New Concepts in Polymeric Materials

### Biological & Biomedical Polymers

C. L. Soles, *Organizer*

L. Gu, *Presiding*

**8:00 PMSE 603.** Characteristic properties of novel organosolv lignin/poly(lactide) copolymers. **S. Harris, U. Tschirner, N. Lemke, J. L. VanLierop**

**8:20 PMSE 604.** Preparation of nanofibers having periodic internal structures made from carbohydrates via electrospinning of glycoconjugate polymers. **I. Otsuka, G. Garg, R. Borsali**

**8:40 PMSE 605.** Preparation and characterization of self-healing dental resin composites. **G. Huyang, J. Sun**

**9:00 PMSE 606.** Cellular delivery of platinum(II)-loaded nanoparticles revealed with combined optical and isotopic nanoscopy. **M.T. Proetto, N.C. Gianneschi**

**9:20 PMSE 607.** Fabrication of chitosan-based hydrogels via enzyme-mediated thiol-ene polymerization. **S.R. Zavada, T. Battsengel, T.F. Scott**

**9:40** Intermission.

**10:00 PMSE 608.** Physical modeling of DNA-looping across genomic scales. **S. Sandholtz, T. Lampo, B. Krajina, A. Spakowitz**

**10:20 PMSE 609.** Supramolecular control of cell adhesion via cucurbit[8]uril on supported lipid bilayer. **E. Cavatorta, M. Verheijden, W. van Roosmalen, J. Voskuhl, J. Huskens, P. Jonkhelijm**

**10:40 PMSE 610.** Graft-through polymerization of complex peptides maintains bioactivity while enabling cellular uptake and protection from proteolysis. **J.K. Kammeyer, A.P. Blum, N.C. Gianneschi**

**11:00 PMSE 611.** Bioinspired catalysts: Mimicking the active site of enzymes. **M. Nothing, A. Espinosa, Z. Xiao, C.J. Hawker, L.A. Connal**

**11:20 PMSE 612.** Laccase-mediated catechin grafting to chitosan for modulating antioxidant, antimicrobial activities and controlled release. **S. Kim, J. Nakamatsu, F. Torres, A. Ribeiro, A.F. Gomes, A. Cavaco-Paulo**

**11:40 PMSE 613.** Mimicking articular cartilage with polymer brushes grown by a surface diffusion approach. **R. Mohammadi Sejoudsari, D.H. Adamson**

### Applications of Polymer Surfaces & Interfaces

### Low Energy Surfaces & De-Icing

*Sponsored by POLY, Cosponsored by COLL and PMSE*

### Anionic Polymerisation: Still Living After 60 Years

*Sponsored by POLY, Cosponsored by PMSE and RUBB*

## PROF

## Division of Professional Relations

**R. D. Libby, Program Chair**

### SOCIAL EVENTS:

**Henry Hill Award, 4:30 PM: Tue**

### BUSINESS MEETINGS:

**Business Meeting, 2:30 PM: Tue**

## SUNDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Balboa

### Ethics 101

*Cosponsored by CHED, CINF and ETHC*

**K. M. Lopez, L. McEwen, S. M. Schelble, Organizers, Presiding**

**11:00 PROF 1.** Ethics education resources. **S.M. Schelble**

**11:25 PROF 2.** Academic research ethics in the 21st century. **K.M. Lopez**

### Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences

*Sponsored by IAC, Cosponsored by CHED, PROF and YCC*

### Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Scott D. Allen, Geoffrey W. Coates & Anthony R. Eisenhut

### Starting a Company on University Technology

*Sponsored by POLY, Cosponsored by PROF and SCHB*

## SUNDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
Rancho Santa Fe 1 & 2

### Enough to be Dangerous: A Chemist's Handbook to Cross-Functional Development

*Cosponsored by YCC*

**M. Grandbois, N. A. LaFranzo, Organizers, Presiding**

**1:00** Introductory Remarks.

**1:05 PROF 3.** Enough project management to be dangerous. **R.D. Simmons**

**1:35 PROF 4.** Market research: What is it, and why should I care? **N.A. LaFranzo**

**2:05 PROF 5.** What will it cost and can we afford it? **J.E. Anderson**

**2:35** Intermission.

**2:45 PROF 6.** Do I have an invention? Some types for figuring it out. **B. Crawford**

**3:15 PROF 7.** Presentations in the digital age: How to make exceptional presentations in spite of PowerPoint. **M.E. Jones**

**3:45** Concluding Remarks.

### Discussions with the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

### Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Scott D. Allen, Geoffrey W. Coates & Anthony R. Eisenhut

### Starting a Company on University Technology

*Sponsored by POLY, Cosponsored by PROF and SCHB*

## SUNDAY EVENING

### My Comments to the President's Task Force on Employment

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

### My Experience with & Advice for Improving Diversity in Chemistry

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

### My Experiences in & Advice for Organic Chemistry Courses

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

## MONDAY MORNING

## Section A

Marriott Marquis San Diego Marina  
Marina Salon E

### Women in Innovation: Science & Technology

*Cosponsored by BMGT and WCC; Financially supported by CIEC*

**J. L. Bryant, Organizer**

**J. C. Giordan, Presiding**

**9:30 PROF 8.** Innovating women: Science and technology - opening overview. **J.C. Giordan**

**9:45 PROF 9.** Innovating women: Science and technology - moderated panel presentations and questions and answers. **J.C. Giordan, J.L. Bryant**

**10:45** Facilitated Q&A.

**11:45** Concluding Remarks and Networking.

### Is There a Crisis in Organic Chemistry Education?

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

### GSSPC: Resolving the Big Picture: Bringing Molecules into Focus

*Sponsored by CHED, Cosponsored by ANYL, MPPG and PROF*

### How to Foster Diversity in the Chemical Sciences: Lessons Learned & Taught from the Stories of Recipients of the Stanley C. Israel Award

*Sponsored by PRES, Cosponsored by CMA and PROF*

### Excellence in Graduate Polymer Research

*Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC*

## MONDAY AFTERNOON

## Section A

Marriott Marquis San Diego Marina  
Marina Salon E

### LGBT Chemists' Symposium on Chemical Biology

*Cosponsored by BIOL, BIOT, MEDI, ORGN, PRES and WCC*  
*Financially supported by Immediate Past President Schmidt*

**J. S. Nowick, Organizer, Presiding**

**1:45** Introductory Remarks.

**1:50 PROF 10.** Why do cancer cells have altered glycosylation? **C.R. Bertozzi**

**2:20 PROF 11.** Controlling biological pathways with unnatural chromophores. **D. Trauner**

**2:50 PROF 12.** Understanding amyloid diseases with chemical model systems. **J.S. Nowick**

**3:20** Intermission.

**3:30 PROF 13.** Engineering microbes for production of chemicals and fuels. **J.D. Keasling**

**4:00 PROF 14.** Panel discussion: Why LGBT issues matter in the chemical sciences. **C. Bertozzi, J.D. Keasling, D. Trauner, C.M. Rubert Pérez, J.S. Nowick**

**Diversity-Quantification-Success?**

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CIN, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

**GSSPC: Resolving the Big Picture: Bringing Molecules into Focus**

Sponsored by CHED, Cosponsored by ANYL, MPPG and PROF

**Excellence in Graduate Polymer Research**

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

**TUESDAY MORNING****Section A**

Marriott Marquis San Diego Marina  
Mission Hills

**Successful REU Programs**

Cosponsored by CHED and CMA

L. M. Watkins, Organizer

K. L. Buchmueller, Presiding

8:15 Introductory Remarks.

8:20 PROF 15. From REU to PUI: One person's perspective. S. Poland

8:30 PROF 16. Benjamin McDonald REU alumni panel. B. McDonald

8:40 PROF 17. My experience participating in international research as an undergraduate. J.I. Medina

8:50 Panel Discussion: Building a Strong REU Cohort from the REU Participant Perspective.

9:15 Intermission.

9:30 PROF 18. Importance of a truly cohesive theme in a research experience for undergraduates (REU) program. N. Hammer

9:45 PROF 19. Lessons from running a chemistry REU site for nine years. J.R. Morrow

10:00 Panel Discussion: Building a Cohesive REU Program.

10:25 Intermission.

10:40 PROF 20. Strategic targeting of diverse cohorts: A glimpse into the Georgia Tech REU program. S.A. France, D.M. Collard, J.C. Tyson, K.A. Johnson

10:55 PROF 21. Research-incubator REU site. T.W. Hanks, K.L. Buchmueller

11:10 PROF 22. Chemistry connections for community college students (4Cs) at UC San Diego: A NSF-REU program. H. Weizman, S. Brydges

11:25 Panel Discussion: Approaches to Broadening Participation at REU Sites.

11:50 Concluding Remarks.

**Excellence in Graduate Polymer Research**

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Technical program information known at press time.

The official technical program for the 251st ACS National Meeting is available at: [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

**TUESDAY AFTERNOON****Section A**

Marriott Marquis San Diego Marina  
Mission Hills

**Chemical Angel Network**

Cosponsored by BMGT and SCHB

J. L. Bryant, M. Vreeke, Organizers

S. S. White, Organizer, Presiding

1:30 Introductory Remarks.

1:35 PROF 23. News and updates from the Chemical Angel Network (CaN). M. Vreeke, S.S. White, J.C. Giordan

2:00 Company Presentations.

3:00 Investment Discussion.

3:30 Open Forum.

4:00 Concluding Remarks.

**Excellence in Graduate Polymer Research**

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

**TUESDAY EVENING****Excellence in Graduate Polymer Research**

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

**RUBB****Rubber Division**

T. Delapa, Program Chair

**MONDAY EVENING****Potpourri of Polymer Projects: Take a Byte out of the NGSS**

Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB

**TUESDAY AFTERNOON****Anionic Polymerisation: Still Living After 60 Years**

Sponsored by POLY, Cosponsored by PMSE and RUBB

**TUESDAY EVENING****Anionic Polymerisation: Still Living After 60 Years**

Sponsored by POLY, Cosponsored by PMSE and RUBB

**WEDNESDAY MORNING****Anionic Polymerisation: Still Living After 60 Years**

Sponsored by POLY, Cosponsored by PMSE and RUBB

**WEDNESDAY AFTERNOON****Anionic Polymerisation: Still Living After 60 Years**

Sponsored by POLY, Cosponsored by PMSE and RUBB

**THURSDAY MORNING****Anionic Polymerisation: Still Living After 60 Years**

Sponsored by POLY, Cosponsored by PMSE and RUBB

**SCHB****Division of Small Chemical Businesses**

J. Sabol, Program Chair

**OTHER SYMPOSIA OF INTEREST:**

The Role of Scientific Patent information in the Innovation Process (see CHAL, Mon)

Building & Protecting Intellectual Property (see CHAL, Wed)

Tomayto vs. Tomahto: Overcoming Incompatibilities in Scientific Data (see CIN, Sun)

Science & Perception of Climate Change (see ENVR, Tue, Wed)

Enough to be Dangerous: A Chemist's Handbook to Cross-Functional Development (see PROF, Sun)

Perspectives on Climate Change Literacy & Education: Local to International (see CHED, Sun)

**SOCIAL EVENTS:**

Social Hour, 5:00 PM: Mon

Reception, 5:00 PM: Mon

Luncheon, 11:30 AM: Sun, Mon, Tue

**BUSINESS MEETINGS:**

Executive Committee Meeting, 5:30 PM: Sun

Business Meeting, 12:00 PM: Mon

**SUNDAY MORNING****Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Scott D. Allen, Geoffrey W. Coates & Anthony R. Eisenhut****Starting a Company on University Technology**

Sponsored by POLY, Cosponsored by PROF and SCHB

**SUNDAY AFTERNOON****Discussions with the President's Task Force on Employment**

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CIN, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

**Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Scott D. Allen, Geoffrey W. Coates & Anthony R. Eisenhut****Starting a Company on University Technology**

Sponsored by POLY, Cosponsored by PROF and SCHB

**SUNDAY EVENING****My Comments to the President's Task Force on Employment**

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CIN, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

**MONDAY MORNING****Section A**

Marriott Marquis San Diego Marina  
Santa Rosa

**Entrepreneurs' Poster Session**

G. W. Ruger, Organizer

**8:00 - 10:00**

SCHB 1. ACS Small Chemical Businesses

Division membership: A valuable tool for the entrepreneur. A. Rahman, M. Chorghade, P.C. Lauro, D.J. Deutsch, A. Kantak, S.V. Vercellotti, J.E. Sabol, J.L. MacLachlan, C.A. Burton, N.A. Vaidya, E. Oltermann, P.C. Kearney, G.W. Ruger

SCHB 2. Chemical Angel Network: Chemists investing in chemical companies. S.S. White, M. Vreeke, J.C. Giordan

SCHB 3. Palladium Science Academy partners with other groups to spread science education. G.W. Ruger, J.R. Berk

**Section A**

Marriott Marquis San Diego Marina  
Santa Rosa

**Start-up Businesses in Drug Discovery**

Cosponsored by ORGN

P. C. Kearney, Organizer, Presiding

10:00 SCHB 4. CDD vault: Successful product case study. B.A. Bunin, C. Weatheral, P. Gund

10:30 SCHB 5. Virtual collaborations for developing Sanfilippo syndrome treatments on a shoestring. S. Ekins, D. Moen, J. Wood

11:00 SCHB 6. Managing drug discovery collaborations: Perspectives from both sides of the partner relationship. J. Nuss

11:30 SCHB 7. Oncology drug discovery at H3 biomedicine: Combining recent advances in synthetic chemistry and cancer genomics. L.A. Marcaurrelle

**Cannabis: Exploring the Chemistry, History & Future**

Sponsored by AGFD, Cosponsored by CHAS and SCHB

**MONDAY AFTERNOON****Section A**

Marriott Marquis San Diego Marina  
Santa Rosa

**Computers in Chemistry: Bridging the Gap between Clients & Software**

*Cosponsored by CINF and ORGN*

M. Johnson, *Organizer, Presiding*

1:05 Introductory Remarks.

1:10 **SCHB 8.** Connecting the needs of the customer with what a small chemical software company has to offer. M. Johnson, J.D. Clark, C. Cannon

1:40 **SCHB 9.** Perspectives on selling custom software development services to R&D scientists in large organizations. E. Milgram

2:10 **SCHB 10.** Sometimes the mountain has to move... but you cannot let it realise it's happening. E. Champness, M.D. Segall

2:40 **SCHB 11.** Vendors are from Venus, clients are from Mars: How to build a successful partnership. C.L. Waller

3:10 Intermission.

3:25 **SCHB 12.** Creative market solutions from customer requests: Simple ideas can lead to big products. T. Cheeseright, R. Scoffin

3:55 **SCHB 13.** Enabling large-scale ligand discovery on the cloud. P.C. Hawkins

4:25 **SCHB 14.** From CDD vault, CDD vision to CDD models: Software for biologists and chemists doing drug discovery. S. Ekins, B. Bunin

4:55 Concluding Remarks.

**Chemical Information for Small Businesses & Startups**

*Sponsored by CINF, Cosponsored by CPRM and SCHB*

**Cannabis: Exploring the Chemistry, History & Future**

*Sponsored by AGFD, Cosponsored by CHAS and SCHB*

**MONDAY EVENING****Section A**

San Diego Convention Center  
Halls D/E

**Sci-Mix**

G. W. Ruger, *Organizer*

8:00 - 10:00

1-3. See previous listings.

**TUESDAY MORNING****Section A**

Marriott Marquis San Diego Marina  
Santa Rosa

**Cannabis: Exploring the Chemistry, History & Future**

*Cosponsored by AGFD, CHAS and ORGN*

E. M. Pryor, *Organizer*

R. Ford, *Organizer, Presiding*

8:00 Networking.

8:30 Introductory Remarks.

8:35 **SCHB 15.** Servicing the cannabis extraction market. E.M. Pryor

9:05 **SCHB 16.** Patient advocacy for cannabis standards creates jobs in industry. S. Sherer, J. Marcu, K. Nevedal

9:35 **SCHB 17.** Findings on blending hemp with thermal coal for power generation. R. Ford

10:05 Intermission.

10:25 **SCHB 18.** Report from a Colorado private laboratory on regional cannabis potency from using UPLC analysis. H. Despres, J. Marcu

10:55 **SCHB 19.** Rapid quantitative chemical analysis of cannabinoids in seized cannabis using heated headspace solid-phase microextraction and gas chromatography/mass spectrometry. A. Brown, J. Sweet, C.C. Yu

11:25 **SCHB 20.** Analytical testing for the cannabis industry: Consumer safety vs. regulatory requirements. C.J. Hudalla

11:55 Concluding Remarks.

**TUESDAY AFTERNOON****Chemical Angel Network**

*Sponsored by PROF, Cosponsored by BMGT and SCHB*

**CCS****Committee on Chemical Safety**

E. Howson, *Program Chair*

**SUNDAY AFTERNOON****Safety Begins in the Classroom: Demonstrations, Awareness & Pre-Lab Planning**

*Sponsored by CHAS, Cosponsored by CCS and CHED*

**Ask Dr. Safety: About Incident Reporting**

*Sponsored by CHAS, Cosponsored by CCS*

**MONDAY AFTERNOON****How Texas Tech & UCLA Have Affected Laboratory Safety Nationwide**

*Sponsored by CHAS, Cosponsored by CCS*

**TUESDAY MORNING****Developing, Implementing & Teaching Hazard Assessment Tools**

*Sponsored by CHAS, Cosponsored by CCS and CHED*

**TUESDAY AFTERNOON****Developing, Implementing & Teaching Hazard Assessment Tools**

*Sponsored by CHAS, Cosponsored by CCS and CHED*

**WEDNESDAY MORNING****Chemical, Sample & Asset Management Tools**

*Sponsored by CHAS, Cosponsored by CCS and CINF*

**WEDNESDAY AFTERNOON****Chemical, Sample & Asset Management Tools**

*Sponsored by CHAS, Cosponsored by CCS and CINF*

**CCA****Committee on Community Activities**

M. McGinnis, *Program Chair*

**SUNDAY MORNING****Fundamentals of Chemistry Outreach Education: From Program Design to Assessment**

*Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC*

**SUNDAY AFTERNOON****Fundamentals of Chemistry Outreach Education: From Program Design to Assessment**

*Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC*

**MONDAY MORNING****Fundamentals of Chemistry Outreach Education: From Program Design to Assessment**

*Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC*

**DAC****Committee on Divisional Activities**

R. Bennett, *Program Chair*

**SUNDAY MORNING****New Horizons in Sustainable Materials Nanocellulose**

*Sponsored by CELL, Cosponsored by DAC† and POLY*

**SUNDAY AFTERNOON****Discussions with the President's Task Force on Employment**

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

**New Horizons in Sustainable Materials****Lignocellulosics**

*Sponsored by CELL, Cosponsored by DAC† and POLY*

**SUNDAY EVENING****My Comments to the President's Task Force on Employment**

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC*

**My Experience with & Advice for Improving Diversity in Chemistry**

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC*

**My Experiences in & Advice for Organic Chemistry Courses**

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

**MONDAY MORNING****Is There a Crisis in Organic Chemistry Education?**

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, DAC, GEOC, I&EC, INOR, MEDI, ORGN, POLY and PROF*

**New Horizons in Sustainable Materials****Glycoscience**

*Sponsored by CELL, Cosponsored by DAC† and POLY*

**MONDAY AFTERNOON****Diversity-Quantification-Success?**

*Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, I&EC, ORGN, PHYS, POLY, PROF and WCC*

**New Horizons in Sustainable Materials****Polysaccharide Materials**

*Sponsored by CELL, Cosponsored by DAC† and POLY*

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## CEI

## Committee on Environmental Improvement

C. Middlecamp, Program Chair

### SUNDAY AFTERNOON

#### Perspectives on Climate Change Literacy & Education: Local to International

Sponsored by CHED, Cosponsored by CEI

### MONDAY MORNING

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Environmental Chemistry/ Water Chemistry

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### WCC 2016 Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE

#### Innovative Materials & Technologies for Water Purification

#### Photochemical Process & Desalination

Sponsored by ENVR, Cosponsored by CEI

#### Treatment of Contaminants of Emerging Concern & Their Transformation Products

Sponsored by ENVR, Cosponsored by CEI

#### Water Treatment Technologies to Support Food-Energy-Water Nexus Water Conservation Needs

Sponsored by ENVR, Cosponsored by CEI

### MONDAY AFTERNOON

#### WCC 2016 Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by CATL, CEI, COMP, ENFL and PMSE

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Environmental Chemistry/ Water Chemistry

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Innovative Materials & Technologies for Water Purification

#### Oxidation, Reduction & Disinfection

Sponsored by ENVR, Cosponsored by CEI

#### Treatment of Contaminants of Emerging Concern & Their Transformation Products

Sponsored by ENVR, Cosponsored by CEI

#### Chemistry of Materials Management: Mitigation & Reuse for Sustainable Environment

Sponsored by ENVR, Cosponsored by CEI

### Undergraduate Research Posters

#### Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored by CEI, I&EC and SOCED

### TUESDAY MORNING

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Microbial Processes & Treatment

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Green Chemistry: Theory & Practice

Sponsored by CHED, Cosponsored by CEI, I&EC and SOCED

#### Innovative Materials & Technologies for Water Purification

#### Adsorption

Sponsored by ENVR, Cosponsored by CEI

#### Treatment of Contaminants of Emerging Concern & Their Transformation Products

Sponsored by ENVR, Cosponsored by CEI

#### ACS-CEI Award for Incorporating Sustainability into Chemistry Education

Sponsored by CHED, Cosponsored by CEI

### TUESDAY AFTERNOON

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Geochemistry

Sponsored by ENVR, Cosponsored by CEI and GEOC

#### Green Chemistry: Theory & Practice

Sponsored by CHED, Cosponsored by CEI, I&EC and SOCED

#### Innovative Materials & Technologies for Water Purification

#### Electrochemical & Biological Process

Sponsored by ENVR, Cosponsored by CEI

#### Treatment of Contaminants of Emerging Concern & Their Transformation Products

Sponsored by ENVR, Cosponsored by CEI

#### Science & Perception of Climate Change

Sponsored by ENVR, Cosponsored by CEI

### WEDNESDAY MORNING

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Water Use & Reuse

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CEI

### WEDNESDAY AFTERNOON

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Water Use & Reuse/Water Treatment

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Citizens First!

Sponsored by CHED, Cosponsored by CEI

#### Membrane Technology for Water-Energy Sustainability

Sponsored by ENVR, Cosponsored by CEI

#### Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CEI

### WEDNESDAY EVENING

#### Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CEI

#### Science & Perception of Climate Change

Sponsored by ENVR, Cosponsored by CEI

#### Treatment of Contaminants of Emerging Concern & Their Transformation Products

Sponsored by ENVR, Cosponsored by CEI

### THURSDAY MORNING

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Modeling

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Membrane Technology for Water-Energy Sustainability

Sponsored by ENVR, Cosponsored by CEI

### THURSDAY AFTERNOON

#### Environmental Aspects of Unconventional Oil & Gas Production & Hydraulic Fracturing

#### Regulatory Aspects

Sponsored by ENVR, Cosponsored by CEI, ENFL and GEOC

#### Membrane Technology for Water-Energy Sustainability

Sponsored by ENVR, Cosponsored by CEI

## ETHC

## Committee on Ethics

K. Vitense, Program Chair

### SUNDAY MORNING

#### Ethics 101

Sponsored by PROF, Cosponsored by CHED, CINF and ETHC

## LSAC

## Committee on Local Section Activities

M. Rudd, Program Chair

### SUNDAY MORNING

#### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

### SUNDAY AFTERNOON

#### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

### MONDAY MORNING

#### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

## CMA

## Committee on Minority Affairs

J. Sarquis, Program Chair

### MONDAY MORNING

#### How to Foster Diversity in the Chemical Sciences: Lessons Learned & Taught from the Stories of Recipients of the Stanley C. Israel Award

Sponsored by PRES, Cosponsored by CMA and PROF

### TUESDAY MORNING

#### Successful REU Programs

Sponsored by PROF, Cosponsored by CHED and CMA



## CPRM

## Committee on Patents &amp; Related Matters

S. Shah, Program Chair

## MONDAY AFTERNOON

## Chemical Information for Small Businesses &amp; Startups

Sponsored by CINF, Cosponsored by CPRM and SCHB

## COMSCI

## Committee on Science

M. Berman, Program Chair

## SUNDAY AFTERNOON

## Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&amp;EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## SUNDAY EVENING

## My Comments to the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&amp;EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## My Experience with &amp; Advice for Improving Diversity in Chemistry

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&amp;EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

## MONDAY MORNING

## Section A

San Diego Convention Center  
Room 31C

## Computational Design of Advanced Materials

Cosponsored by COMP and PHYS

M. Berman, Organizer, Presiding

## 8:30 Introductory Remarks.

9:00 COMSCI 1. Materials genome initiative—an industrial perspective. C. Wadia

9:20 COMSCI 2. Design of integrated functional soft matter systems. J. De Pablo

9:40 COMSCI 3. Design principles for solid catalysts. J. Norskov

10:00 COMSCI 4. Extracting materials information from the literature—harder than you might think. J. Pitera

10:20 Intermission.

10:35 COMSCI 5. Growth of nanoscale materials: Insights from simulation. K. Fichthorn

10:55 COMSCI 6. Accelerating materials discovery with data-driven atomistic computational tools. C. Wolverton

11:15 Panel Discussion.

## MONDAY AFTERNOON

## Diversity-Quantification-Success?

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&amp;EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

## CTA

## Committee on Technician Affairs

K. Allen, Program Chair

## MONDAY MORNING

## New Reality of the Chemical Enterprise: Traditional &amp; Non-traditional Career Paths

## Chemistry Professionals Working "Outside the Box"

Sponsored by I&amp;EC, Cosponsored by CTA, PRES and SOCED

## MONDAY AFTERNOON

## New Reality of the Chemical Enterprise: Traditional &amp; Non-traditional Career Paths

## Chemistry Professionals Working "Outside the Box"

Sponsored by I&amp;EC, Cosponsored by CTA, PRES and SOCED

## TUESDAY MORNING

## New Reality of the Chemical Enterprise: Traditional &amp; Non-traditional Career Paths

## Chemistry Professionals Working in the Government

Sponsored by I&amp;EC, Cosponsored by CTA, PRES and SOCED

## TUESDAY AFTERNOON

## New Reality of the Chemical Enterprise: Traditional &amp; Non-traditional Career Paths

## Chemistry Professionals are Entrepreneurs &amp; More

Sponsored by I&amp;EC, Cosponsored by CTA, PRES and SOCED

## IAC

## International Activities Committee

E. Contis, Program Chair

## SOCIAL EVENTS:

Reception, 5:30 PM: Sun

## SUNDAY MORNING

## Section A

Hilton San Diego Bayfront  
Aqua 310A

## Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences

Cosponsored by CHED, PROF and YCC

A. Rimando, E. Tratras Contis, Organizers

C. LaPrade, Organizer, Presiding

9:00 Introductory Remarks - Christopher LaPrade.

9:15 IAC 1. Summer chemistry research in Hannover, Germany: Synthesis of a unique adventure catalyzed by fungal biosynthetic enzymes. L. Qiao, R. Cox

9:35 IAC 2. Synthesis of Argyrin B in Hannover, Germany: My introduction to natural compound modification and cultural diversity. L. Lotti Diaz

9:55 IAC 3. Collaboration in Germany: Bench-top flow reactors and a little bit of curry. S. Dickinson

10:15 IAC 4. Undergraduate research in Jena: Scientific and personal discovery in Germany. B. Snyder, R. Freund, H. Arndt

10:35 Intermission.

10:50 IAC 5. Microfluidics research in Jena, Germany: Lessons in communication, culture, and continuous processes. C. Dobson, M. Leiske, S. Schubert, U. Schubert

11:10 IAC 6. Theoretical study of hydrogen adsorption on Ag/Pt(111) in Ulm, Germany. E. Bringley, J. Mueller, T. Jacob

11:30 IAC 7. Summer research in Ulm, Germany: Ordered protein assembly via a DNA origami scaffold. A. Osunsade, Y. Tokura, Y. Wu, T. Weil

11:50 IAC 8. POM-photosensitizer systems for hydrogen reduction in Ulm um Ulm und um Ulm herum. W.C. Howland, S. Schönweiz, C. Streb

## SUNDAY AFTERNOON

## Section A

Hilton San Diego Bayfront  
Aqua 310A

## Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences

Cosponsored by CHED, PROF, and YCC

A. Rimando, E. Tratras Contis, Organizers

C. LaPrade, Organizer, Presiding

1:30 IAC 9. Summer in Singapore: Purifying water and exploring Southeast Asia. S. Padgaonkar, S. Vallyaveettill

1:50 IAC 10. Undergraduate research in Singapore: Cultural exploration of Southeast Asia and Hf/Zr-fumarate metal-organic framework synthesis and optimization. I. Castano, D. Zhao, Z. Hu

2:10 IAC 11. Exploring Singapore through electrocatalysts and Katong Laksa. J. Cavanaugh, Y. Qian, D. Zhao

2:30 IAC 12. Undergraduate research in Glasgow, Scotland: A study on magnetic nanoparticles and life beyond the United States. M. Hayes, D. Graham, S. Mabbott

2:50 IAC 13. Synthesis of small molecules for improved organic solar cell efficiency. S. Chapman, N. Findlay, P. Skabara

3:10 Intermission.

3:25 IAC 14. Beyond chromatography: investigating the Catellani Reaction in the Italian Countryside. A. Kahler-Quesada, L. Vaccaro, S. Santoro

3:45 IAC 15. International research experience in Perugia, Italy: The effect of concentration, solvent, and nanoparticle concentration on the photophysical behavior of 9ACA. A. Davis, G. Zampini, L. Latterini

4:05 IAC 16. Undergraduate research in Perugia, Italy: Extending cultural horizons and human vision through fuzzy logic photochromic systems. A. Rightler, P. Gentili

4:25 IAC 17. My IREU Experience in Perugia, Italy: Studying iridium catalysts for light-driven experimentation. K. Ellingwood

4:45 Concluding Remarks.

## Discussions with the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&amp;EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## SUNDAY EVENING

## My Comments to the President's Task Force on Employment

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&amp;EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

## TUESDAY MORNING

## Section A

Hilton San Diego Bayfront  
Aqua 310A/B

## Eli Pearce Memorial Symposium

Cosponsored by CHAS and POLY

D. Walters, P. Zarras, Organizers, Presiding

8:30 Welcome and Introductory Remarks.

8:40 IAC 18. Eli Pearce: A man for all seasons and causes. M. Jacobs

9:00 IAC 19. Eli Pearce, the pioneer. A. Pavlath

9:20 IAC 20. Eli Pearce— A global leader and humanitarian. H. Cheng

9:40 IAC 21. Eli Pearce: A mensch for all seasons. M. Hoffman, Z. Lerman

10:00 Intermission.

10:20 IAC 22. Professor Eli Pearce- Our permanent adviser. C. Do

**10:40 IAC 23.** He made it in New York!  
N. Jespersen

**11:00 IAC 24.** Eli Pearce, the Director of  
Polymer Research Institute. K. Levon

**11:20 IAC 25.** Observe the good man:  
A personal tribute to Eli M. Pearce.  
D. Pearce-McCall, L. Brown

**11:50** Audience Comments and Concluding  
Remarks.

## TUESDAY AFTERNOON

### International & Multicultural Perspective

Sponsored by CHED, Cosponsored by IAC

## SOCED

### Society Committee on Education

S. Emory, Program Chair

#### SOCIAL EVENTS:

**Making the Most of Your First  
National Meeting**, 9:00 AM: Sun

**Graduate School Reality Check:  
Getting In**, 10:00 AM: Sun

**Chem Demo Exchange**, 11:00 AM: Sun

**Graduate School Reality Check: You're  
In- Now What?**, 11:15 AM: Sun

**Networking Social with Graduate  
School Recruiters**, 1:00 PM: Sun

**Workshop: Effective Chemistry Demos for  
Community Outreach**, 2:45 PM: Sun

**Student Chapter Awards  
Ceremony**, 7:00 PM: Sun

**Undergraduate Social**, 8:30 PM: Sun

**Speed Networking with Chemistry  
Professionals**, 3:45 PM: Mon

## SUNDAY MORNING

### High School Program

Sponsored by CHED, Cosponsored by SOCED

### Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored  
by CCA, LSAC, SOCED and YCC

### The Two Year Guidelines: What's New

Sponsored by CHED, Cosponsored by SOCED

Technical program information  
known at press time.

The official technical program  
for the 251st ACS National

Meeting is available at:

[www.acs.org/sandiego2016](http://www.acs.org/sandiego2016)

## SUNDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom C

### Trends in Computational Chemistry: Biophysical to Materials Chemistry

Cosponsored by COMP

S. Emory, Organizer, Presiding

**1:00 SOCED 1.** Computational design of  
perovskite nanostructures for solar energy  
conversion. R. Berger

**1:30 SOCED 2.** Seeing the unseen: Chemical  
discovery through the lens of a computa-  
tional microscope. R. Amaro

**2:00 SOCED 3.** Hacking the Aufbau principle  
to simulate electronic excitations in  
organic materials. T. Kowalczyk

### High School Program

Sponsored by CHED, Cosponsored by SOCED

### Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored  
by CCA, LSAC, SOCED and YCC

## MONDAY MORNING

### Section A

San Diego Convention Center  
Room 33C

### Frontiers in Inorganic Chemistry

Cosponsored by INOR

S. Emory, Organizer

C. Daley, Presiding

**9:30 SOCED 4.** Developing ligands for use in  
metal-mediated enantioselective catalysis.  
C. Daley

**10:00 SOCED 5.** Dihydrogen complexes:  
Methods for characterization. D. Heineke

**10:30 SOCED 6.** Redox-active ligands for  
the transformation of small molecules.  
J. Gilbertson

**11:00 SOCED 7.** Inorganic nanoparticles in  
medicine. M. Sailor

### Section B

San Diego Convention Center  
Room 33B

### Advances in Chemical Imaging: Ultra-Resolution to Single Molecules

Cosponsored by ANYL and PHY5

S. Emory, Organizer

X. Qian, Presiding

**9:00 SOCED 8.** Development of SERS  
nanoparticles for biomedical applications.  
S. Nie, L. Lane, X. Qian

**9:30 SOCED 9.** Chemical imaging at  
100nm and single molecule sensitivity:  
Photochemistry of organic semiconduc-  
tors probed by a combination of high res-  
olution fluorescence microscopy and ion  
mobility mass spectrometry. S. Buratto

**10:00 SOCED 10.** Imaging the genome in  
living cells. B. Huang

### New Reality of the Chemical Enterprise: Traditional & Non- traditional Career Paths

### Chemistry Professionals Working "Outside the Box"

Sponsored by I&EC, Cosponsored  
by CTA, PRES and SOCED

### Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by  
PRES, PROF, SOCED and YCC

### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored  
by CCA, LSAC, SOCED and YCC

## MONDAY AFTERNOON

### Section A

Marriott Marquis San Diego Marina  
San Diego Ballroom A

### Eminent Scientist Lecture: Richard N. Zare, Stanford University

S. Emory, Organizer, Presiding

**2:30 SOCED 11.** My life with lasers. R. Zare

### New Reality of the Chemical Enterprise: Traditional & Non- traditional Career Paths

### Chemistry Professionals Working "Outside the Box"

Sponsored by I&EC, Cosponsored  
by CTA, PRES and SOCED

### Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by  
PRES, PROF, SOCED and YCC

### Undergraduate Research Posters

### Agricultural & Food Chemistry

Sponsored by CHED, Cosponsored  
by AGFD and SOCED

### Undergraduate Research Posters

### Analytical Chemistry

Sponsored by CHED, Cosponsored  
by ANYL and SOCED

### Undergraduate Research Posters

### Biochemistry

Sponsored by CHED, Cosponsored  
by BIOL and SOCED

### Undergraduate Research Posters

### Biotechnology

Sponsored by CHED, Cosponsored  
by BIOT and SOCED

### Undergraduate Research Posters

### Chemical Education

Sponsored by CHED, Cosponsored by SOCED

### Undergraduate Research Posters

### Computational Chemistry

Sponsored by CHED, Cosponsored  
by COMP and SOCED

### Undergraduate Research Posters

### Environmental Chemistry

Sponsored by CHED, Cosponsored  
by ENVR and SOCED

### Undergraduate Research Posters

### Geochemistry

Sponsored by CHED, Cosponsored  
by GEOG and SOCED

### Undergraduate Research Posters

### Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored  
by CEI, I&EC and SOCED

### Undergraduate Research Posters

### Inorganic Chemistry

Sponsored by CHED, Cosponsored  
by INOR and SOCED

### Undergraduate Research Posters

### Medicinal Chemistry

Sponsored by CHED, Cosponsored  
by MEDI and SOCED

### Undergraduate Research Posters

### Nanochemistry

Sponsored by CHED, Cosponsored by SOCED

### Undergraduate Research Posters

### Organic Chemistry

Sponsored by CHED, Cosponsored by SOCED

### Undergraduate Research Posters

### Physical Chemistry

Sponsored by CHED, Cosponsored by SOCED

### Undergraduate Research Posters

### Polymer Chemistry

Sponsored by CHED, Cosponsored  
by PMSE, POLY and SOCED

## MONDAY EVENING

### Successful Student Chapters

Sponsored by CHED, Cosponsored by SOCED

## TUESDAY MORNING

### New Reality of the Chemical Enterprise: Traditional & Non- traditional Career Paths

### Chemistry Professionals Working in the Government

Sponsored by I&EC, Cosponsored  
by CTA, PRES and SOCED

### Green Chemistry: Theory & Practice

Sponsored by CHED, Cosponsored  
by CEI, I&EC and SOCED

### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by  
PRES, PROF, SOCED and YCC

## TUESDAY AFTERNOON

### New Reality of the Chemical Enterprise: Traditional & Non- traditional Career Paths

### Chemistry Professionals are Entrepreneurs & More

Sponsored by I&EC, Cosponsored  
by CTA†, PRES and SOCED

**Green Chemistry: Theory & Practice**

Sponsored by CHED, Cosponsored by CEI, I&EC and SOCED

**Excellence in Graduate Polymer Research**

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

**TUESDAY EVENING****Excellence in Graduate Polymer Research**

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

**WCC****Women Chemists Committee**

K. Wozniak and A. Debaille, Program Chairs

**OTHER SYMPOSIA OF INTEREST:**

**Women in Innovation: Science & Technology** (see PROF, Mon)

**LGBT Chemists' Symposium on Chemical Biology** (see PROF, Mon)

**SOCIAL EVENTS:**

**Breakfast**, 7:30 AM: Mon

**Social Hour**, 4:00 PM: Mon

**Luncheon**, 12:00 PM: Tue

**BUSINESS MEETINGS:**

**WCC Business Meeting**, 5:30 PM: Fri

**WCC Business Meeting**, 7:30 AM: Sat

**Eli Lilly Travel Award Poster Session**, 11:00 AM: Tue

**SUNDAY MORNING****Computational Chemistry Across Catalysis****Modeling Complex Reaction Networks in Catalysis**

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

**ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg**

Sponsored by INOR, Cosponsored by WCC

**Catalysis at the Sub-Nanometer Scale****Subnanometer (Selective) Oxidation Catalysts**

Sponsored by CATL, Cosponsored by WCC

**SUNDAY AFTERNOON****Discussions with the President's Task Force on Employment**

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

**Computational Chemistry Across Catalysis****QMMM & Reaction Pathway Sampling**

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

**ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg**

Sponsored by INOR, Cosponsored by WCC

**Catalysis at the Sub-Nanometer Scale****Challenges in Catalyst Synthesis, Stability & Characterization**

Sponsored by CATL, Cosponsored by WCC

**SUNDAY EVENING****My Comments to the President's Task Force on Employment**

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, IAC, INOR, MEDI, ORGN, PHYS, PMSE, POLY, PROF, SCHB and WCC

**My Experience with & Advice for Improving Diversity in Chemistry**

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

**MONDAY MORNING****Section A**

San Diego Convention Centr  
Room 12

**WCC 2016 Rising Stars Awards Symposium**

Cosponsored by CATL, CEI, COMP, ENFL and PMSE

M. Kane, Organizer, Presiding

9:30 Introductory Remarks.

9:40 **WCC 1.** From iodine-mediated hydration of terminal alkynes to 1,2,3-triazole chemosensors: The rewards of mentorship and invaluable collaborations. K. Aiken

10:00 **WCC 2.** Journey for the perfect tools of polyolefin structure determination. R. Cong

10:20 **WCC 3.** Multiscale modeling in materials chemistry. A. Alexandrova

10:40 Intermission.

10:55 **WCC 4.** From bench top to utility scale: An adventure in development and commercialization from a national laboratory perspective. E. Fox

11:15 **WCC 5.** Exploring the Permissive Stromal Microenvironment. A. Hummon, P. Zorlutuna, E. Weaver

**Women in Innovation: Science & Technology**

Sponsored by PROF, Cosponsored by BMGT and WCC

**Computational Chemistry Across Catalysis****Towards Chemical Accuracy**

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

**Catalysis at the Sub-Nanometer Scale Selectivity**

Sponsored by CATL, Cosponsored by WCC

**MONDAY AFTERNOON****Section A**

Hilton San Diego Bayfront  
Cobalt 520

**WCC 2016 Rising Stars Awards Symposium**

Cosponsored by CATL, CEI, COMP, ENFL and PMSE

M. Kane, Organizer, Presiding

1:30 **WCC 7.** Expanding the imaging toolbox and lessons learned along the way. J. Prescher

1:50 **WCC 8.** Why being a consumer and a mom has made me a better scientist. S. Chirch

2:10 **WCC 9.** On supramolecular organic chemistry, breastfeeding, and commuting: Life as a chemistry professor, mom of three, and half of a dual career couple. M. Levine

2:30 Intermission.

2:45 **WCC 10.** New methods in nucleoside phosphorylation. R. Ruck

3:05 **WCC 11.** Pathway towards engineering artificial proteins and the lessons learned. J. Montclare

3:25 Concluding Remarks.

**Diversity-Quantification-Success?**

Sponsored by PRES, Cosponsored by BIOL, CELL, CHED, CINF, COLL, COMSCI, DAC, GEOC, I&EC, INOR, MEDI, ORGN, PHYS, POLY, PROF and WCC

**LGBT Chemists' Symposium on Chemical Biology**

Sponsored by PROF, Cosponsored by BIOL, BIOT, MEDI, ORGN, PRES and WCC

**Computational Chemistry Across Catalysis****Oxide Catalysts & Key Industrial Reactions**

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

**ACS Award in Organometallic Chemistry: Symposium in honor of Karen I. Goldberg**

Sponsored by INOR, Cosponsored by WCC

**TUESDAY MORNING****Section A**

Hilton San Diego Bayfront  
Cobalt 520

**ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in honor of Carol A. Fierke**

Cosponsored by BIOL

A. Mapp, Organizer, Presiding

9:30 Introductory Remarks.

9:40 **WCC 12.** Dissecting dynamic transcriptional coactivator complexes with small molecule modulators. A. Mapp

10:00 **WCC 13.** Taking RNA in a new direction: 3'-5' polymerases in biology. J. Jackman

10:20 **WCC 14.** Ribosomes pause and slide on lysine-encoding homopolymeric A stretches. K. Koutmou, A. Schuller, J. Brunelle, A. Radhakrishnan, S. Djuranovic, R. Green

10:40 Intermission.

10:55 **WCC 15.** Increasing complexity of mammalian serine palmitoyltransferases. T. Dunn

11:15 **WCC 16.** Quality control during 40S ribosome assembly. K. Karbstein

11:35 **WCC 17. Award Address** (ACS Award for Encouraging Women into Careers in the Chemical Sciences sponsored by The Camille and Henry Dreyfus Foundation, Inc.). Diversification: Faculty at the University of Michigan and tRNA processing enzymes. C. Fierke

**Computational Chemistry Across Catalysis****Electrocatalysis & Photocatalysis**

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

**Polyethylene****Catalysis**

Sponsored by PMSE, Cosponsored by WCC

**TUESDAY AFTERNOON****Computational Chemistry Across Catalysis****From Metallic Nanoparticles to Isolated Metal Active Site**

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

**Polyethylene****Crystallization**

Sponsored by PMSE, Cosponsored by WCC

**WEDNESDAY MORNING****Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of Donna G. Blackmond**

Sponsored by ORGN, Cosponsored by CATL and WCC

**Computational Chemistry Across Catalysis****From Heterogeneous to Homogeneous Catalysis**

Sponsored by CATL, Cosponsored by COMP, ENFL and WCC

**Polyethylene****Fracture & Mechanical Properties**

Sponsored by PMSE, Cosponsored by WCC

**WEDNESDAY AFTERNOON****Polyethylene****Characterization & Reaction Engineering**

Sponsored by PMSE, Cosponsored by WCC

YCC

## Younger Chemists Committee

M. Druelinger, Program Chair

### SUNDAY MORNING

#### Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored by CHED, PROF and YCC

#### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

### SUNDAY AFTERNOON

#### Section A

Hilton San Diego Bayfront  
Cobalt 520

#### Starting a Successful Research Program at a Predominantly Undergraduate Institution

T. Matos, Organizer

M. Druelinger, Organizer, Presiding

1:00 Introductory Remarks – M. Druelinger.

1:05 YCC 1. What is undergraduate research and why do research at a predominantly undergraduate institution?  
M. Malachowski

1:15 YCC 2. Collaborative research with undergraduates: Research project and research group design.  
M. Malachowski

1:35 YCC 3. Balancing teaching, research, service and life in the context of primarily undergraduate institutions (PUIs).  
B. Gourley

1:55 YCC 4. Art and necessity of gaining internal support from institutional administrators.  
M. Druelinger

2:15 Intermission.

2:30 YCC 5. Undergraduate new investigator grants at the ACS Petroleum Research Fund.  
T. Clancy

2:55 YCC 6. Funding opportunities at the National Science Foundation of particular interest to faculty at primarily undergraduate institutions (PUIs).  
M. Bushey

3:25 YCC 7. Writing more competitive grant proposals.  
T. Wenzel

3:45 YCC 8. Using small grant opportunities to jump-start your research.  
B. Gourley

4:05 Questions and Open Panel Discussion.

4:25 Concluding Remarks.

#### Enough to be Dangerous: A Chemist's Handbook to Cross-Functional Development

Sponsored by PROF, Cosponsored by YCC

#### Going Global with International Scientific Training: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored by CHED and YCC

#### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

### MONDAY MORNING

#### Preparing for the Real World: Challenges Faced by Young Investigators

#### Choosing Grad Research Advisors & A Career in Academia or Industry

Sponsored by MPPG, Cosponsored by CHED, CINF, COMP, PHYS and YCC

#### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

#### Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

### MONDAY AFTERNOON

#### Preparing for the Real World: Challenges Faced by Young Investigators

#### Research at PUI's

Sponsored by MPPG, Cosponsored by CHED, CINF, COMP, PHYS and YCC

#### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

### TUESDAY MORNING

#### Young Investigators in Nuclear & Radiochemistry

Sponsored by NUCL, Cosponsored by YCC

#### Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

### TUESDAY AFTERNOON

#### Young Investigators in Nuclear & Radiochemistry

Sponsored by NUCL, Cosponsored by YCC

#### Excellence in Graduate Polymer Research

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### TUESDAY EVENING

#### Excellence in Graduate Polymer Research

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### WEDNESDAY MORNING

#### Young Investigators in Nuclear & Radiochemistry

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# EXPOSITION HIGHLIGHTS

**SEE WHAT'S NEW INSIDE THE EXPOSITION.** Visit the ACS National Exposition at the San Diego Convention Center (SDCC), Halls B/C, from Sunday, March 13, through Tuesday, March 15. The show hours will be Sunday, 6:00 to 8:30 PM, and Monday and Tuesday, 9:00 AM to 5:00 PM.

Companies will showcase services, instruments, books, computer hardware, scientific software, and an array of chromatographic, lab, and safety equipment. Technical personnel will give demonstrations, answer questions, and discuss your needs and interests.

You can also visit the ACS Career Fair Recruiters Row inside the exposition, where employers will showcase their products and services. Also, join us at the ACS Booth in the middle of the exposition floor, where ACS staff members will present the many benefits, services, products, and merchandise offered by ACS.

**Online Exposition.** The Online Exposition is a component within the Exhibitor

Directory that enables attendees to view videos, press releases, brochures, and flyers of participating exhibitors. Access the Online Exposition at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016) to learn more about exhibiting companies and download product information that meets your needs.

**Free Exhibitor Workshops.** Free workshops will be hosted by exhibitors on the exposition floor and in private rooms inside the San Diego Convention Center. These workshops will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications that may improve your productivity. Register at [www.acs.org/sandiego2016](http://www.acs.org/sandiego2016) to reserve your seat.

**Presentations & Special Events.** Join us on Sunday from 6:00 to 8:30 PM for the Attendee Welcome Reception. Also, visit the Town Center inside the exposition for poster sessions, to connect with colleagues, and to relax during the Tuesday afternoon break from 3:00 to

5:00 PM. Refreshments available while supplies last.

**Internet & Technology.** Get free Internet access and leave messages for one another at the Meeting Mail terminals inside the Town Center. Enjoy free Wi-Fi service at designated areas in the San Diego Convention Center.

**Admission Requirements & Expo-Only Registration.** Exposition admission is complimentary for all national meeting registrants; however, you are required to wear your badge. Individuals who want to visit the exhibits without registering for the technical component of the national meeting can obtain an expo-only badge for \$60. Students with school identification can obtain an expo-only badge for \$30. Registration can be handled online or in person at ACS Attendee Registration in the San Diego Convention Center, Lobby D, and at our satellite registration areas at the Manchester Grand Hyatt, Hilton San Diego Bayfront, and Westin San Diego.



ACS Exposition

## EXHIBITORS

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PROTO Manufacturing	327
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Waters Corp.	912
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# EXPOSITION

## 2016 NEW PRODUCT LISTINGS

### ACS Member Insurance Program

**Booth # 427**  
Chemical Educators Legal Liability  
Life Insurance  
Disability Income  
International Term Life Insurance

### AdValue Technology

**Booth # 1200**  
Ceramic membrane  
single crystal sapphire substrate  
polycrystalline sapphire tube  
cerium oxide polishing powder  
quartz cuvettes

### Ark Pharm, Inc.

**Booth # 804**  
2-Bromo-5H-pyrrolo[2,3-b]pyrazine,  
875781-43-4  
2,6-Dichloro-4-methyl-3-nitropyridine,  
5043-79-8  
5-Fluoropicolinaldehyde, 31181-88-1  
2-Amino-4-bromobenzaldehyde, 59278-65-8  
4-Iodo-1H-pyrrole-2-carbaldehyde, 33515-62-7

### Avantor Performance Materials

**Booth # 714**  
J.T. Baker HPLC Sugars  
J.T. Baker Direct Dispense Packaging  
J.T. Baker Process Chromatography

### BioChromato (Amuza Inc.)

**Booth # 329**  
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Smart Evaporator C10

### Biolin Scientific

**Booth # 100**  
QCM-D QTools

### BrandTech Scientific

**Booth # 917**  
Dispensette® S Bottletop Dispenser

### Camag Scientific, Inc.

**Booth # 121**  
TLC-MS Interface  
DBS-MS 500  
Automatic TLC Sampler 4 (ATS4)  
TLC Visualizer  
Automatic Developing Chamber 2 (ADC2)

### Cambridge Crystallographic Data Ctr.

**Booth # 926**  
CSD-System  
CSD-Enterprise  
CSD-Discovery  
CSD-Materials  
CSD-Community

### Carbosynth LLC

**Booth # 1217**  
IPTG  
EDAC  
OG  
X-GAL

### ChemAxon LLC

**Booth # 328**  
Plexus Suite  
MarvinSketch  
Marvin Live  
ChemCurator  
JChem for Office

### Chemrus Inc.

**Booth # 1334**  
disposable filter funnels  
multi-flask reaction kit  
Liu flasks  
reaction blocks

### Combi-Blocks, Inc.

**Booth # 1407**  
Deuterated boronic acids  
Amino acids  
Chiral compounds

### CombiPhos Catalysts, Inc.

**Booth # 805**  
Deuterated Reagents  
Deuterated Drugs  
Novel Boronic acids  
Cross-coupling products  
Cross-coupling catalysts

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Torch  
Spark  
Forge  
Blaze

### CrunchYard

**Booth # 1437**  
ADF  
AMBER  
GROMACS  
CP2K  
GAMNESS

### CrystalMaker Software Ltd.

**Booth # 831**  
CrystalMaker 9.2  
CrystalViewer 9.2  
CrystalDiffract 6.5  
SingleCrystal 2.3

### Delong America

**Booth # 1414**  
LVEM5 (TEM/SEM/STEM)  
LVEM25 (TEM/STEM)

### Ecodyst, Inc.

**Booth # 1442**  
EcoChyll  
Self cooling technology  
coolant free chiller

### FEI Company

**Booth # 1518**  
Teneo (VolumeScope) Scanning Electron  
Microscope  
Quanta Scanning Electron Microscope Family  
with  
Talos Scanning/Transmission Electron  
Microscope  
Titan Themis Transmission Electron Microscope  
Titan ETEM Themis

### Focus Synthesis, LLC

**Booth # 1535**  
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Cheminformatic Gap Fillers

### Gamry Instruments

**Booth # 800**  
Reference 600+ Potentiostat/Galvanostat/ZRA  
Interface 1000T Potentiostat

### Gaussian

**Booth # 719**  
Gaussian  
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### Grace Discovery Sciences

**Booth # 417**  
Reveleris Prep

### GlycoSurface LLC

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Workshop Publication Techniques  
Course Scientific Publication Techniques  
Computational Biophysics  
Epithelial Cell Culture Training

### Harrick Scientific

**Booth # 1418**  
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ConcentratIR2 ATR/FTIR accessory

### Hielscher Ultrasonics

**Booth # 813**  
MPC48 - Insert for Ultrasonic Reactor  
Ultrasonic Closed Batch Reactor  
UIP400St: Digital Ultrasonic Lab Homogenizer  
(400W)  
UIP2000hdT: Digital Ultrasonicator for Industry  
UIP4000hdT: Digital Power-Ultrasound Device  
(4kW)

### HORIBA Scientific

**Booth # 1016**  
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LabRAM HR Evolution  
FluoroMax and FluoroMax Plus  
Aqualog  
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### Inert

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PureLab  
I-Lab  
ClearLab  
PureSolv  
PureSolv Micro

### InfoChem GmbH

**Booth # 815**  
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ICFRP  
SPRESImobile  
Patent databases  
ICC cartridge

### Inte:Ligand GmbH

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### Japan Analytical Industry Co. Ltd.

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5060  
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### Kimble Chase LLC

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Universal Tube Rack  
Media Bottle Starter Pack  
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### KNF Neuberger

**Booth # 1026**  
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Vacuum Controller VC 900  
Vacuum Pump N 920 G  
Dual Vacuum System SCC 950

### Knauer

**Booth # 211**  
AZURA Bio LC system  
Analytical HPLC/UHPLC  
Preparative LC system  
Educational HPLC system  
LC columns

### Magna-Safe International

**Booth # 107**  
Microreactor

### Malvern Instruments, Inc.

**Booth # 1410**  
OMNISEC  
MicroCal PEAQ-ITC

### Materials Design, Inc.

**Booth # 1104**  
Medea® atomistic modeling environment  
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Services  
Medea® Instrument hardware

### Mettler-Toledo AutoChem, Inc.

**Booth # 206**  
EasySampler

### MicroLAB, Inc.

**Booth # 226**  
FS-528 Laboratory Data System  
Visual Spectrometer  
Energy of Light/Planck's Constant module

**Minesoft**  
**Booth # 310**  
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PatBase  
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PatBase Express  
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**Nacalai USA, Inc.**  
**Booth # 1433**  
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cosmocore  
Cholesterol  
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**Oakwood Products Inc.**  
**Booth # 1404**  
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1-Isocyanato-1-(trifluoromethyl)cyclopropane  
5-Chloro-4-(trifluoromethyl)pyridin-2-amine  
hydroc  
1-Chloro-3-(2,2,2-trifluoroethyl)benzene

**Parr Instrument Co.**  
**Booth # 1401**  
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**Particle Sizing Systems**  
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POLAR3 Polarimeter  
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Instrument

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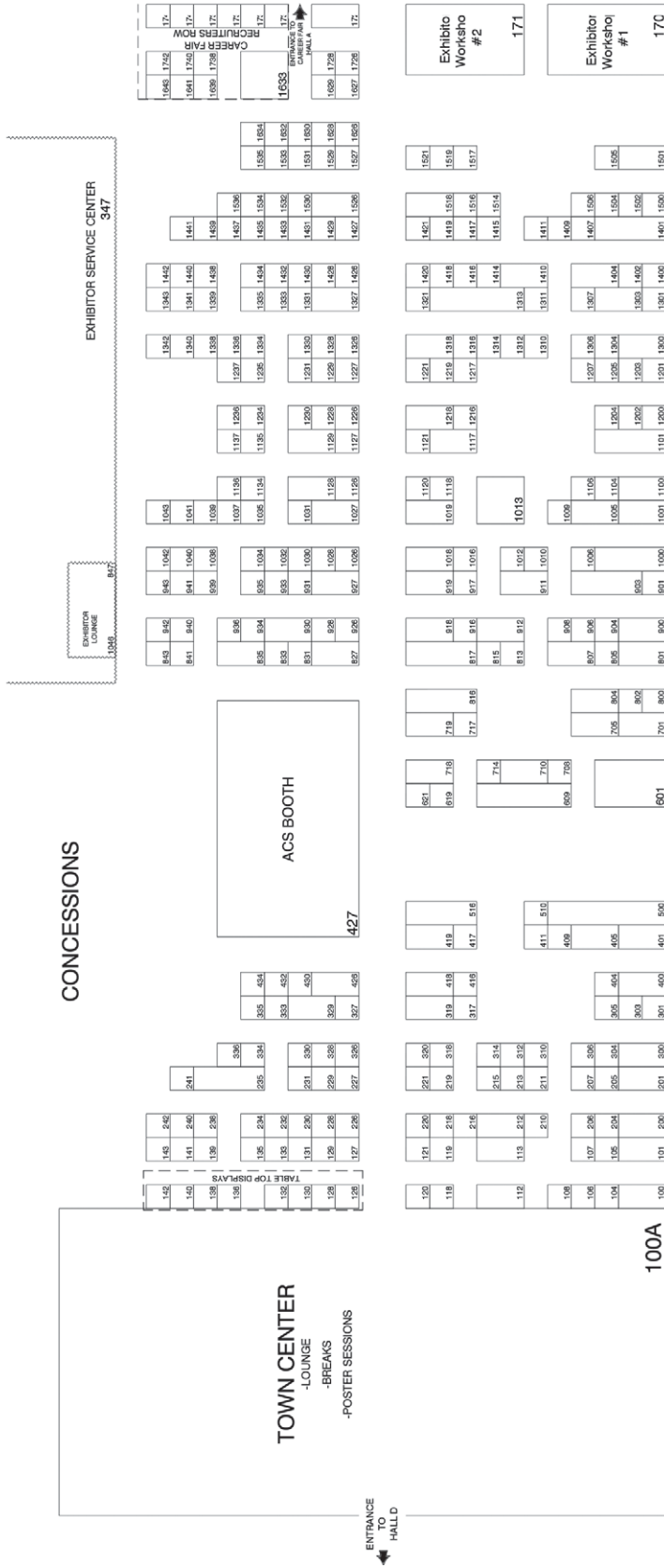
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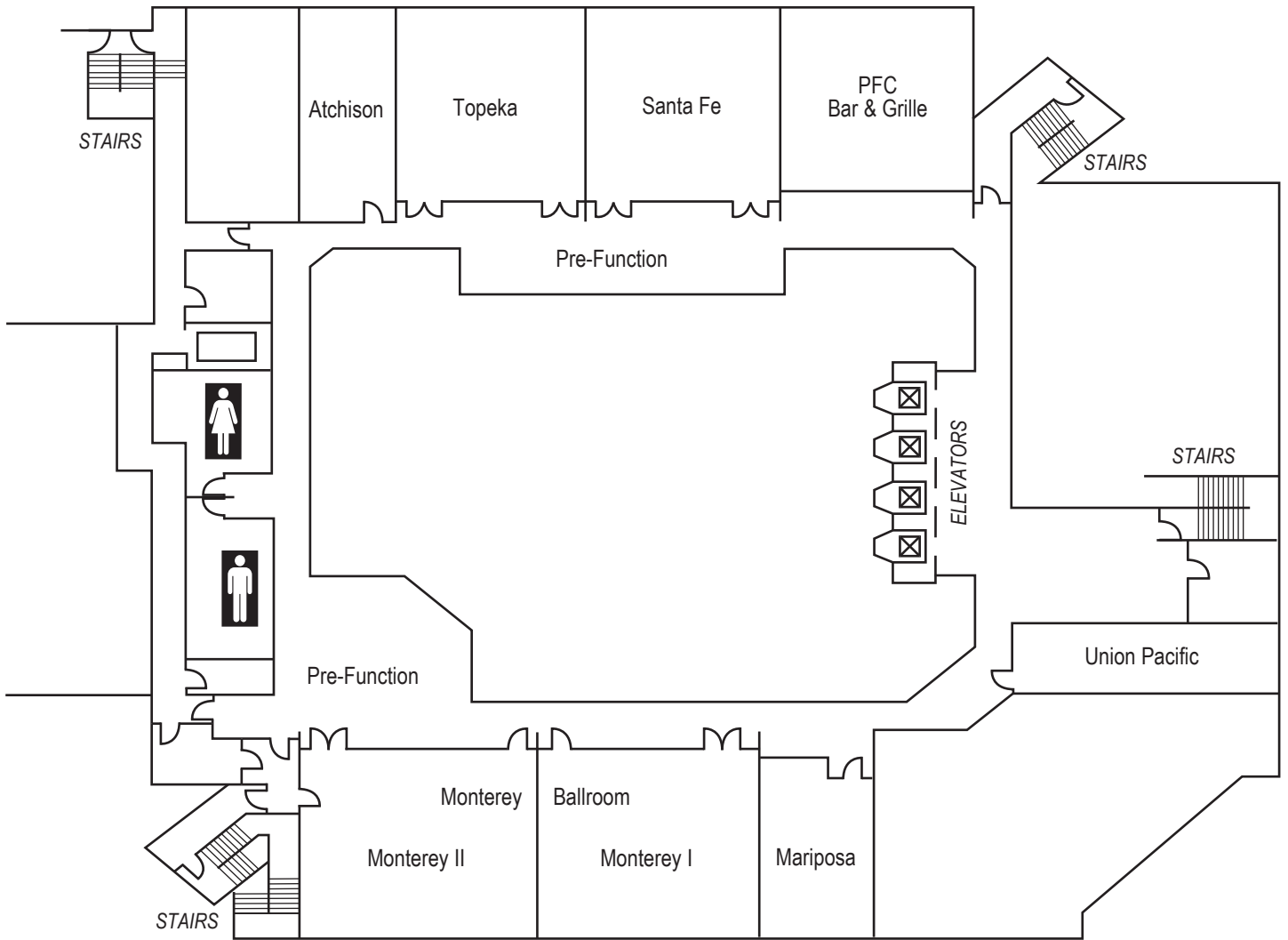
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# Authors

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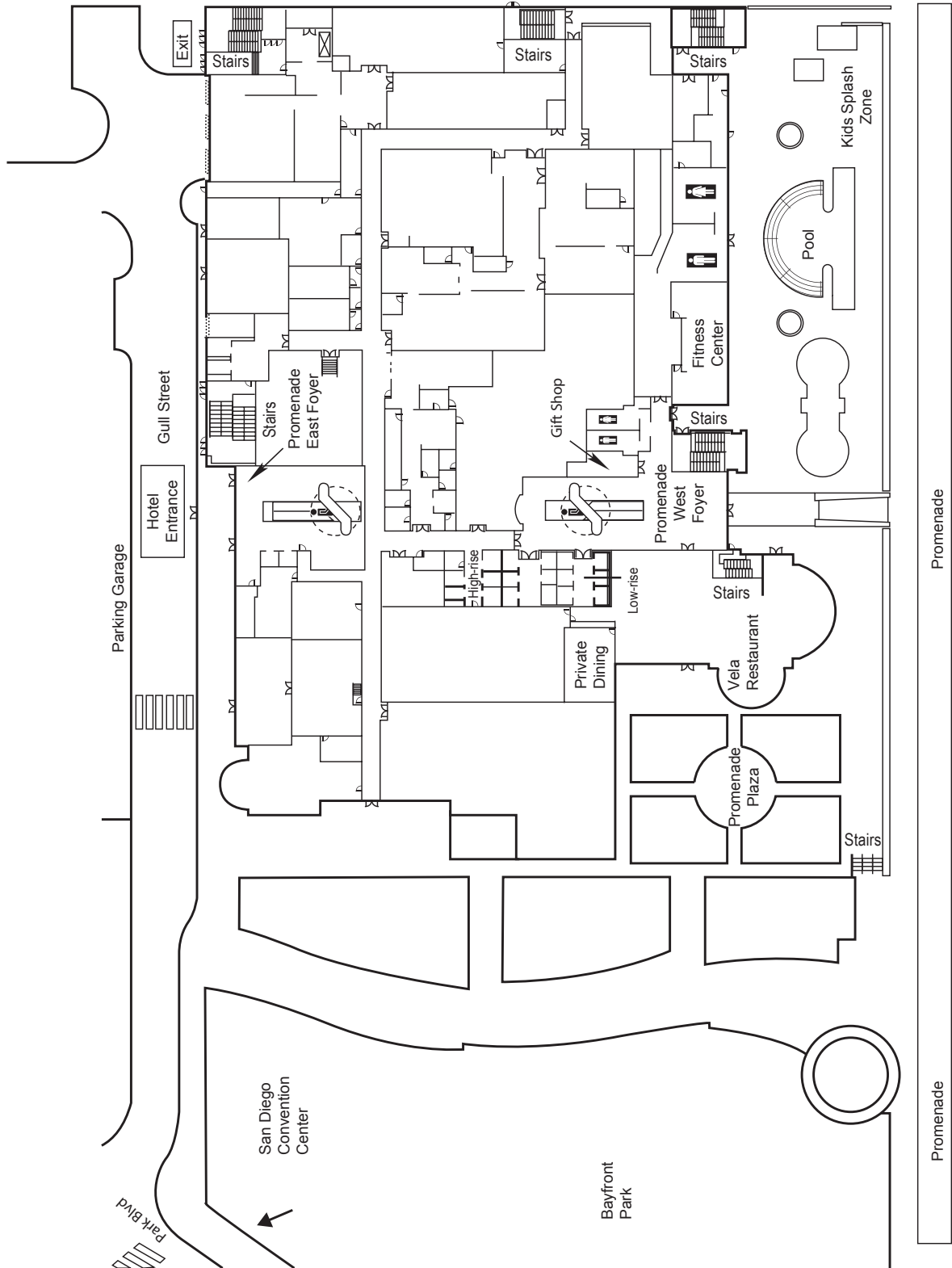




# HILTON BAYFRONT

## Promenade Level

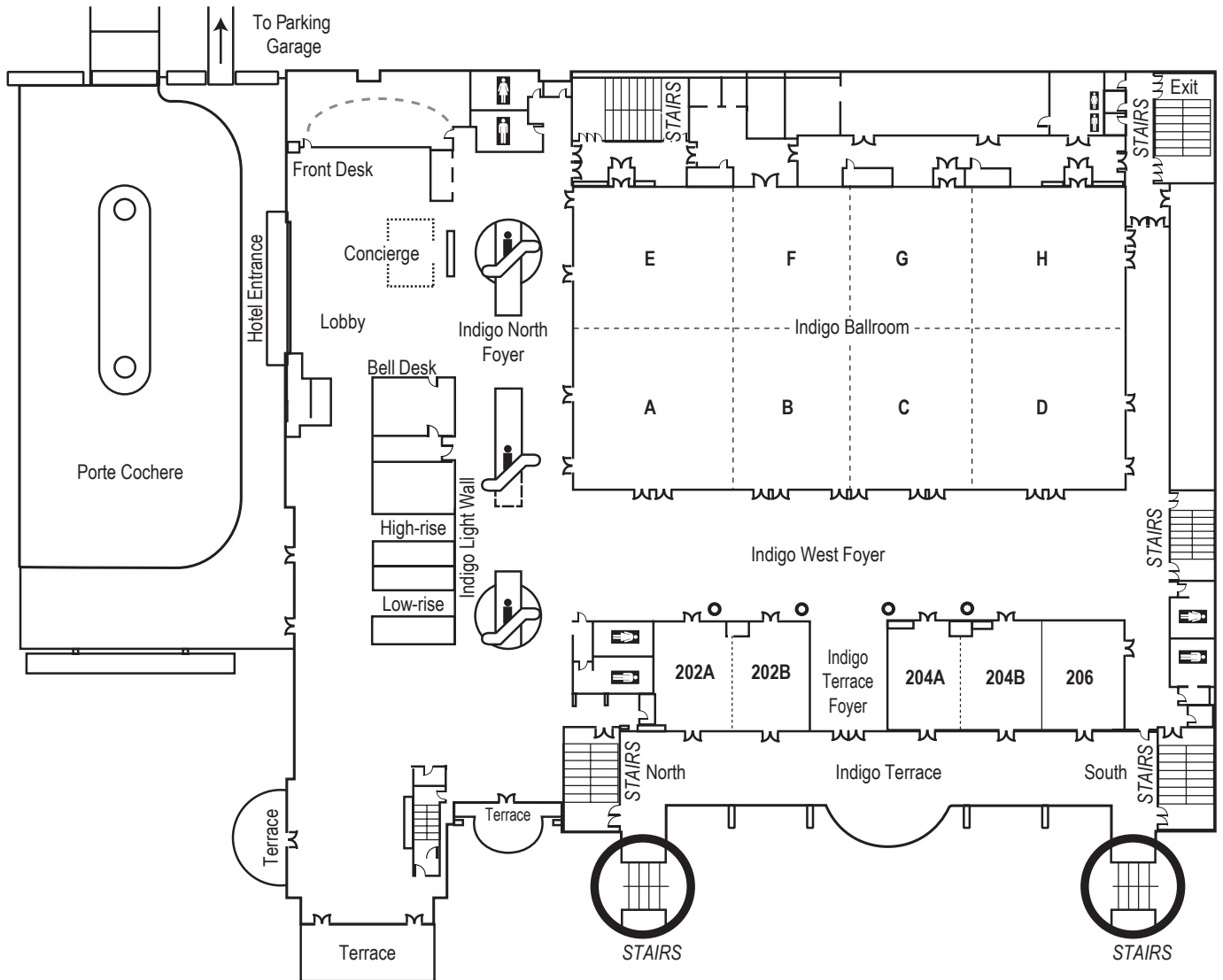
First Floor



# HILTON BAYFRONT

## Indigo Level

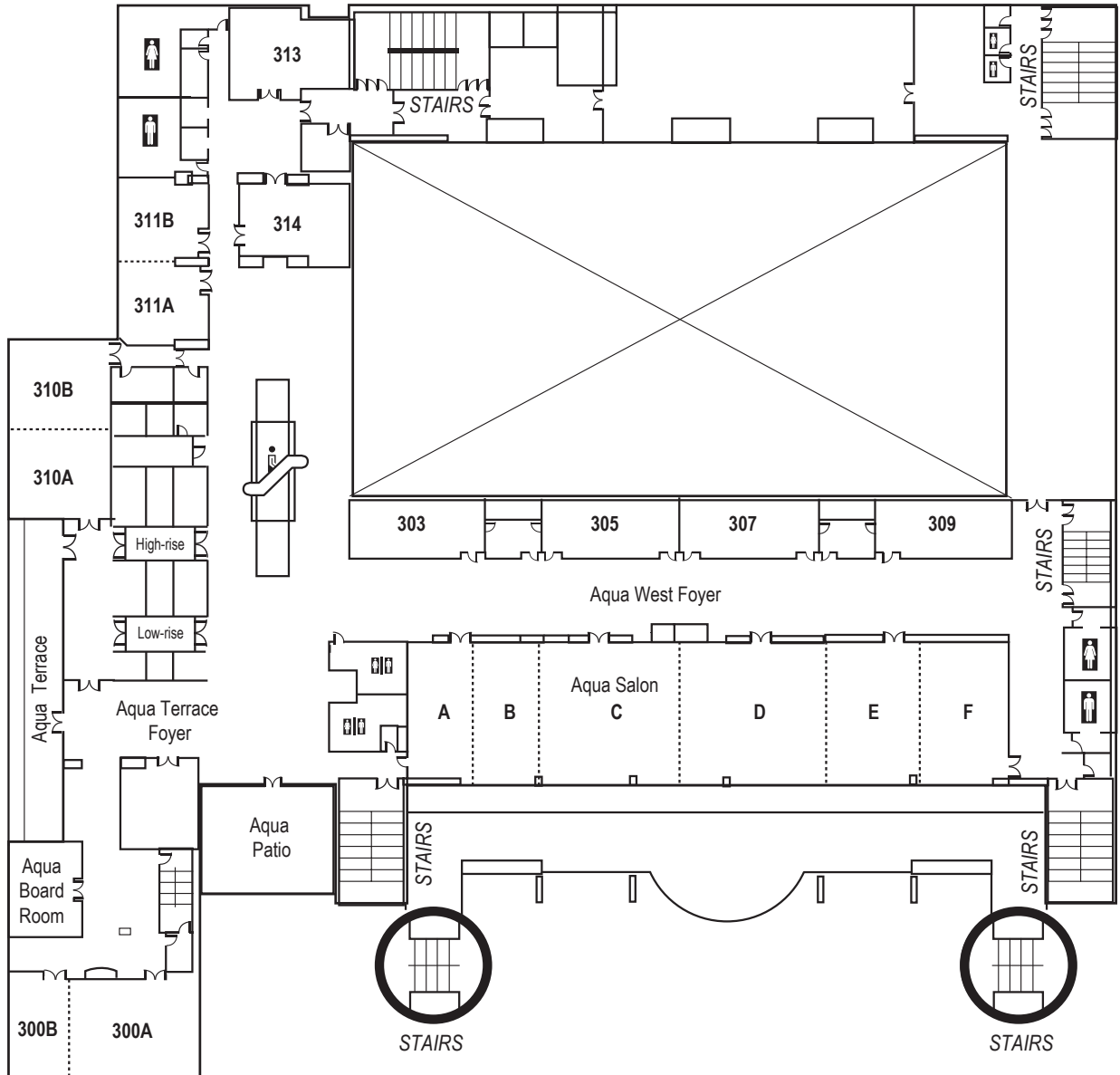
Second floor



# HILTON BAYFRONT

## Aqua Level

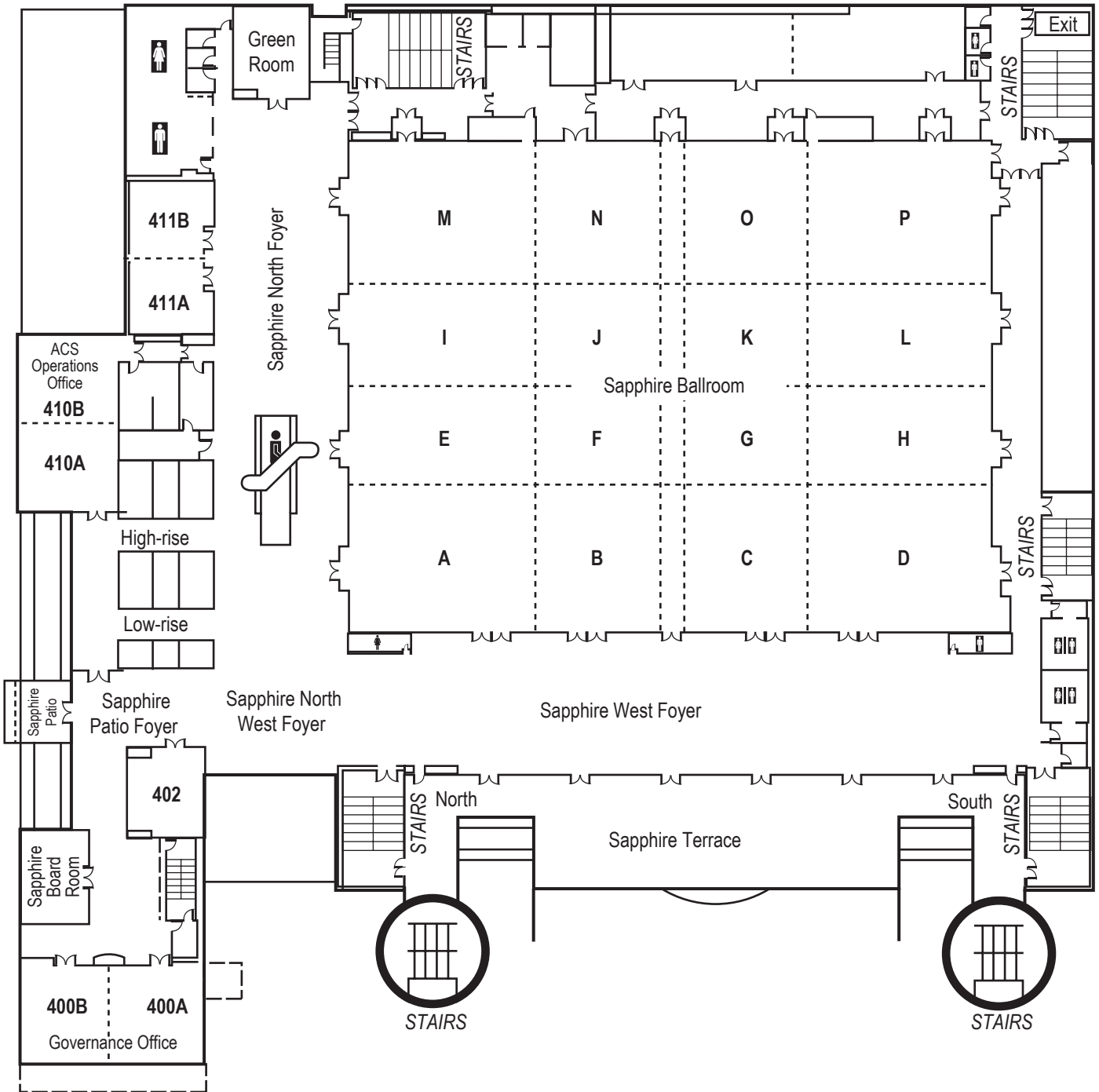
### Third Floor



# HILTON BAYFRONT

## Sapphire Level

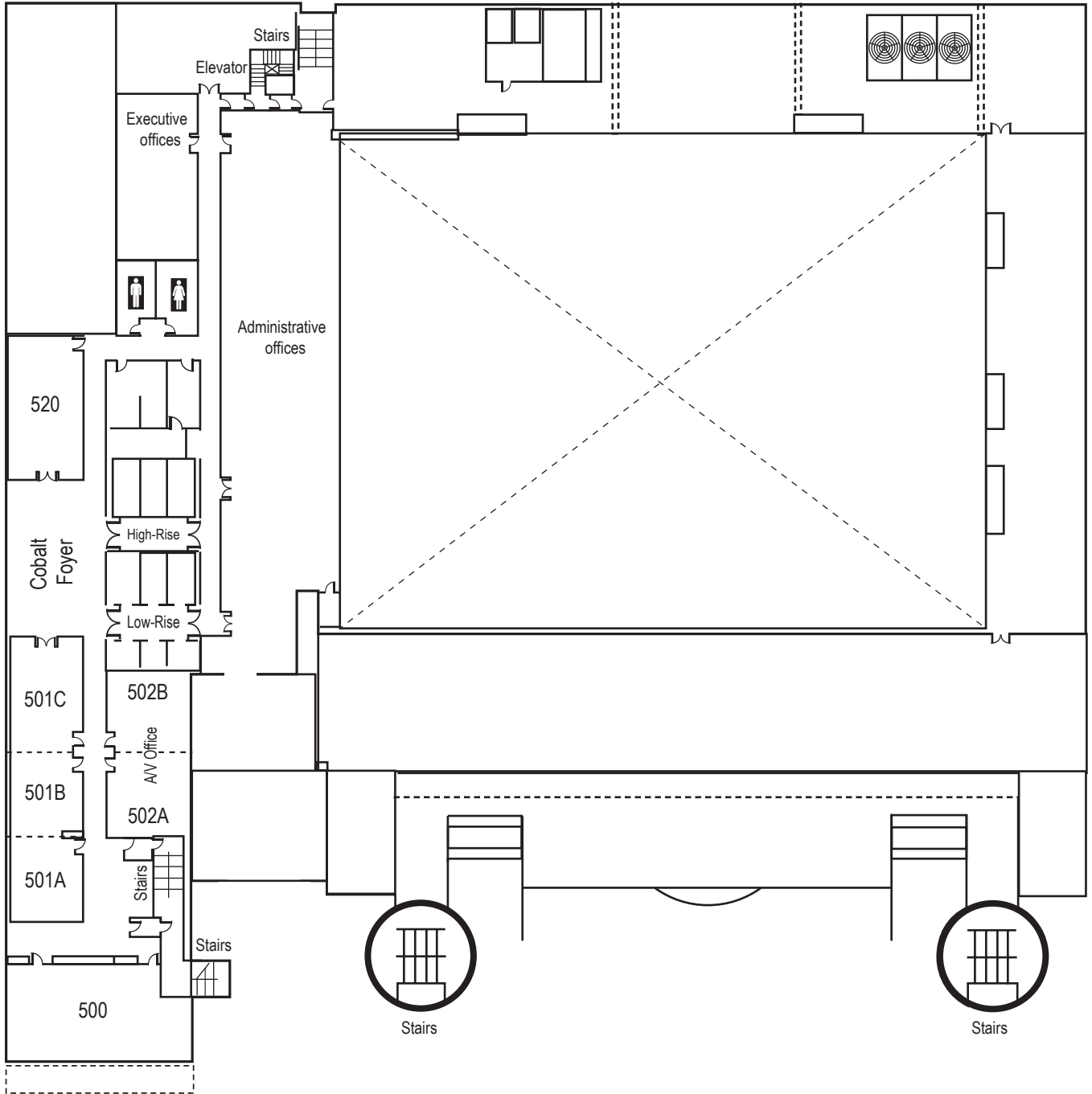
Fourth Floor



# HILTON BAYFRONT

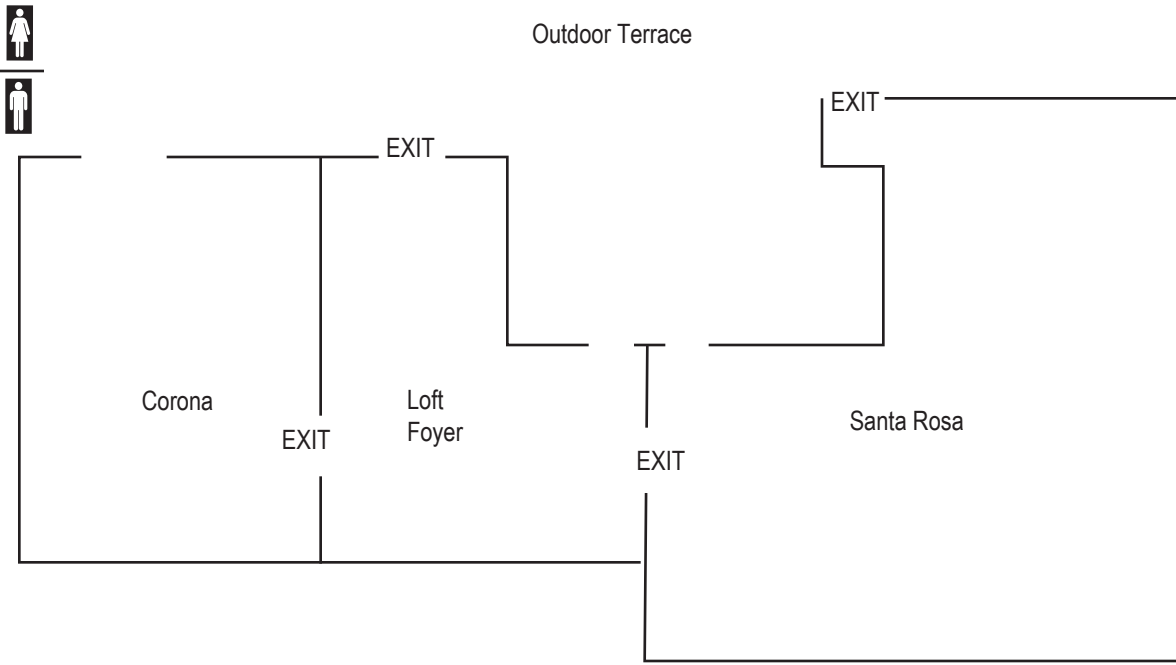
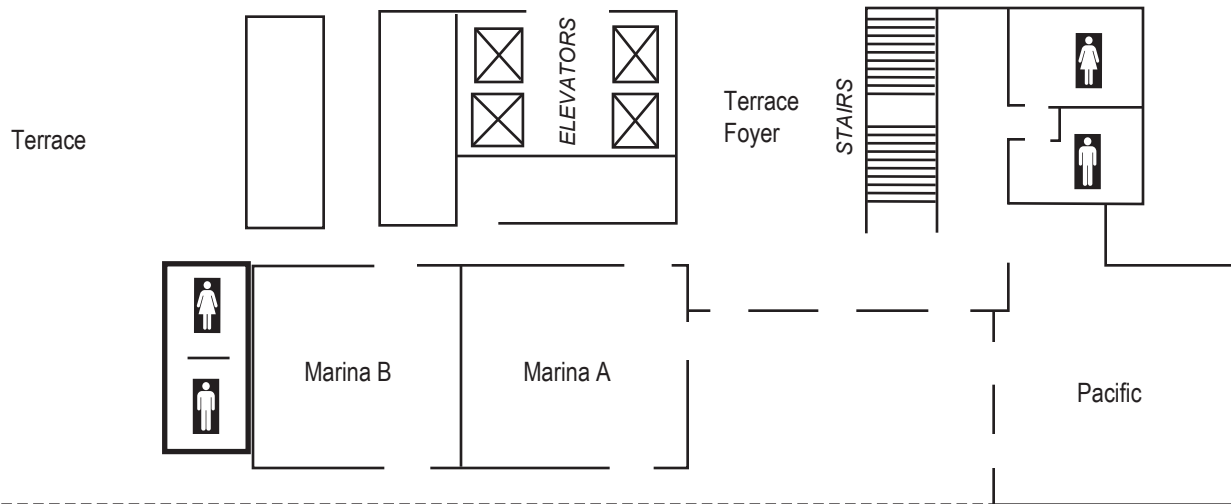
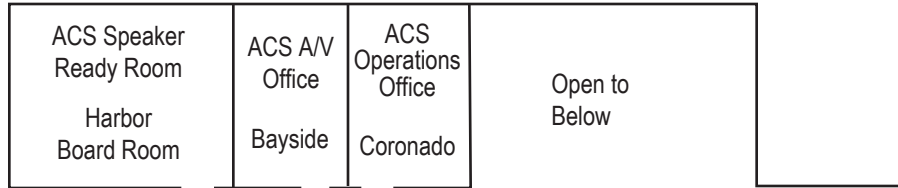
## Cobalt Level

### Fifth Floor



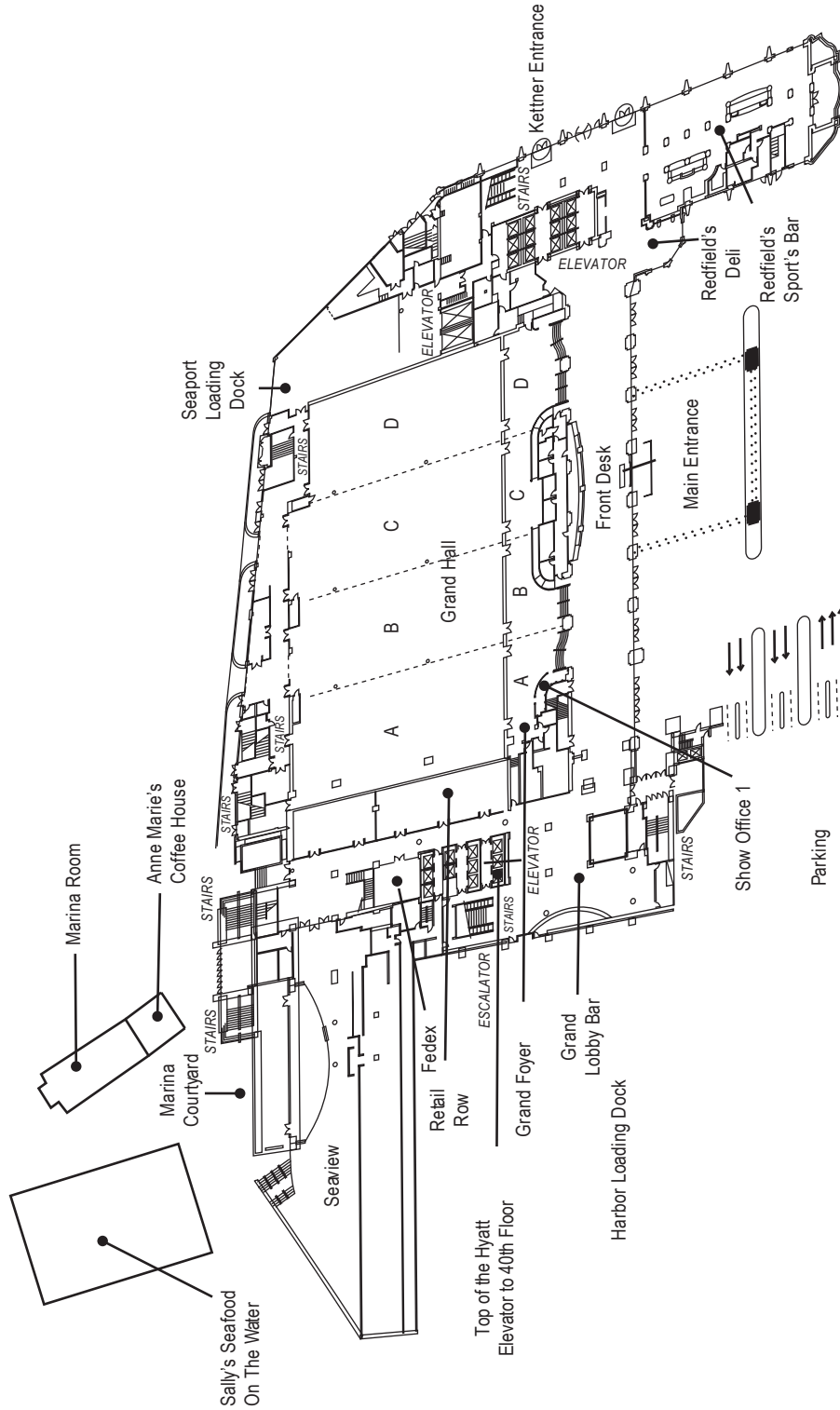
# Hilton Gaslamp

## Function Space



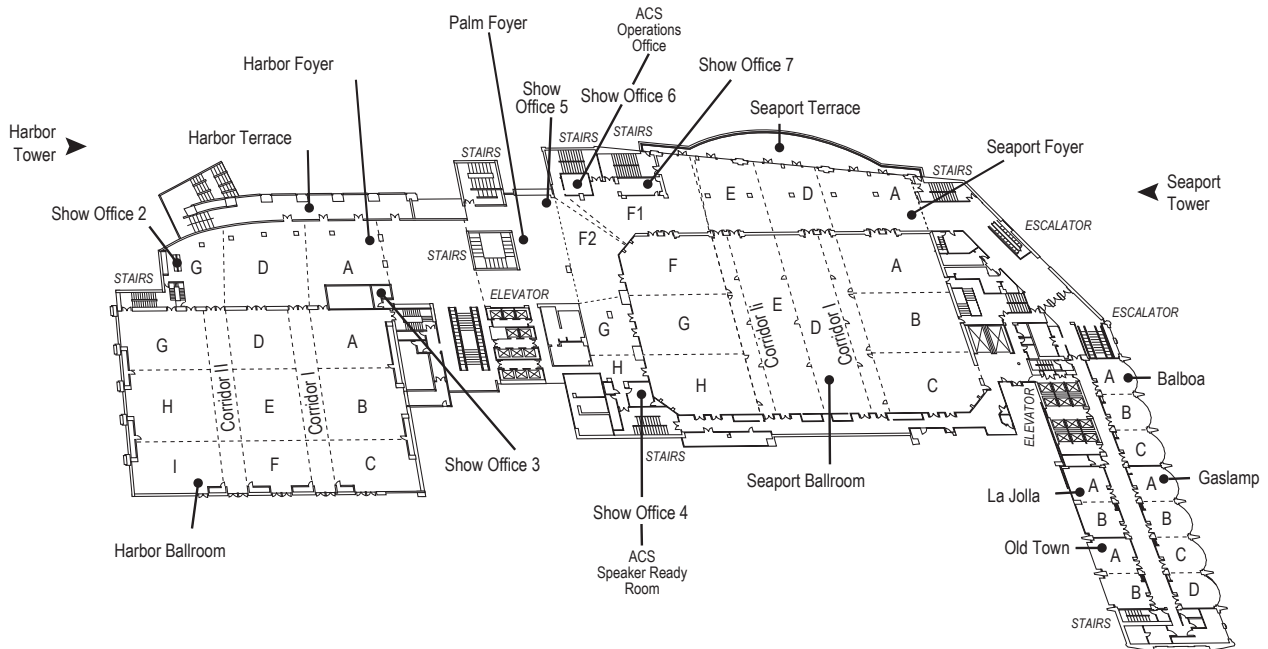
# MANCHESTER GRAND HYATT

## Lobby Level

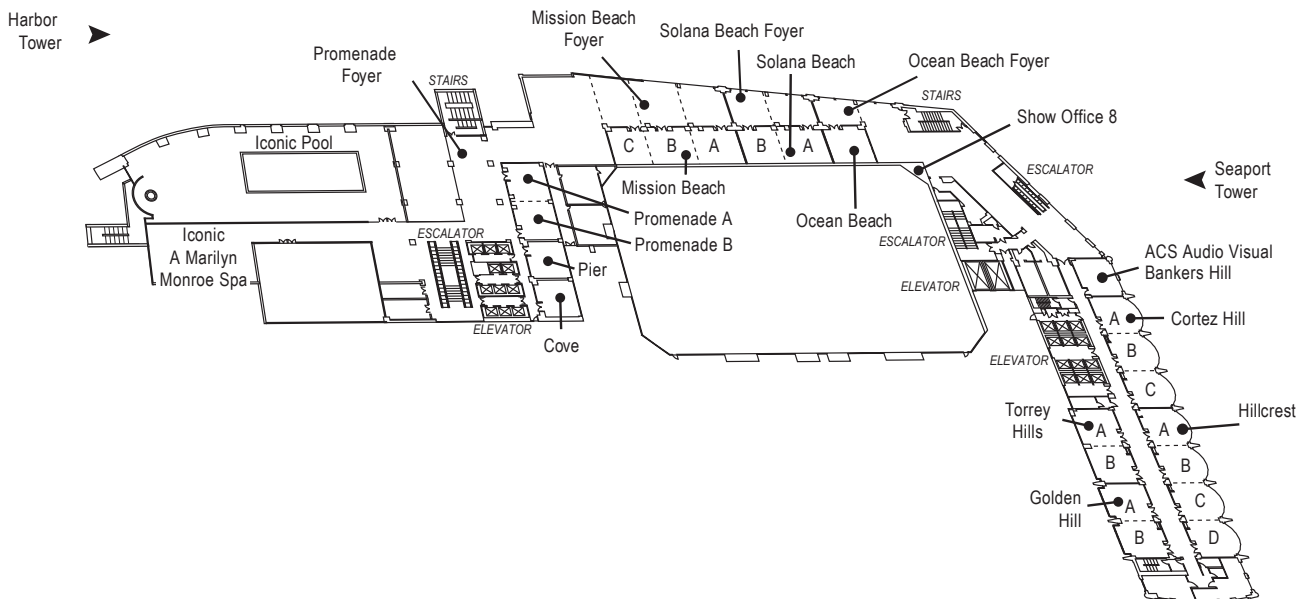


# MANCHESTER GRAND HYATT

## Second level



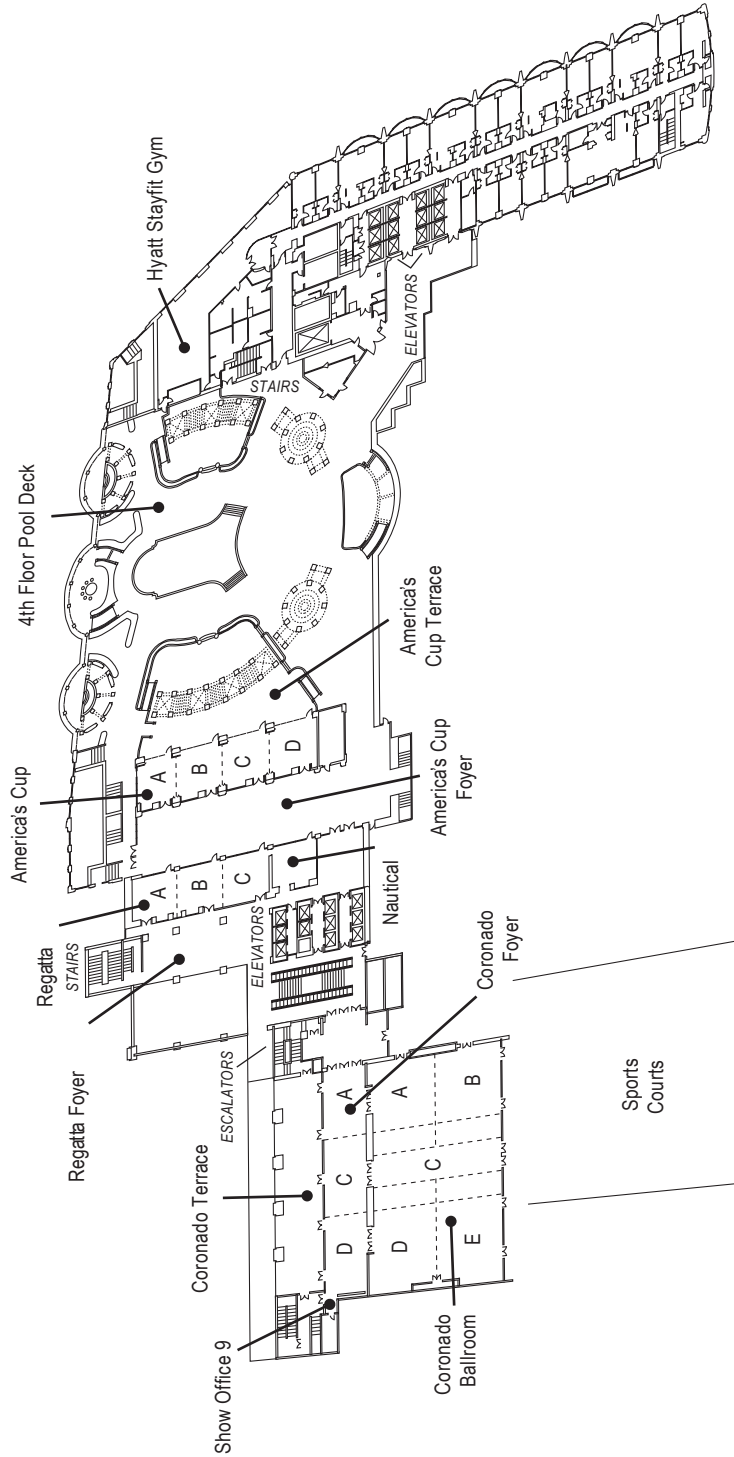
## Third Level





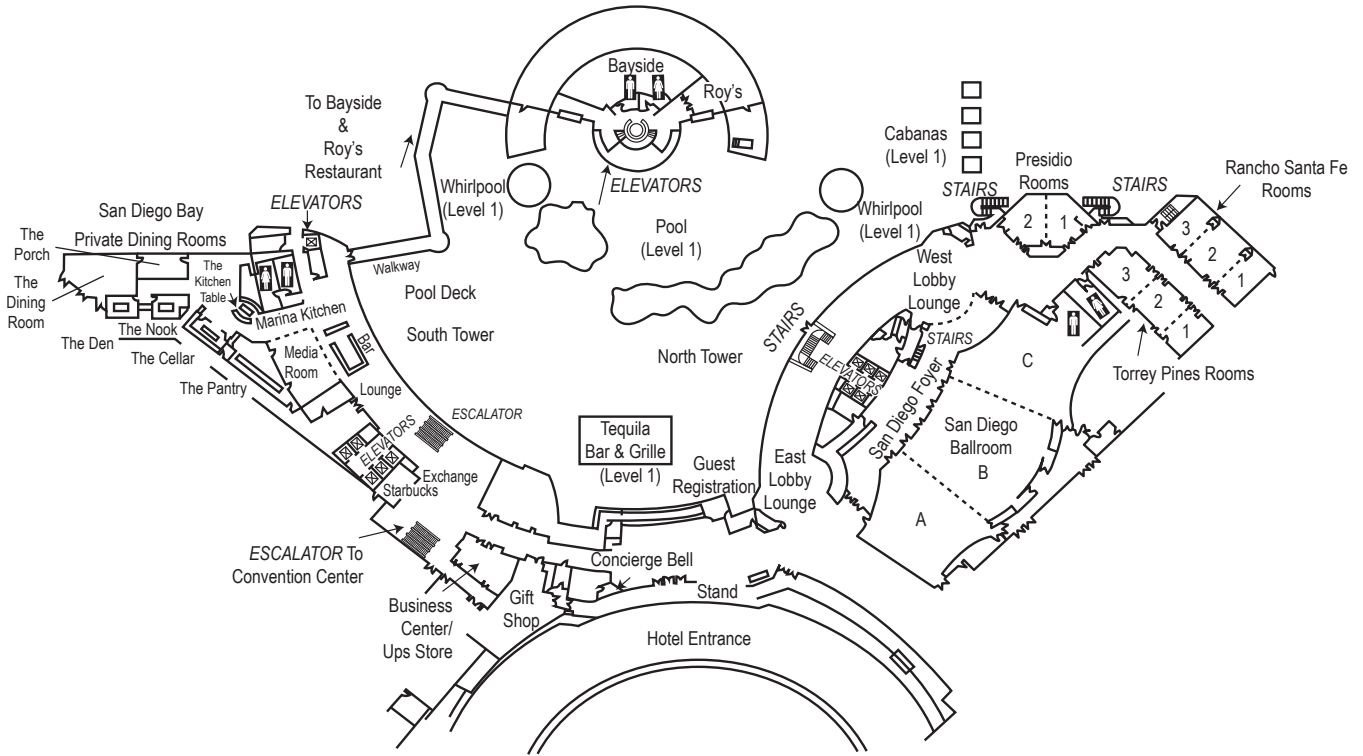
# MANCHESTER GRAND HYATT

## Fourth Level



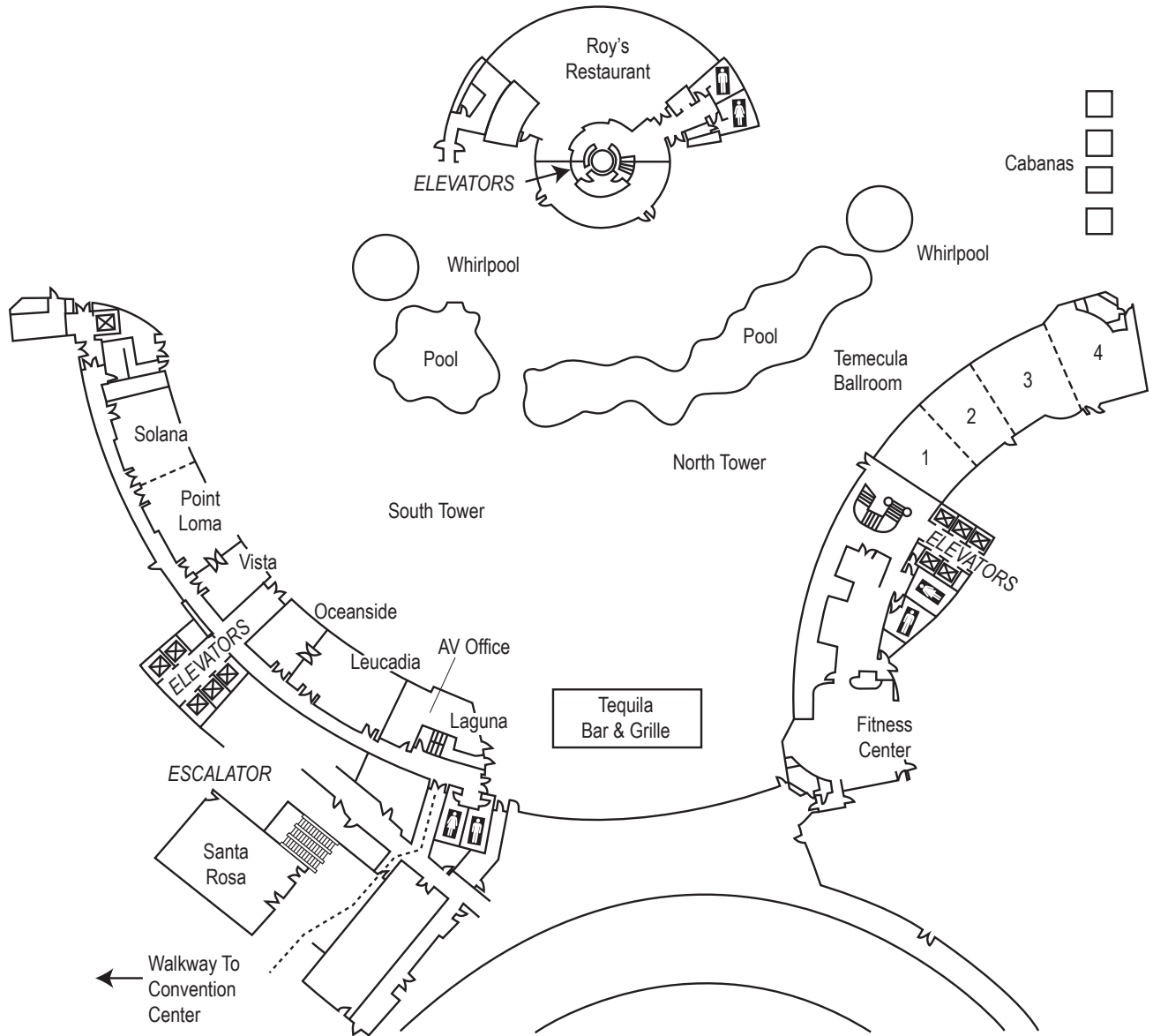
# MARRIOTT MARQUIS

## Lobby Level



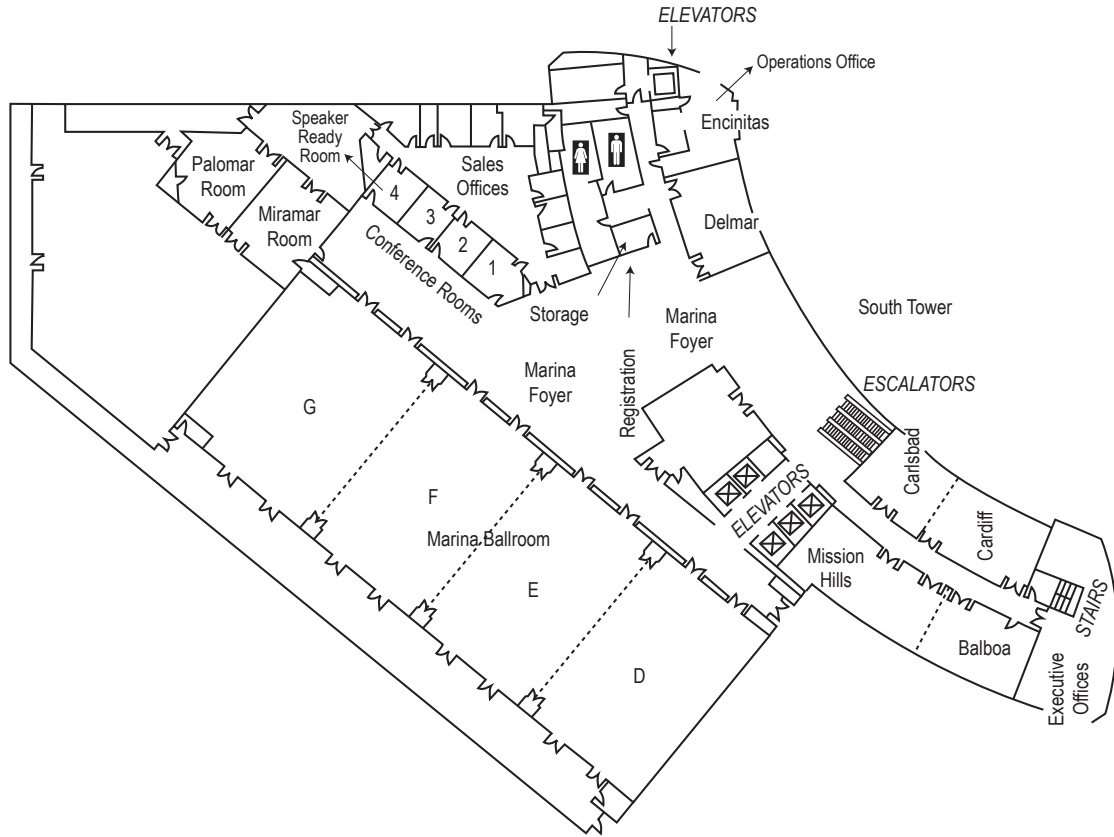
# MARRIOTT MARQUIS

## First Floor

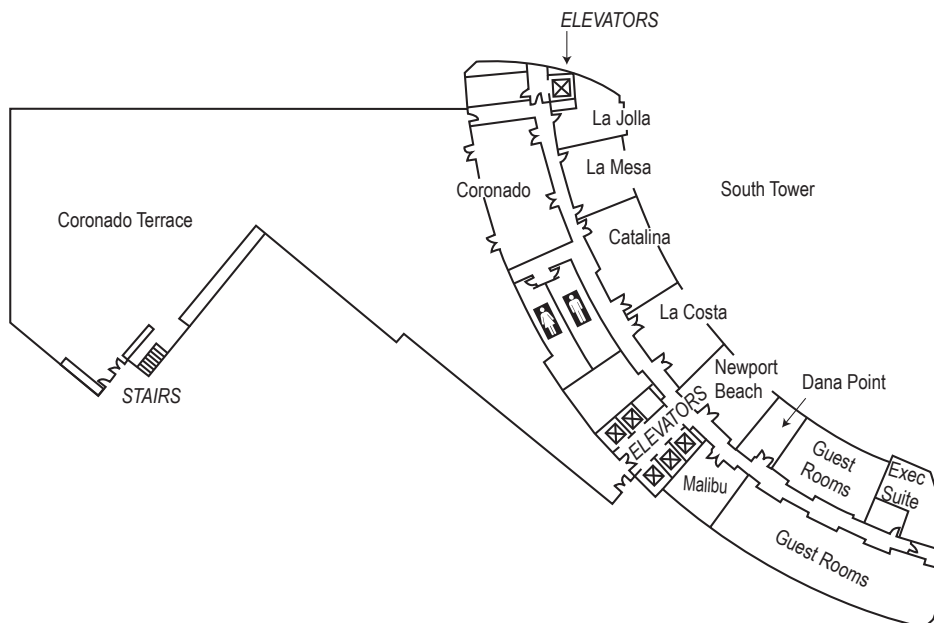


# MARRIOTT MARQUIS

## Third Floor

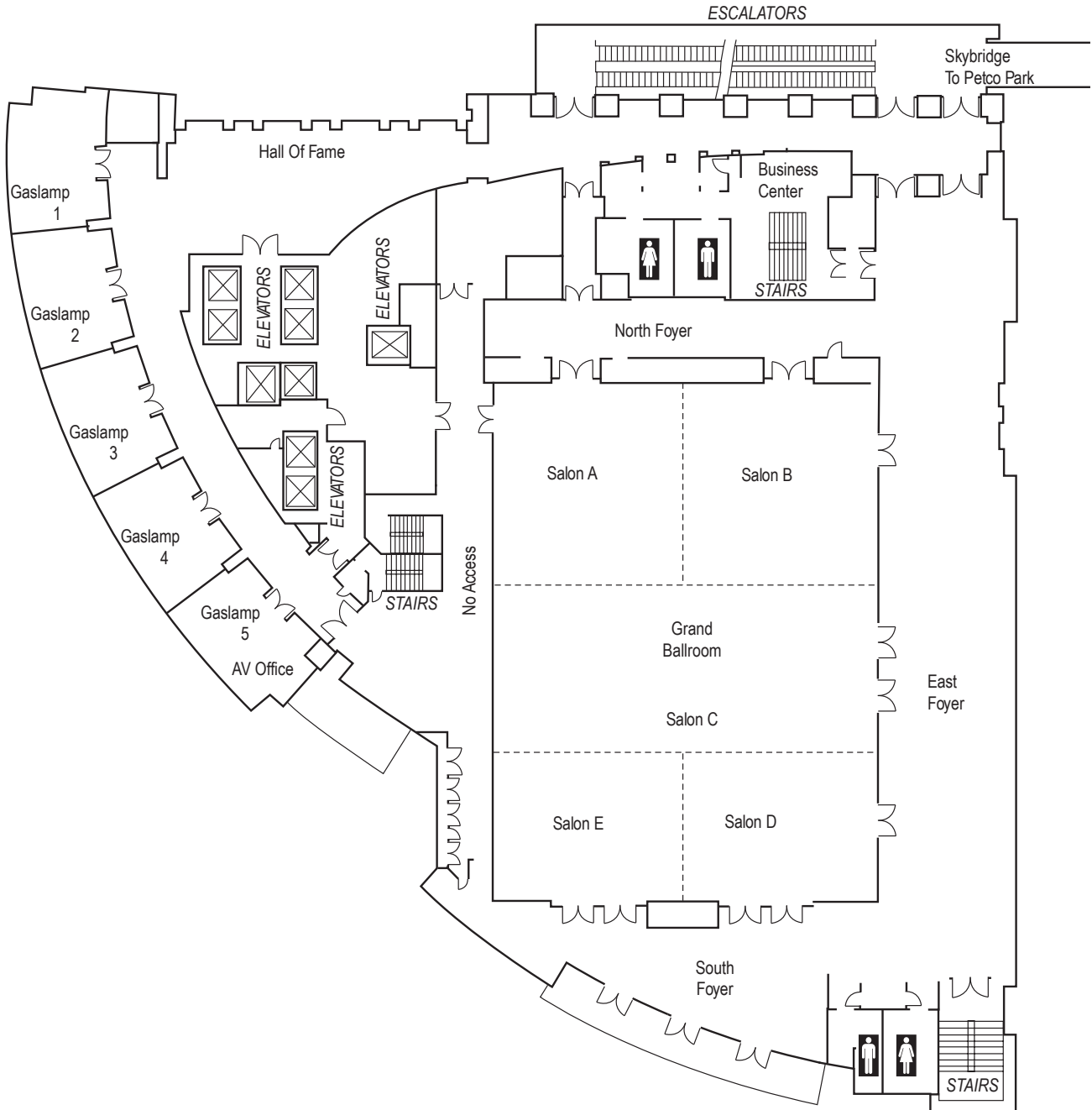


## Fourth Floor



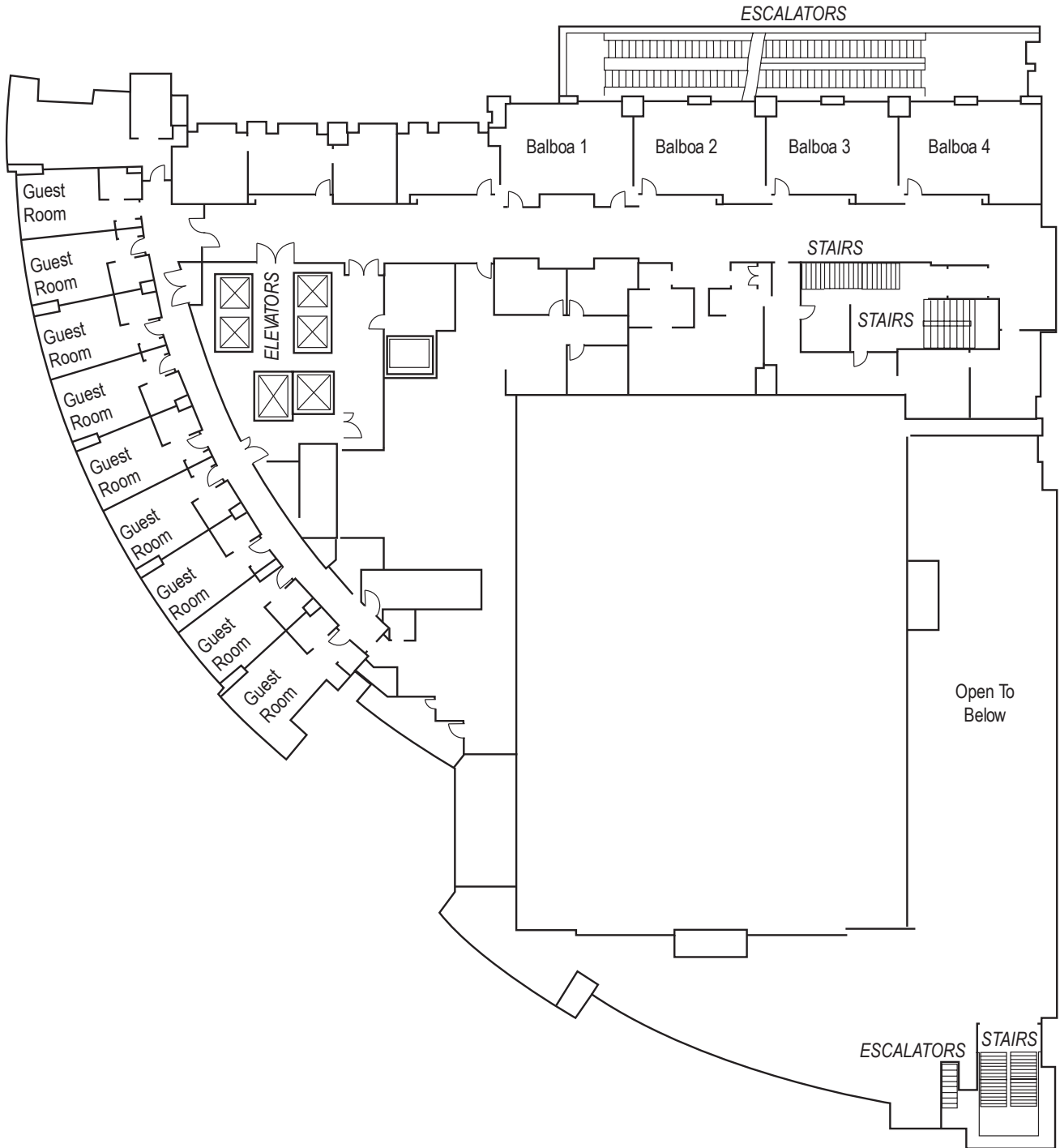
# OMNI

## Fourth Floor



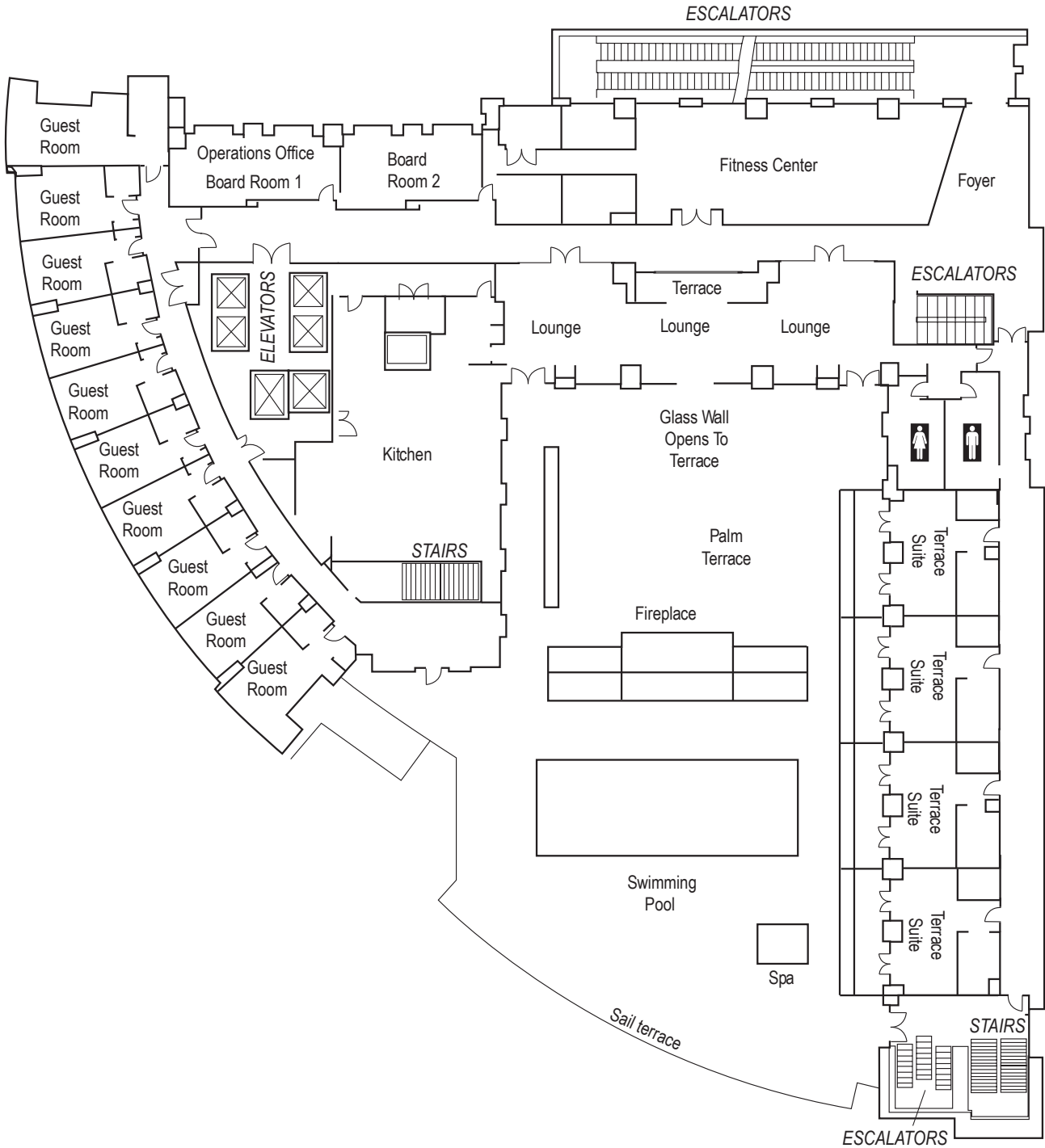
# OMNI

## Fifth Floor



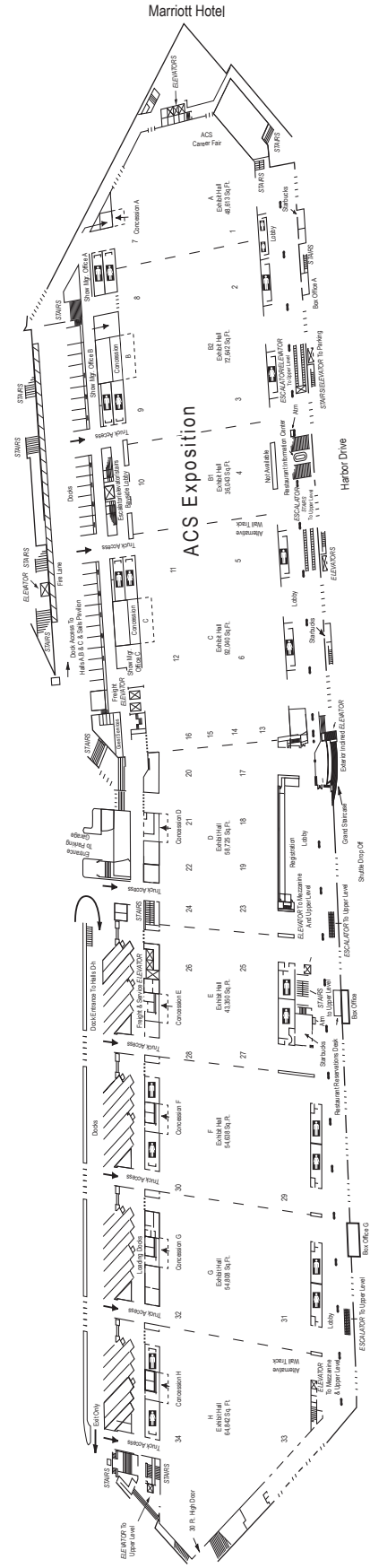
# OMNI

## Sixth Floor



# SAN DIEGO CONVENTION CENTER

## Ground Level View

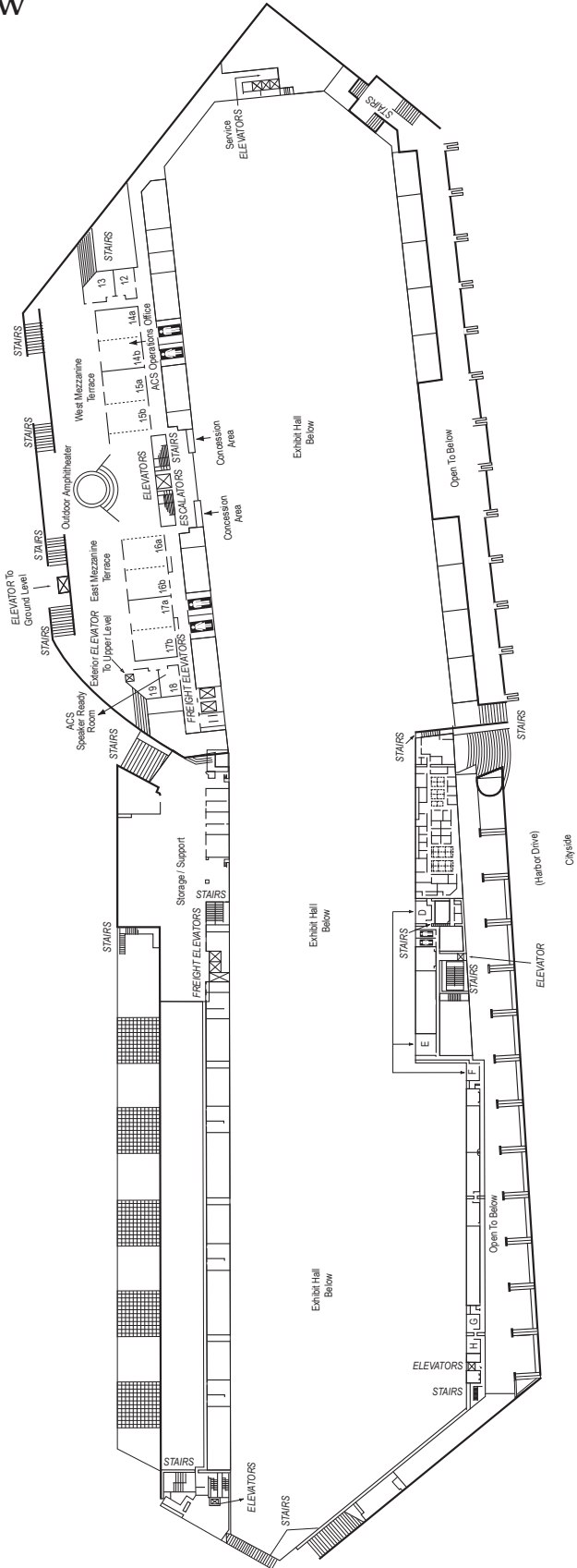




# SAN DIEGO CONVENTION CENTER

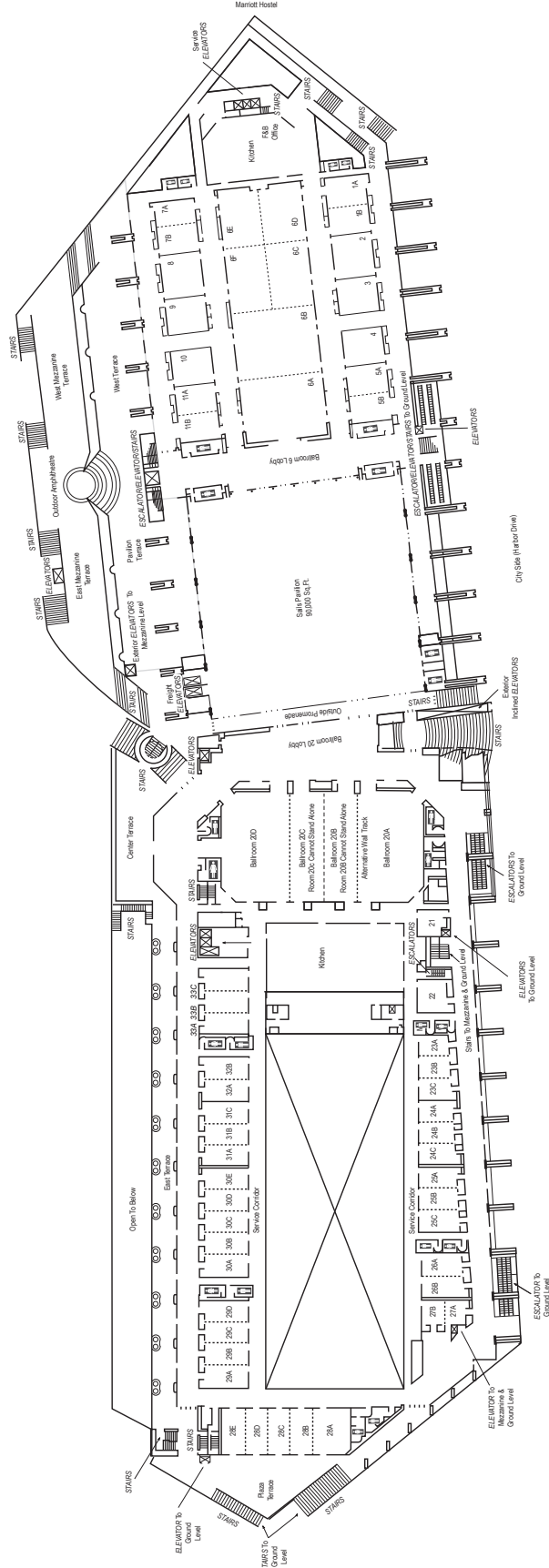
## Mezzanine Level View

Marriott Hotel



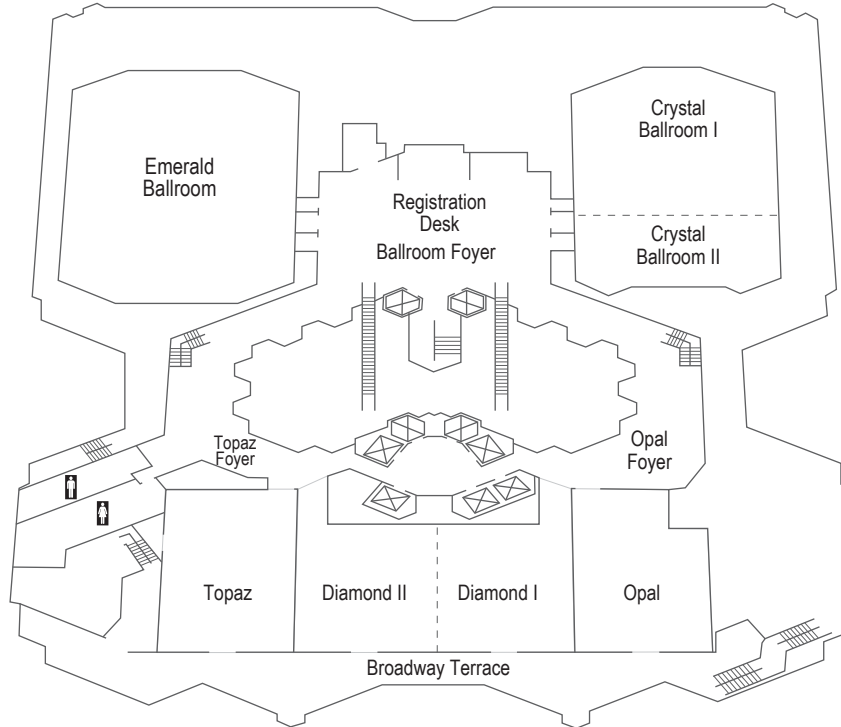
# SAN DIEGO CONVENTION CENTER

## Upper Level View

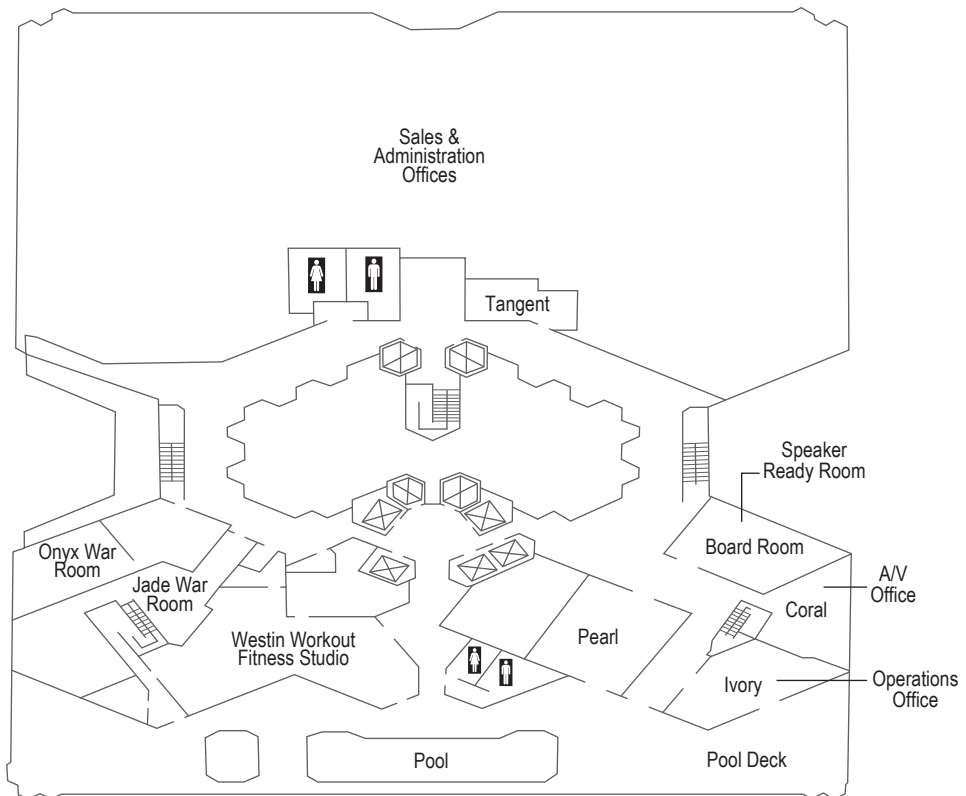


# THE WESTIN SAN DIEGO

## Level 2

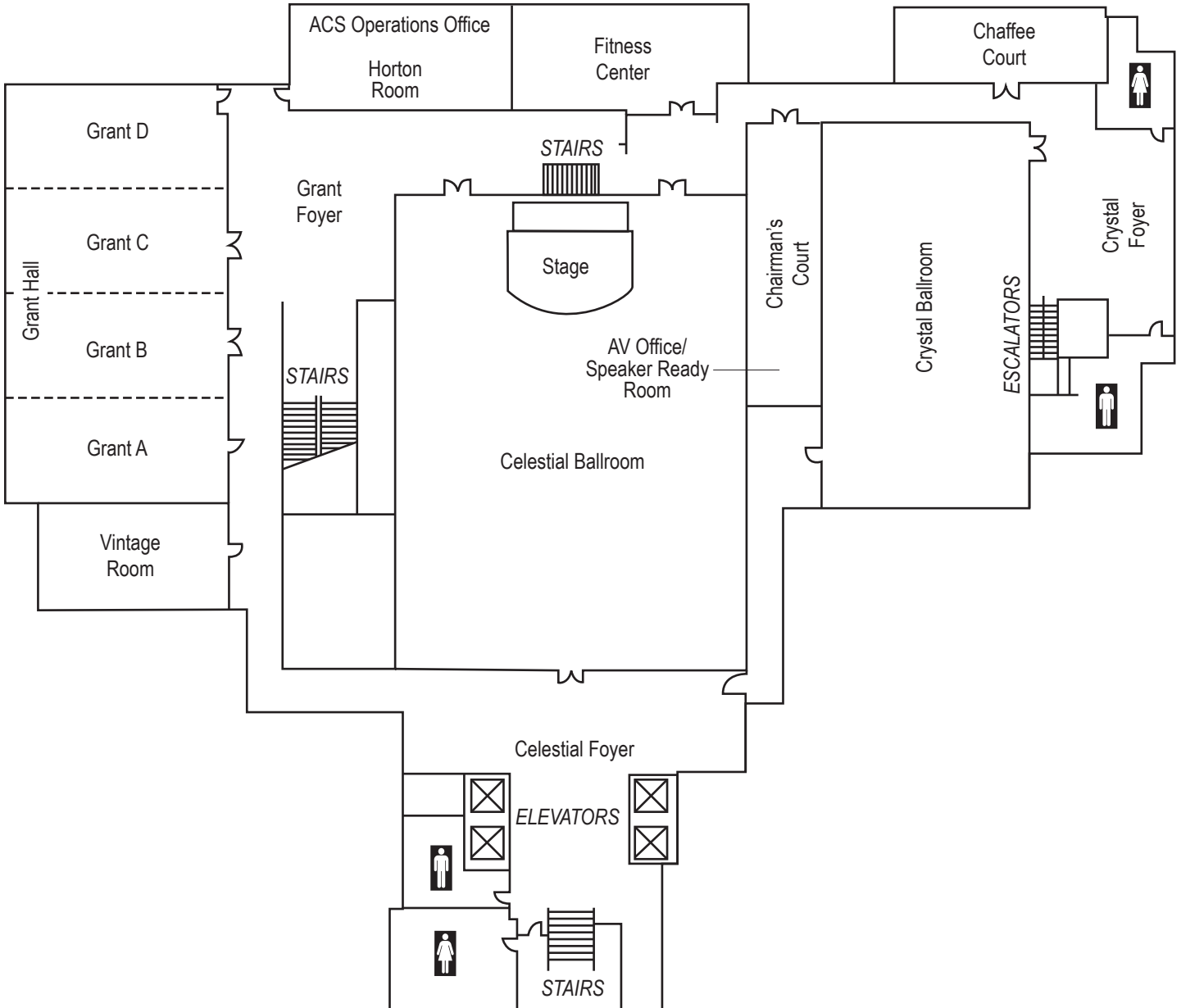


## Level 3



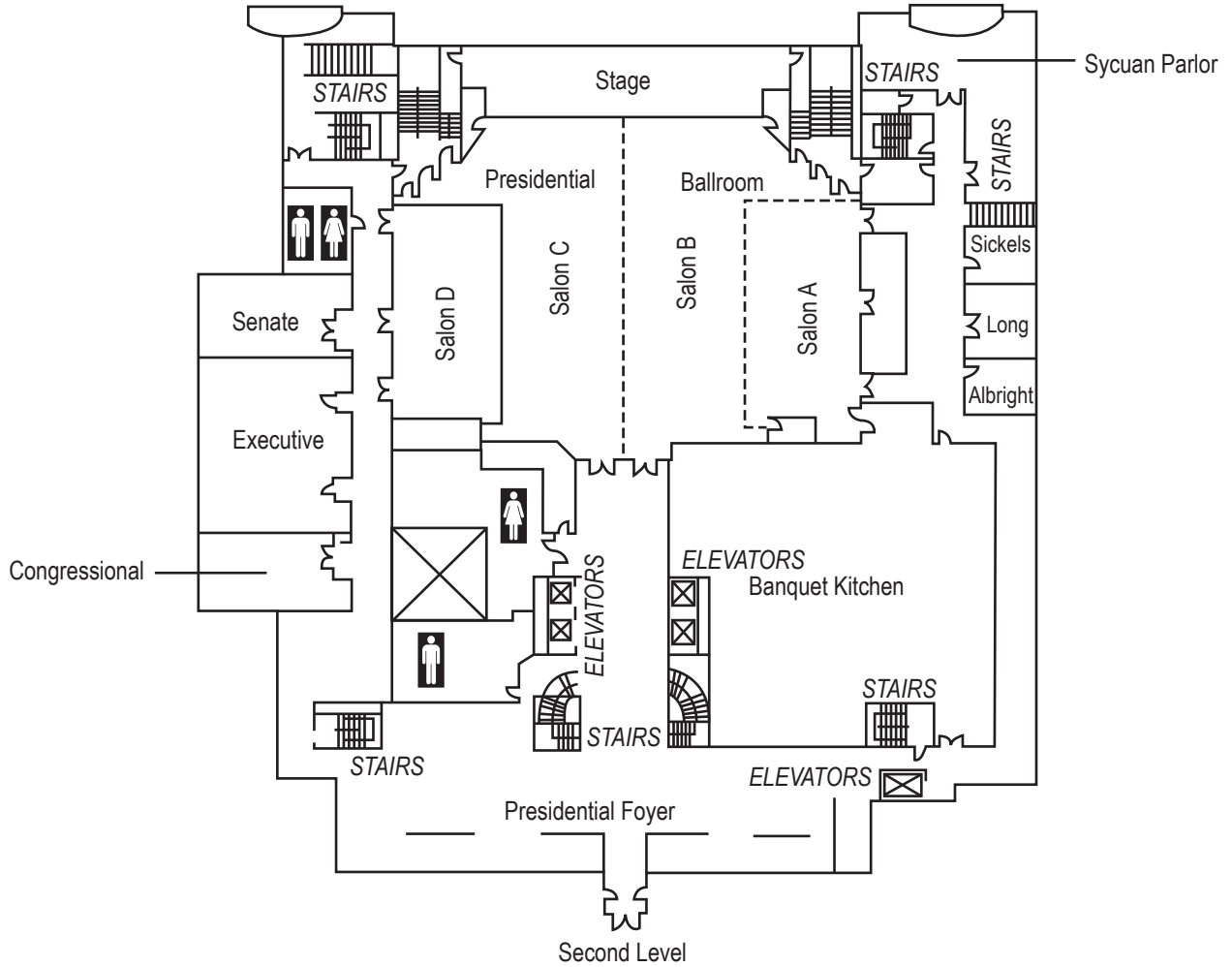
# US GRANT

## Lower Level



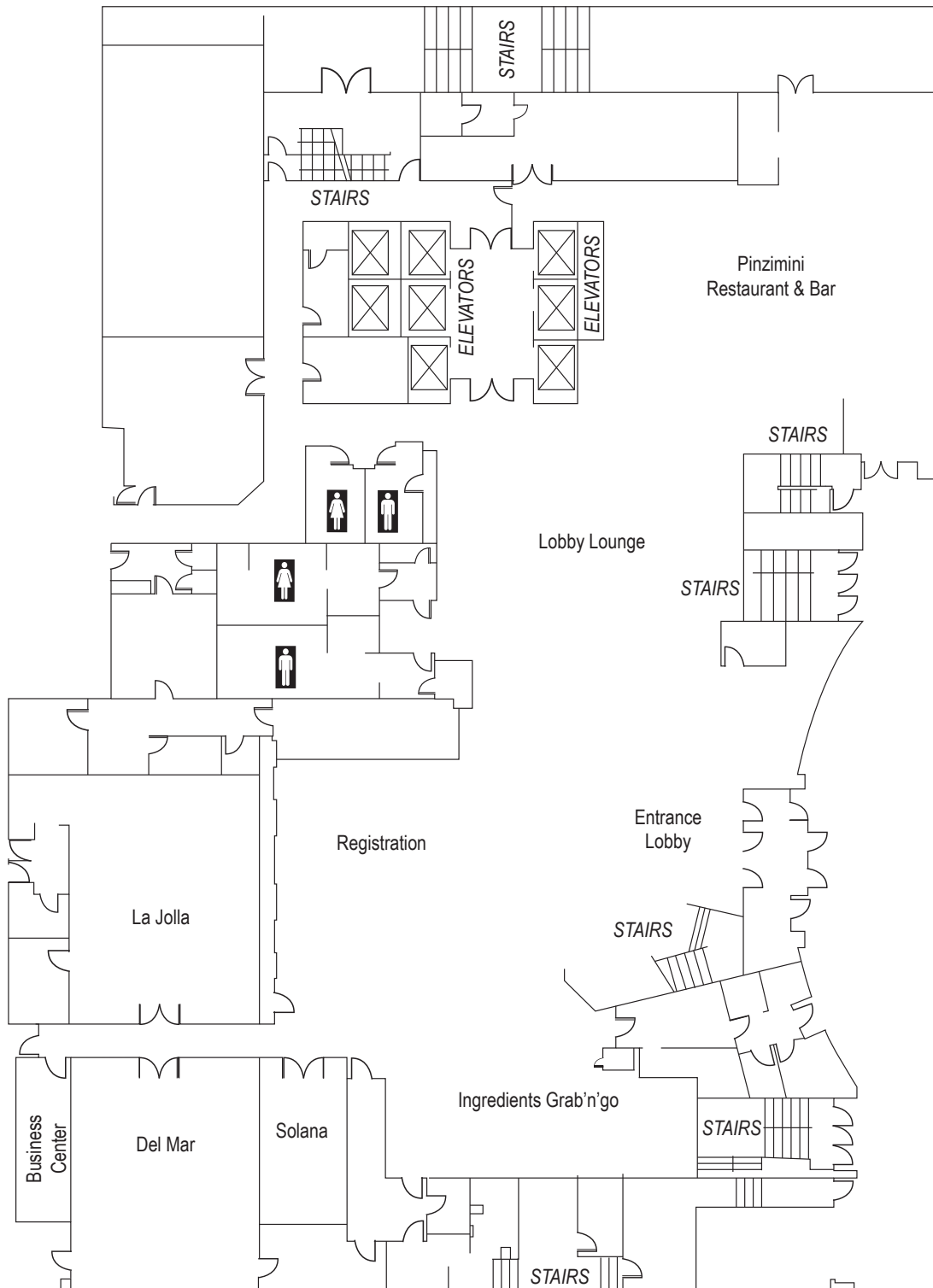
# US GRANT

## Second Floor



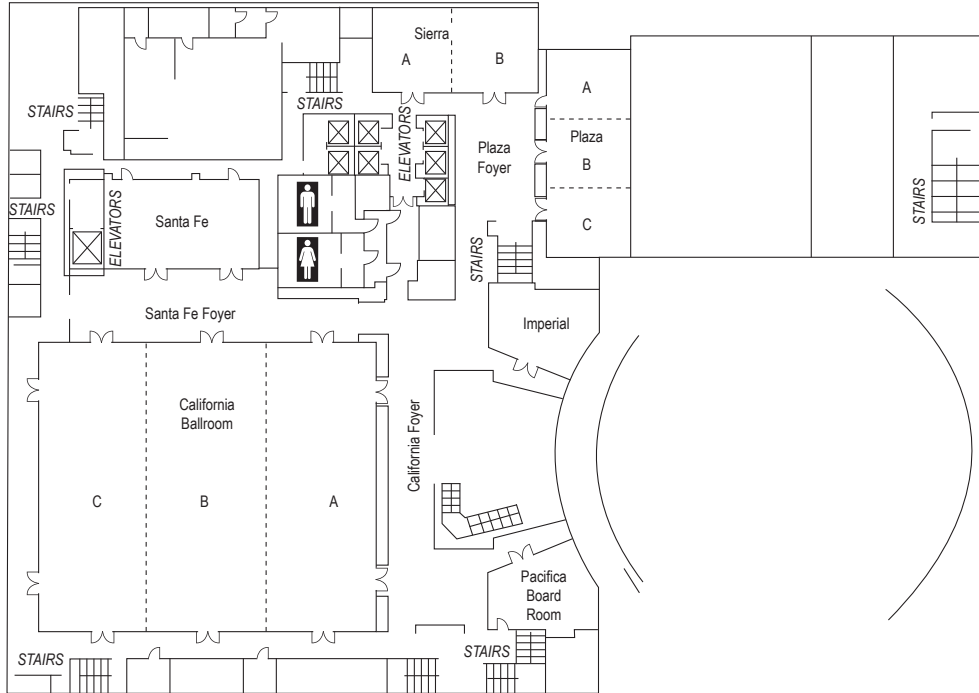
# WESTIN GASLAMP

## Lobby Floor

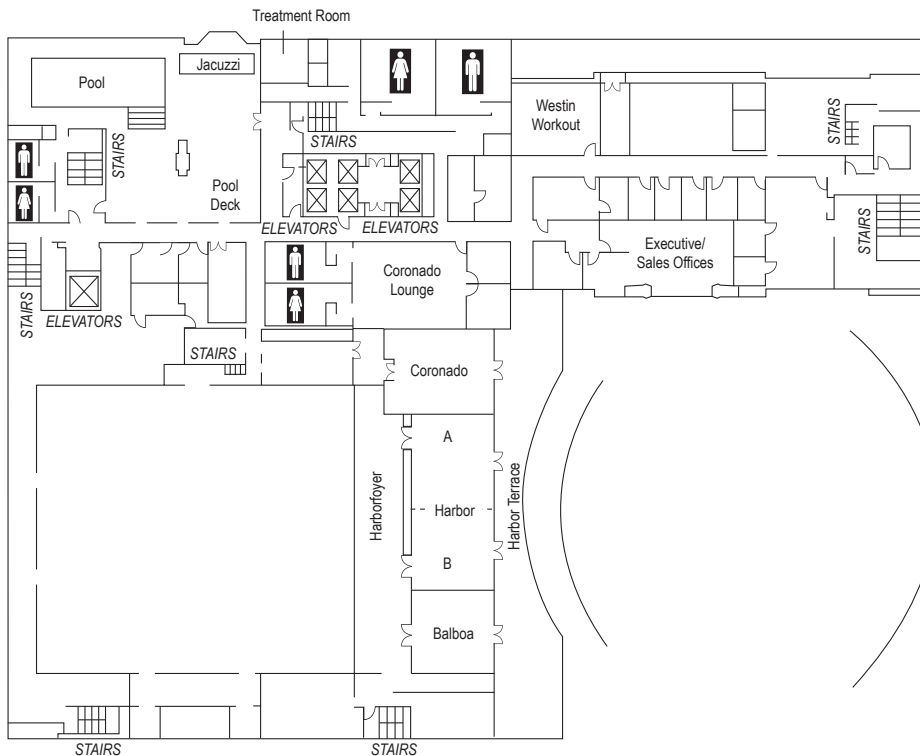


# WESTIN GASLAMP

## Second Floor

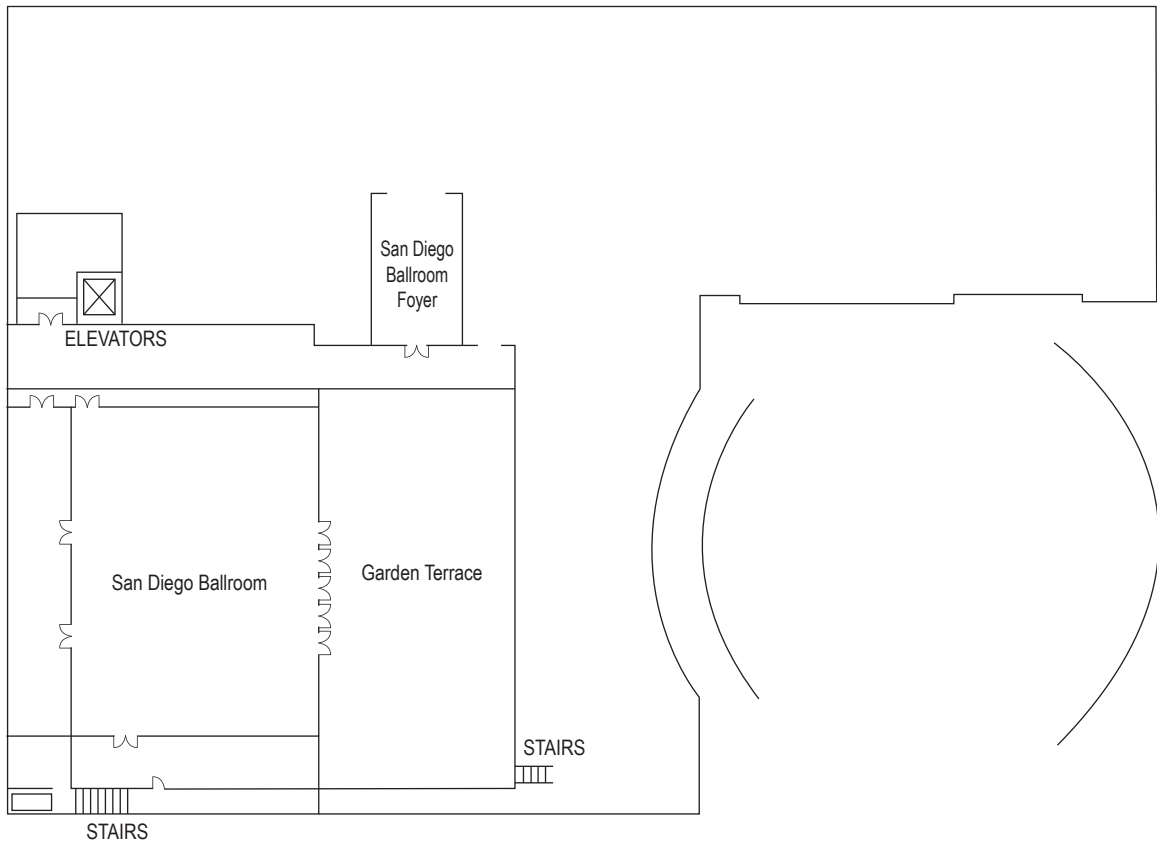


## Third Floor



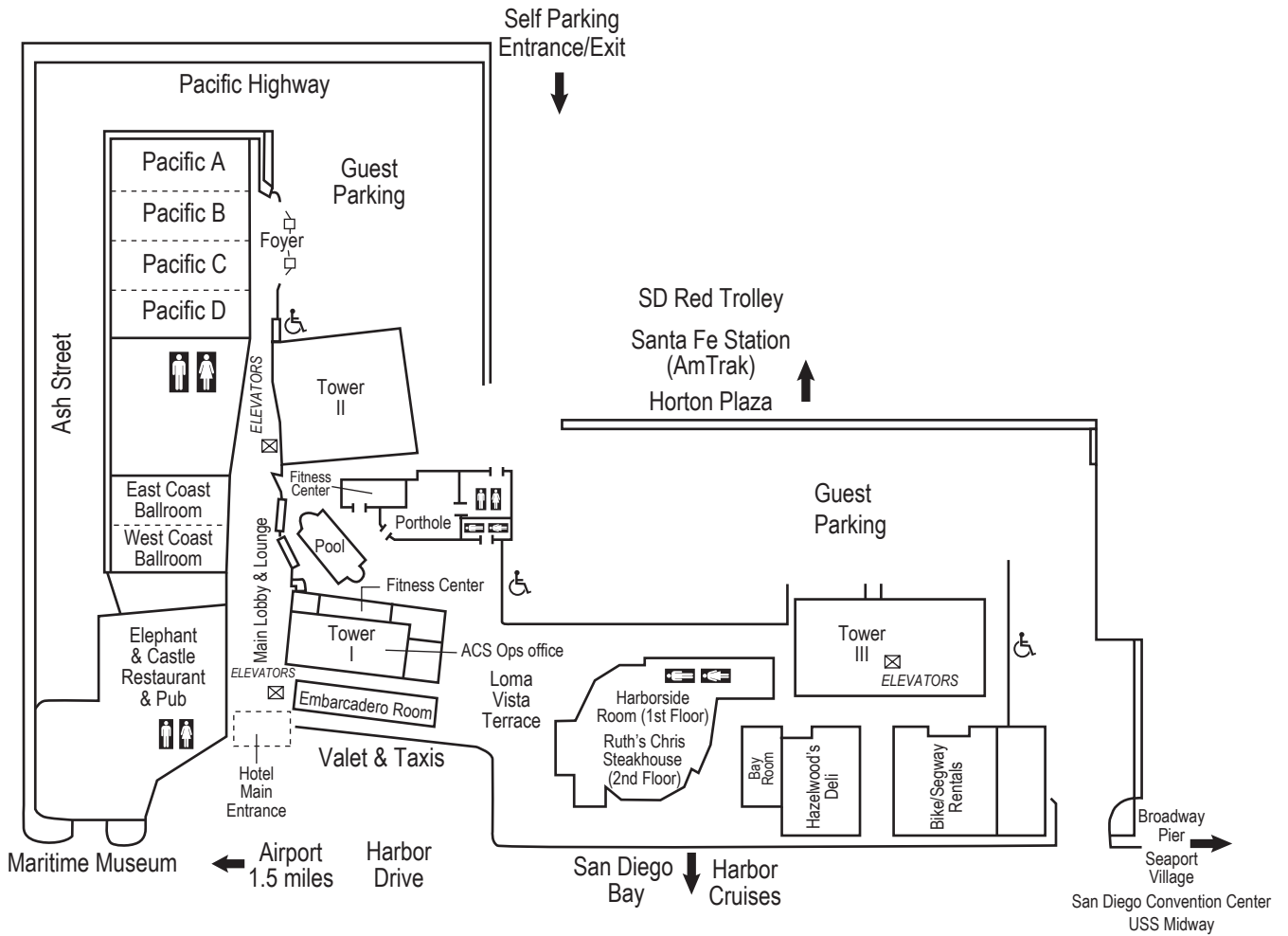
# WESTIN GASLAMP

## Fourth Floor





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ACS Volunteers contribute thousands of hours of service to create and implement programs that promote our science, benefit our members, and contribute to the development of our communities. Thanks to your contributions, the Society provides its members with:

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- Expansive career enhancement materials;
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- Meetings & expositions that set industry standards for excellence.

We salute the outstanding volunteer efforts that have contributed to the suc-

cess of this year's national and regional meetings, including division officers and national meeting program chairs, regional meeting organizers and program chairs, symposium organizers, session and award presiders, short course and workshop instructors, career counselors, and all members of our Society's governance. To get involved, visit [www.acs.org](http://www.acs.org).

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## Shuttle Schedule

### SUNDAY, MARCH 13\*

7:00 AM – 10:00 AM .....	15 minute service
10:00 AM – 4:00 PM .....	30 minute service
4:00 PM – 7:00 PM .....	15 minute service
7:00 PM – 11:00 PM .....	30 minute service

*\*Due to SD Half Marathon, please expect variations in traffic patterns & boarding locations. Check your hotel or lobby sign onsite for details.*

### MONDAY, MARCH 14

7:00 AM – 10:00 AM .....	15 minute service
10:00 AM – 4:00 PM .....	30 minute service
4:00 PM – 11:00 PM .....	15 minute service

### TUESDAY, MARCH 15

7:00 AM – 10:00 AM .....	15 minute service
10:00 AM – 4:00 PM .....	30 minute service
4:00 PM – 11:00 PM .....	15 minute service

### WEDNESDAY, MARCH 16

6:30 AM – 11:00 PM .....	30 minute service
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### THURSDAY, MARCH 17

7:00 AM – 6:00 PM.....	60 minute service
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● Route 1   ● Route 2   ● Route 3  
● Walk to Convention Center   X Boarding Location  
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Join the Editors of *ACS Nano* and *Nano Letters* for the next semi-annual joint session in conjunction with the ACS National Meeting. The 2016 spring symposium is specially designed for the National Meeting theme with world-renowned speakers from the nanoscience and nanotechnology community presenting their ground-breaking research.



**PAUL WEISS**  
EDITOR-IN-CHIEF, *ACS NANO*



**PAUL ALIVISATOS**  
CO-EDITOR, *NANO LETTERS*

## GUEST SPEAKERS & PRESENTATIONS

**Kenneth Merz**, Editor-in-Chief, *Journal of Chemical Information & Modeling*, Michigan State University

*Thermodynamics of Virus Capsid Assembly*

**Carlton Willson**, University of Texas at Austin

*Polymers for Microelectronics: A View of the Future*

**Philip Kim**, Harvard University

*Electron Transport across the van der Waals Interfaces*

**Julia Greer**, California Institute of Technology

*Fractal Arrangement of Atomic Structures in Metallic Glasses*

**Paul Weiss**, University of California, Los Angeles

*New approaches to multimodal nanoscale imaging and analyses*

# American Chemical Society

## Volunteer/National Meeting Attendee Conduct Policy

One of the key strengths of the ACS has been the enduring and varied contributions made by its thousands of dedicated volunteers.

Another unassailable strength of the ACS is its outstanding national meetings program. ACS national meetings are among the most respected scientific meetings in the world. ACS national meetings offer scientific professionals a legitimate platform to present, publish, discuss, and exhibit the most exciting research discoveries and technologies in chemistry and its related disciplines. Furthermore, ACS national meetings facilitate networking opportunities, career development and placement, and provide organizations with opportunities to exhibit products and services to targeted audiences.

The Society's Congressional Charter explicitly lists among its objectives "the improvement of the qualifications and usefulness of chemists through high standards of professional ethics, education and attainments...." The ACS expects its volunteers and national meeting attendees to display the highest qualities of personal and professional integrity in all aspects of their ACS-related activities. Indeed, every chemical professional has obligations to the public, to volunteer and staff colleagues, and to science.

Accordingly, and to foster a positive environment built upon a foundation of trust, respect, open communications, and ethical behavior, the ACS Board of Directors has issued this Conduct Policy. It applies to ACS Volunteers, i.e., it applies to individuals conducting the business and affairs of the ACS without compensation for that conduct. It also applies to attendees at ACS national meetings. Volunteers and national meeting attendees should at all times abide by this Conduct Policy. Specifically:

1. Volunteers should understand and support ACS's vision and mission.
2. Volunteers and national meeting attendees should contribute to a collegial, inclusive, positive, and respectful environment for their fellow volunteers and attendees, as well as for other stakeholders, including national meeting vendors and ACS staff.
3. Volunteers and national meeting attendees must avoid taking any inappropriate actions based on race, gender, age, religion, ethnicity, nationality, sexual orientation, gender expression, gender identity, marital status, political affiliation, presence of disabilities, or educational background. They should show consistent respect to colleagues, regardless of the level of their formal education and whether they are from industry, government or academia, or other scientific and engineering disciplines.
4. Volunteers and national meeting attendees should interact with others in a cooperative and respectful manner. Volunteers and national meeting attendees should refrain from using insulting, harassing, or otherwise offensive language in their ACS interactions. Disruptive, harassing, or inappropriate behavior toward other volunteers, stakeholders, or staff is unacceptable. Personal boundaries set by others must be observed. Harassment of any kind, including but not limited to unwelcome sexual advances, requests for sexual favors, and other verbal or physical harassment will not be tolerated.
5. Volunteers must obey all applicable laws and regulations of the relevant government authorities while acting on behalf of the ACS. Likewise, national meeting attendees must obey all applicable laws and regulations of the relevant government authorities while attending ACS national meetings. Volunteers and national meeting attendees alike should also ensure that they comply with all applicable safety guidelines relating to public chemistry demonstrations.
6. Volunteers and national meeting attendees should only use ACS's trademarks, insignia, name, logos, and other intellectual property in compliance with ACS regulations and directives as may be issued from time to time.
7. Violations of this Conduct Policy should be reported promptly to the ACS Secretary and General Counsel or to the Chair of the ACS Board of Directors. In cases of alleged persistent and/or serious violations of this Conduct Policy, the Board shall review the evidence and shall take such actions as may be appropriate, including but not limited to requiring volunteers to leave their volunteer position(s); precluding volunteers from serving in Society volunteer roles in the future; requiring national meeting attendees to leave the meeting; and, precluding meeting attendees from attending future ACS national meetings. ACS, through its Board of Directors, reserves the right to pursue additional measures as it may determine are appropriate.



252nd American Chemical Society National Meeting & Exposition

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