

249th American Chemical Society National Meeting & Exposition

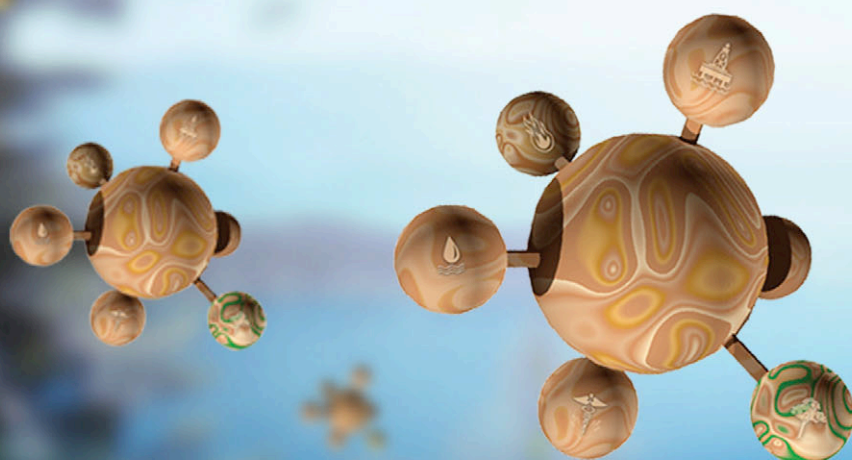
www.acs.org/denver2015

#acsdenver

CHEMISTRY OF NATURAL RESOURCES

Denver, CO • March 22-26, 2015

WWW.ACS.ORG/DENVER2015



Put this book in your pocket!

Download the free ACS Denver 2015 mobile app at
www.acs.org/meetingapp



Available at
amazon

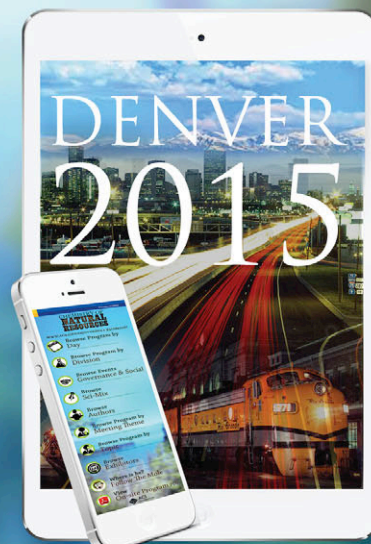


ANDROID APP ON
Google play



Download on the
App Store

*Online version is also available for internet enabled devices.



IMPORTANT NOTICE

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.

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

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.

To continue to increase our support of sustainability efforts through engagement, education and reporting, we would like to remind you of the significant investments that we have made. One huge step in 2014 was the introduction of the mobile application for the National Meetings. The app received overwhelmingly positive feedback having over 6,500 downloads per meeting. The National Meetings app was also recognized in PCMA's *Convene* as Best in Show.

Additional 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 features
- Decreased print-run of the Onsite Program book due to digital and mobile applications
- Reformatted National Meeting website based on viewer analytics
- Increased Meeting Mail terminals at the Convention Center
- 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

Thank you for your support in making ACS a leader in sustainability. Further information can be found at: www.acs.org/greenermeetings. There you will find the ACS 2014 Sustainability Report including information on how to join the Greener Meetings Challenge.



249th American Chemical Society National Meeting & Exposition

TABLE OF CONTENTS

ACS Volunteer/National Meeting	
Attendee Conduct Policy	2
ACS President's Welcome	4
Thematic Organizer's Welcome	5
Governor's Welcome	6
Mayor's Letter	7
General Meeting Information	
• Registration.....	11
• Accommodations	12
• Travel & Transportation.....	14
• Member Services.....	15
• On-Site Arrangements	15
Governance & Business Meetings	
• Board of Directors & Council Meetings	19
• Division Officers & Councilor Caucus Meetings	21
• Governance Committee Meetings & Agendas.....	21
• Division Meetings & Social Events	26
Social & Educational Events	
• Presidential Events	30
• Awards.....	30
• Social & Ticketed Events	33
• Student & Teacher Activities	38
• Workshops	39
• ACS Career Navigator	42
• ACS Professional Educational Short Courses	43
• 2015 Leadership Development System Course Offerings.....	43
• ACS Career Fair	44
• Exposition	45
• Exhibitor Workshops	45
Technical Program Summary	
• Speaker Instructions	73
• Abstracts & Preprints	73
• Technical Program Summary.....	75
Full Technical Program	
• How to Read the Technical Program.....	94
• Technical Program (Listing of Papers)	96
Exposition	
• Exposition Highlights.....	253
• Exhibitor Directory (Listing of Exhibitors)	254
• Exposition Floor Plan.....	267
Attendee Resources	
• Floor Plans (Convention Center & Meeting Hotels).....	270
• Official ACS Properties & Shuttle Schedule (Addresses, Phone Numbers & Map).....	293
• Acknowledgements & Thank You to Our Volunteers.....	297

ACS OPERATIONS OFFICES

- **Colorado Convention Center – Room 210/212** 303-228-8400
- **Hyatt Regency Denver at Colorado Convention Center – Quartz A** 303-489-4976
- **Grand Hyatt Denver – Blanca Peak** 303-603-4305
- **Marriott City Center Denver - Homestead** 303-291-3657
- **Sheraton Denver Downtown Hotel – Aspen & Plaza Reg.** 303-352-2447
- **Embassy Suites Denver—Downtown Convention Center – Quartz Boardroom** 720-587-0988
- **The Curtis—a DoubleTree by Hilton – Paper Room** 720-889-4753

INFORMATION CONTACTS

- **Attendee Registration – Colorado Convention Center, Lobby A/F** 303-228-8411
- **Career Fair Information Center, Colorado Convention Center, Hall B1** 303-228-8417
- **Exhibitor Registration, Colorado Convention Center, A/F Upper Lobby** 303-228-8414
- **Finance Office, Colorado Convention Center, Room 101** 303-228-8412
- **Host Local Section Booth, Colorado Convention Center, Lobby A/F** 303-228-8419
- **Housing Assistance, Colorado Convention Center, Lobby A/F** 303-228-8413
- **Member Services, Colorado Convention Center, Lobby A/F** 303-228-8418
- **Press Center, Colorado Convention Center, Room 104** 303-228-8406
- **Shuttle Desk, Colorado Convention Center, Outside Lobby F** 303-228-8420
- **Society Program Office, Hyatt Regency Denver at Colorado Convention Center** 303-486-4978
- **Governance Office, Hyatt Regency Denver at Colorado Convention Center** 303-486-4915

ACS OFFICERS

Diane Grob Schmidt, President
Donna J. Nelson, President-Elect
Tom Barton, Immediate Past President
Pat N. Confalone, Chair, Board of Directors
Thomas M. Connelly, Executive Director & CEO
Flint H. Lewis, Secretary & General Counsel
Brian A. Bernstein, Treasurer & CFO

American Chemical Society

1155 16th Street, NW, Washington, DC 20036
Tel: 800-227-5558 (US only) or 202-872-4600

Fax: 202-872-4615 E-mail: help@acs.org Website: www.acs.org

The American Chemical Society is a self-governed individual membership organization of more than 158,000 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 249th National Meeting & Exposition, refer to www.acs.org/denver2015. All San Francisco photos in this program are courtesy of the San Francisco Convention and Visitors Bureau and Shutterstock.



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.

CHEMISTRY OF NATURAL RESOURCES

Denver, CO • March 22-26, 2015

WWW.ACS.ORG/DENVER2015

Where to Find Meeting Information

Official Meeting Website
www.acs.org/denver2015

Announcements & Changes
www.acs.org/meetingupdates

Digital Meeting Program
www.acs.org/denver2015



follow us @acsnatlmtg
tweet using #acsdenver



[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

Text your question to
754.227.2012 (Standard text rates apply)



ACS
Chemistry for Life®

Welcome to Denver and the 249th ACS National Meeting

It is my pleasure to join all of you in the Mile High City, one of the most gorgeous locales for our meetings.

Twenty-nine technical divisions and eight committees are hosting original programming based on the meeting theme of Chemistry of Natural Resources. More than 10,000 papers will be presented, and nearly 4,000 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 Open Session will be an opportunity to hear from Deborah Blum, bestselling author of *The Poisoner's Handbook*, discuss her thoughts on communicating chemistry. Please join your colleagues from noon to 1:00 p.m. in the Four Seasons Ballroom 4 of the Colorado Convention Center.

There are three Presidential Symposia I encourage you to attend as well as several others I am recommending. The first is on the morning of Sunday, March 22, titled *Chemistry Without Borders: The Transnational Practice of Chemistry and Allied Sciences and Engineering* (8:00 a.m.–12:00 p.m., Colorado Convention Center, Ballroom 3A.). The other two presidential symposia focus on nanotechnology, with the first beginning later that afternoon on Sunday, March 22, and continuing all day on Monday. *Nanotechnology: Delivering on the Promise* will highlight the fascinating research, development, and commercialization of nanochemistry and nanotechnology and will include 16 senior-level speakers from industry, academe, and government. The third presidential symposium (Tuesday, 8:30–11:30 a.m.), *DOE Nanoscience Research Centers: National Resources for the Nanoscience Community*, will feature the five heads of chemistry at U.S. national laboratories. This is the first symposium of its type to highlight these speakers collectively.



Diane Grob Schmidt
ACS President

On Monday afternoon, Theodore Betley, Professor of Chemistry and Chemical Biology at Harvard University will deliver The Kavli Foundation Emerging Leader in Chemistry Lecture on 'Radical Frontiers in Catalysis.' He is followed by Laura Kiessling, at the University of Wisconsin - Madison with The Fred Kavli Innovations in Chemistry Lecture (Colorado Convention Center, Bellco Theater) who will speak on 'Us Versus Them: Distinguishing Humans from Microbes with Carbohydrates.'

The entire meeting program is filled with outstanding scientific, educational, and professional content. Please consult the listings in this program or go to

www.acs.org/denver2015 for all the specific details pertaining to these events. There is plenty to select from and I am sure you will find something to satisfy your needs and expectations.

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 the members of the Colorado Local Section; the Committee on Meetings and Expositions; thematic program chair Robert S. Weber of the Pacific Northwest National Laboratory; the divisional program chairs and symposium chairs responsible for organizing this meeting's technical sessions; and the ACS staff for making it all happen. And thanks to you for contributing to the success of this meeting. Of course, thanks to all of you for attending.



Diane Grob Schmidt
ACS President

Welcome Message from Bob Weber, Denver Thematic Program Chair

The Spring 2015 ACS National Meeting, (Denver, March 22-26), will showcase the *Chemistry of Natural Resources*: their extraction, refining and conservation; a theme that resonates well with the history, biology and geology of the Mile-High City.

The plenary session, on Sunday afternoon, March 22, will inaugurate the theme with three invited lectures: Prof. Carolyn Koh (Colorado School of Mines) will discuss “The Fundamentals of Gas Hydrates and Their Role in Energy Transport;” Dr. Paul Bryan (formerly manager of the Biomass program at DOE) will present “The Four Horsemen of the Advanced Biofuels Apocalypse — Sustainability, Technology, Profitability, and Politics,” an overview of challenges and future opportunities for renewable fuels; and Dr. Peter Kareiva (Chief Scientist of The Nature Conservancy) will discuss “Water in the Anthropocene: Too Much, Too Little, Too Dirty.” The afternoon of Monday, March 23 will see the Kavli Foundation Emerging Leader in Chemistry Lecture by Prof. Theodore Betley (Harvard University) “Radical Frontiers in Catalysis” and the Fred Kavli Innovations in Chemistry Lecture by Prof. Laura Kiessling (University of Wisconsin-Madison) “Us Versus Them: Distinguishing Humans from Microbes with Carbohydrate.”

The technical program constructed by the ACS divisions includes both topical sessions and nearly 50 symposia honoring the winners of ACS awards. Symposia that resonate well with the overall theme of the meeting can be found in the sessions sponsored by AGFD, AGRO, ANYL, CATL, CEI, CELL, CINF, COLL, COMP, COMSCI, ENFL, ENVR, GEOC, HIST, I&EC, INOR, PHYS, SCHB, SOCED, and YCC.



Bob Weber
Denver Thematic
Program Chair

Denver and its surroundings evoke many images: the American frontier, mining, forest products, coinage, civic zest, “Rocky Mountain Spring Water” and recently, the production of unconventional fossil fuels. To recollect and celebrate the region’s traditions and resources, the local ACS chapter has put together a great social and enrichment program around local attractions. The Presidential Outreach Event, “Exploring Our World Through Chemistry,” will take place at the Denver Zoo on Saturday, March 21. Denver authorities have also reminded me to note that spring skiing in Colorado is some of the best anywhere, easily reached by shuttles to the ski resorts

(about 1.5 hours away from the meeting venue downtown):
www.coloradomountainexpress.com/downtown-denver

The program for the meeting and other information is available online at the website of the meeting
www.acs.org/denver2015.

I am very grateful to the members of the local section, the program chairs of the divisions listed above, and the ACS staff for their essential help in making the theme of this meeting cogent and coordinated. I look forward to meeting you in Denver.



Bob Weber
Thematic Program Chair

STATE OF COLORADO

EXECUTIVE CHAMBERS

136 State Capitol
Denver, CO 80203 - 1792
Phone (303) 866-2471



John Hickenlooper
Governor



March 22, 2015

Greetings:

On behalf of the State of Colorado, it is my distinct pleasure to welcome you to Denver for the 249th American Chemical Society National Meeting and Exposition.

You could not have chosen a better location to celebrate the chemistry of natural resources, as they are central to Colorado's heritage and an important part of our future. I commend all participants as you recognize and explore the transformative power of chemistry over the coming days. I wish you a productive and successful conference and look forward to learning about your ongoing research and discoveries. Outside of these activities, I hope you have some time to explore and enjoy our wonderful state.

Once again welcome to this exciting and informative event. You have my best wishes, now and in the years to come.

Sincerely,



John W. Hickenlooper

Michael B. Hancock
Mayor



City and County of Denver

OFFICE OF THE MAYOR
CITY AND COUNTY BUILDING
DENVER, CO 80202-5390
TELEPHONE: (720) 865-9090 • FAX: (720) 865-8787
TTY/TTD: (720) 865-9010

March 22, 2015

American Chemical Society's 249th National Meeting
Colorado Convention Center
707 West 14th Street
Denver, CO 80202



Greetings:

On behalf of the City and County of Denver, it is my pleasure to extend a heartfelt welcome to the "Mile High City." We are excited that you have chosen Denver to advance the work of your organization.

The American Chemical Society has a long and rich history of support in the field of chemical science, engineering, and related fields. You are the leading source of authoritative scientific information through the Journal of the American Chemical Society and Chemical & Engineering News, and have been catalyst for education, research and publication, as well as advocate for information protection. Denver is a great location to continue this very important work.

While you are here, we invite you to take advantage of the many amenities that our city has to offer. Denver is one of the nation's most walkable cities and boasts a variety of attractions, including the nation's second largest performing arts complex, three art museums, three sports stadiums, a U.S. Mint, more than 300 restaurants and one of the largest city park systems in the country.

Also, please take advantage of the various transportation options we offer. We've made getting around the Mile High City easy with our 500 rental bikes available at 30 downtown stations, a free hybrid shuttle along the 16th Street pedestrian mall, and FasTracks, the nation's largest light rail initiative with 120 miles of track.

Again, welcome to Denver, have an informative and enjoyable time and please plan to return soon.

Respectfully,

A handwritten signature in black ink, appearing to read "Michael B. Hancock", with a long horizontal flourish extending to the right.

Michael B. Hancock
Mayor

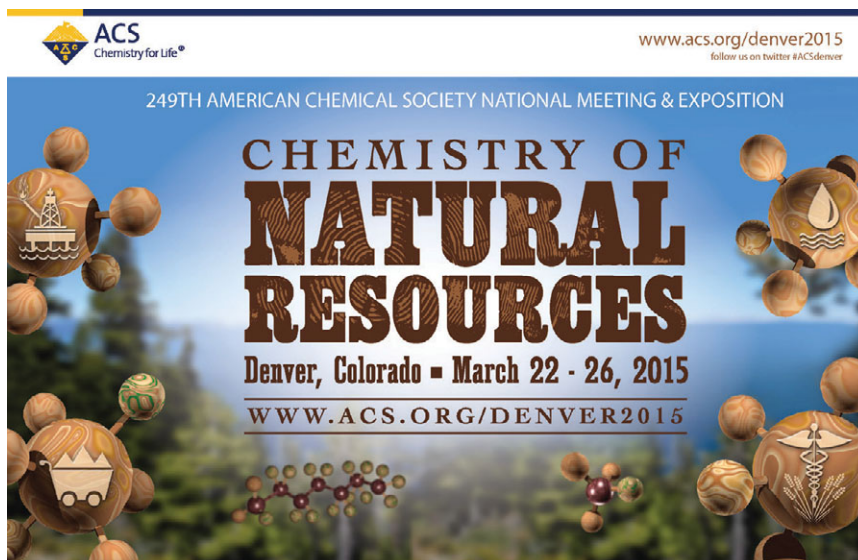
PRESIDENTIAL SYMPOSIA

Sponsored by the ACS President

Photo: Peter Cutts Photography



Diane Grob Schmidt, Ph.D.
ACS President



Sunday and Monday – March 22-23, 2015

Nanotechnology: Delivering on the Promise

(Cosponsored by the following ACS Divisions and Committees and other scientific societies AGFD, AGRO, ANYL, CARB, CHAS, COLL, ENFL, HIST, I&EC, PMSE, POLY, SCHB, MPPG, CA, CCS, CCPA, COMSCI, DAC, IAC, SOCED; American Institute of Chemical Engineers, Gordon Research Conferences, Materials Research Society & National Academy of Engineering)

Sunday, March 22, 2015

1:30-5:30 PM

**Nanotechnology: Delivering
on the Promise – R&D**

Monday, March 23, 2015

8:30-11:45 AM

**Nanotechnology:
Delivering on the Promise –
Opportunities and
Challenges for Health,
Safety, and the Environment**

Monday, March 23, 2015

1:30-4:45 PM

**Nanotechnology: Delivering
on the Promise – Bridging
the Gap to a Thriving U.S.
Marketplace**

Colorado Convention Center, Mile High Ballroom 3A (Lower Level)

249th American Chemical Society National Meeting & Exposition

Download the free ACS Denver 2015 Mobile App

- Quick Access to the full technical program, maps, and search features.
- Build your schedule. Browse by day, division, theme topics, exhibitors or authors.
- Use your ACS ID to sync your schedule.
- Take notes and share them via email. Connect your meeting experience with social media and more!

The ACS Mobile Meeting Application is your free full greener guide to manage your experience at the 249th ACS National Meeting in Denver.



Learn more at
www.acs.org/meetingapp
#acsdenver



Visit the Denver Mobile App Desk for a free app t-shirt — *while supplies last.*
Colorado Convention Center, Lobby A/F

JOIN THE
ACS BOARD OF DIRECTORS
OPEN MEETING



Guest Speaker: Deborah Blum

2015 Grady Stack Award Recipient

Helen Firstbrook Franklin Professor
School of Journalism and Mass Communication
University of Wisconsin-Madison

Sunday, March 22, 2015

Noon – 1:00 PM

Four Seasons Ballroom 4 (Lower Level)
Colorado Convention Center

The Poisoner's Guide to Communicating Chemistry

Join the ACS Board of Directors at its Regular Session as they host lunchtime speaker Deborah Blum. Deborah is an American journalist, a columnist for the *New York Times*, a professor of journalism at the University of Wisconsin-Madison, and a blogger for *Wired*. She is also the author of several books including *The Poisoner's Handbook*. She is a much sought out speaker and has appeared at several very well-attended ACS symposia focused on communicating chemistry/science to the public.

Deborah will be receiving the 2015 Grady-Stack Award at the ACS National Meeting in Denver, March 2015, for her achievements in public outreach, engagement and communications.

Sandwiches available for first 200 attendees.

GENERAL MEETING INFORMATION

YOUR MEETING REGISTRATION

entitles you to a wide range of programming, including 987 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 Feb. 13 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 Feb. 13 must pick up their badge credentials on-site.

MEETING INFO ON THE WEB

Registration, housing, technical programming, special events, participating exhibitors, and other meeting details are available at www.acs.org/denver2015.

Registration Changes. Attendees can modify their existing registration or generate a receipt from the registration website by following the instructions in their confirmation message. Attendees can also update their registration on-site at ACS Attendee Registration. Bring your confirmation and/or badge credentials with you to the meeting for faster processing.

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

Internet. Register online at www.acs.org/meetings until March 26. 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 26 at 800-251-8629 (U.S./Canada only) or 508-743-0192 (international), Monday to Friday, 9:00 AM to 5:00 PM EST.

Fax/Mail. Submit the registration form by fax: 508-743-9605 or mail: ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532. Mailed registrations will be accepted until March 26.

On-site. Register during the meeting at ACS Attendee Registration at standard registration rates. ACS Attendee Registration will be open at the Colorado Convention Center, Lobby A/F, on Saturday, 3:00 to 6:00 PM; Sunday, 7:30 AM to 7:30 PM; Monday, 7:30 AM to 9:30 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.

Registration forms received without payment will not be processed.

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. 30	STANDARD AFTER FEB. 13
MEMBERS		
ACS member or society affiliate	\$390	\$470
Postdoctoral member	390	470
Emeritus or retired member	200	240
50-year member	No fee	No fee
Unemployed member (Dues waiver required)	No fee	No fee
Precollege teacher	110	110
Graduate student	200	200
Undergraduate	110	110
One-day registrant	200	240
NONMEMBERS		
Chemical scientist	\$680	\$820
Postdoctoral scientist	680	820
Visitor: Nonchemical scientist or chemical technician	390	470
Precollege teacher	110	110
Graduate student	390	390
Undergraduate	200	200
One-day registrant	390	470
Guest of registrant ^a	50	50
EXPOSITION-ONLY VISITORS		
Adult, exposition only	\$60	\$60
Student, exposition only	30	30

^a 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

REGISTRATION ASSISTANCE. The ACS National Meeting Registration Center will be available from 9:00 AM to 5:00 PM EST by telephone, fax, mail, or e-mail. Service representatives can be reached at 800-251-8629 (U.S./Canada only) or 508-743-0192 (international); fax: 508-743-9605; e-mail: acs@xpressreg.net; or mail: ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532.

Registration Cancellations/Refunds. All cancellations and refund requests must be submitted in writing to guarantee the registrant a full refund less a \$50 administrative fee. Refund requests made after March 6 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 508-743-9605 (save your fax confirmation sheet).

Social Event Ticket Cancellations/Refunds. Social event cancellations received by March 6 entitle the registrant to a full refund. Refund requests made after March 6 will not be honored. 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), or e-mail: 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 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 e-mail: 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 Colorado Convention Center. For more information, visit 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 \$60 or \$30 for students with school identification. Register online or in person at ACS Attendee Registration.

EXHIBITOR REGISTRATION. Exhibitor registration is handled exclusively through ACS National Expositions at www.acs.org/expositions.

CAREER FAIR EMPLOYER REGISTRATION. ACS Career Fair Employer registration is handled exclusively through ACS Careers at www.acs.org/careers.

ACCOMMODATIONS

ORCHID EVENT SOLUTIONS is the official housing bureau for the ACS national meeting in Denver. ACS does not endorse booking hotel reservations through any other sources. All attendees who made their reservations through Orchid Event Solutions will

receive complimentary internet access in their sleeping rooms and automatically entered in the ACS Housing Drawing.

On-site Housing. During the meeting an on-site housing desk will be located at the Colorado Convention Center in the registration area. Staff will be available to assist with last-minute housing changes or needs.

Reservation Confirmation. All registrants who booked their reservations through Orchid Event Solutions received a confirmation. Each confirmation contains a unique number that is proof of your reservation.

Keep Your Meeting Affordable. Attendee support of the official hotels allows ACS to utilize meeting space at a discount and keep registration fees to a minimum.

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 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 to read about our greener meeting initiatives and access our annual Event Sustainability Report.

For our efforts, ACS has been recognized by the Capital Chapter of the Professional Convention Management Association as a sustainable event leader and received the Trade Show Executive's Gold 100 Award for the Show with the Most Commendable Green Initiatives. Here are a few reasons why:

■ ACS offsets all shuttle transport emissions and staff-related emissions (1,193 tons of carbon dioxide were offset in 2014, equivalent to not driving 2,840,476 miles in an average passenger vehicle).

Take the greener meeting Challenge

Take the Greener Meetings Challenge at www.acs.org/greenermeetings. Tell your story or simply show your support for the ACS Greener Meetings Program. All participants will receive a special thank you (*While supplies last.*). Three participants having the best stories will be awarded prizes on **April 27, 2015**.

To be a catalyst for positive change! Here's what you can do:

1



Take advantage of linen reuse and other initiatives at your hotel, and always turn the lights off when away from your room. If you are staying at the Westin or Sheraton, enroll in their Make A Green Choice program.

2



Responsibly dispose of recyclable materials (paper, plastic, glass, aluminum) at the convention center and hotels.

3



Download the national meeting mobile app or digital program. Limited quantities of the printed Onsite Program are available.

4



Avoid the use of taxis by walking when safe and possible. Stop by the Greener Meetings Booth for your pedometer (*While supplies last*). Burn calories, and enjoy the city.

5



Ride the ACS carbon-neutral shuttle service when walking isn't an option between your hotel and the center. Shuttle service will be provided between many ACS contracted properties.

6



Avoid the use of disposable, plastic water bottles. Stop by the ACS Colorado Host Local Section Booth to pick up a free, reusable water bottle (*While supplies last*). Avoid the cost and waste associated with disposable bottles.

Colorado Convention Center, Lobby A/F

Greener Meetings Booth

Sun., 3 – 6 PM

Mon., 8 – 1PM

Tues., 8 – 1 PM

Colorado Host Local Section Booth

Sat., 3 to 6 PM

Sun., 7:30 AM to 7:30 PM

Mon., 7:30 AM to 9 PM

Tues., 7:30 AM to 5 PM

Wed., 7:30 AM to 4 PM

Thurs., 7:30 AM to 1 PM

■ ACS partnered with conservation group American Forests to offset ACS staff-related emissions (related to travel, accommodations, and show management freight) through tree-planting efforts in Lower Rio Grande Valley National Wildlife Refuge and the Dinky Collaborative Reforestation project.

■ ACS performed on-site walk-throughs for 98% of our hotel room block properties in 2014, surveying hotels on more than 40 sustainability practices.

■ ACS designates Sci-Mix as a “zero waste” event. We achieved nearly 100% diversion for meetings in both Dallas and San Francisco. Help us keep up the great work!

Be A Catalyst For Change In Denver.

Facilities are only as effective as the people who operate and occupy them. That means you! Go to www.acs.org/greenermeetings and take the Greener Meeting Challenge to show your support and share your personal national meeting sustainability story. Challenge participants are eligible to win fantastic prizes. Challenge activities include the following:

■ Take advantage of linen reuse initiatives at your hotel, decline delivery of unread newspapers, and turn off the lights when away from your hotel room.

■ Responsibly dispose of recyclable materials (paper, plastic, glass, aluminum) in the convention center and hotels.

■ Use the meeting mobile app and digital program instead of the printed on-site program.

■ Enjoy the city, burn calories, and travel carbon dioxide-neutral by walking to and from your hotel.

■ When walking isn't an option, use the ACS carbon-offset shuttle service.

■ Bring a reusable water bottle to avoid the cost and waste associated with disposable, petroleum-based plastic water bottles.

Suggestions? end them to ACS National Meetings & Expositions at NationalMeetings@acs.org.

TRAVEL & TRANSPORTATION

DENVER is easily accessible by air or train, and the city offers several options to get around, including the ACS shuttle, taxis, and buses.

AIRPORT. Numerous ground transportation options are available at Denver International Airport. The Ground Transportation Information Counter is located in the central area on Level 5 of Jeppesen Terminal. Counter hours are 6:00 AM to 11:30 PM daily. For more information, call 303-342-4059.

SUPERSHUTTLE. ACS has established a 10% discount for attendees of our meeting. Take advantage of this savings by going to www.supershuttle.com or www.execucar.com and entering the discount code 94D3G in the “Group/Discount Code” box on the first page of the website.

TAXIS are readily available and provide service to the Denver metro area and surrounding counties. From Denver International Airport to downtown Denver there is a flat rate of \$55.15 (one-way fare, airport access fee already included). Taxis pick up and drop off from Jeppesen Terminal, Level 5, Island 1, outside doors 507 through 511 (Terminal East) and doors 506 through 510 (Terminal West).

PUBLIC TRANSPORTATION. Public bus service is scheduled and provided within the local metro area by the Regional Transportation District (RTD). Please contact RTD directly, or visit their booth in the Jeppesen Terminal, for information on specific routes, schedules, and fares. Riders must have exact change. RTD buses pick up and drop off from Jeppesen Terminal Level 5, outside doors 504, 506, and 510 (west side).

TRANSPORTATION DISCOUNTS. ACS has negotiated special travel discounts with the partners listed below. To get the best rates and avoid service fees, it is recommended to make reservations online (except Amtrak).

AIRLINES:

Delta

delta.com; 800-328-1111 (please note that ticketing charges will apply for bookings by phone)

Discount Codes: NMK2Y, NMJTX (international)

United

united.com; 800-426-1122

Offer Code: ZT6E969361

Southwest

swabiz.com

Corporate ID: 99329790

Online Reservations Only

TRAIN:

Amtrak

amtrak.com; 800-872-7245

Convention Fare Discount: #X03V-918

RENTAL CARS:

Advantage Rent A Car

advantage.com; 800-777-5500

Discount Code: CD02C826E8

Avis

avis.com; 800-331-1600

Avis Worldwide Discount (AWD): B923099

Hertz

hertz.com; 800-654-2240

Discount Code: CV# 02UZO014

TRAVELING TO MEETING VENUES

The Colorado Convention Center is located at 700—14th St., Denver, CO 80202.

ACS Shuttle. Complimentary shuttle service will be provided between the Colorado Convention Center and official ACS hotels, with the exception of hotels within walking distance. Buses will run from 7:00 AM to 11:00 PM from Sunday to Wednesday and 7:00 AM to 6:00 PM on Thursday. Buses will run approximately every 15 to 30 minutes. Visit the meeting website for a route map and to download the shuttle schedule.

If you require wheelchair access or for any other inquiries, please e-mail nationalmeetings@acs.org to schedule.

Parking. Daily parking is limited and expensive in downtown Denver. You should contact your hotel to inquire about daily parking policies and fees.

GETTING AROUND THE CITY

Walking. The Colorado Convention Center and ACS hotels are conveniently located in downtown Denver. Do your part to reduce our environmental impact by walking to ACS properties.

Denver's Regional Transportation District (RTD). Denver's Regional Transportation District (RTD) offers

GENERAL INFORMATION

eco-friendly transportation by bus or light-rail services within and around the city of Denver. RTD also offers a shuttle services "skyRide" to and from Denver International Airport. For routes, fares, and other pertinent information, call 303-299-6000 or visit the website at www.rtd-denver.com.

ACS MEMBER SERVICES

ACS MEMBER SERVICES. ACS staff can 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 A/F near registration in the Colorado Convention Center and is open Saturday, March 21, 3:00 to 6:00 PM; Sunday, March 22, 7:30 AM to 7:30 PM; Monday, March 23, 7:30 AM to 9:00 PM; Tuesday, March 24, 7:30 AM to 5:00 PM; Wednesday, March 25, 7:30 AM to 4:00 PM; and Thursday, March 26, 7:30 AM to 1:00 PM.

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.

BUSINESS CENTER. The UPS Store, located in Concourse A, offers in-store and online printing, notary services, document finishing, packing and ship-

ping, and a variety of other services tailored to help you make the best of the convention.

MEMBER INSURANCE PROGRAM. Exposition Booth 624. 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 Station to learn how you can sign up for Life & Health Insurance, Auto & Homeowners Plus, Disability Income, Long-Term Care, Medicare Supplement, Medical Discount Cards, Pet Insurance, and Professional Liability.

Also learn more about two new policies available to ACS members: International Life Insurance and Commercial Business Insurance. We look forward to showing you how you can receive great value for your insurance dollars. For additional information, visit www.acs.org/insurance.

ON-SITE MEETING ARRANGEMENTS

ADA-COMPLIANT MEETING. The Colorado 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 denverconvention.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; fax: 202-872-6128; or phone: 202-872-6111 by Feb. 5 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 Rooms 210/212. 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/denver2015. Use the Meeting Mail terminals located in the Colorado 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 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 22, through Thursday, March 26. 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. For your child's safety, the location of Camp ACS will not be communicated until your registration is confirmed. On-site registration will be accepted at the ACS Operations Office, Colorado Convention Center, room 210/212 and on the space available basis.

Access meeting information
and the On-site Program at
www.acs.org/denver2015

GENERAL INFORMATION

LUGGAGE & COAT CHECK. A luggage and coat check station will be available during registration hours from Sunday through Thursday at the Colorado Convention Center, Lobby A/F. 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 Colorado 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 Colorado Convention Center, Lobby F.

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/denver2015.

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 Colorado 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 Colorado Convention Center:

Attendee Registration: Lobby A/F

Career Fair: Hall B1

Exhibitor Registration: Upper Lobby A/F

Exposition: Halls A/F

Finance Office: Room 101

Host Local Section Center: Lobby F

Member Services: Lobby A/F

Press Center: Room 104

Shuttle Desk: Outside F Lobby

The following offices are located at the identified properties:

Operations Offices: Colorado Convention Center, Hyatt Regency Denver at Colorado Convention Center, Grand Hyatt Denver, Marriott City Center Denver, Sheraton Denver Downtown Hotel, Embassy Suites Denver—Downtown Convention Center, The Curtis—a DoubleTree by Hilton

Governance Office: Hyatt Regency Denver at Colorado Convention Center

TIPS FOR A SAFE STAY IN DENVER

- 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.

Society Programs: Hyatt Regency Denver at Colorado Convention Center

MOTHERS ROOM. For your convenience and privacy, ACS will provide a room for nursing mothers at the Colorado Convention Center. Please see the Operations Office in Room 210/212 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.

THANK YOU

The society thanks the many volunteers of the Colorado local section who are contributing to the 249th 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.

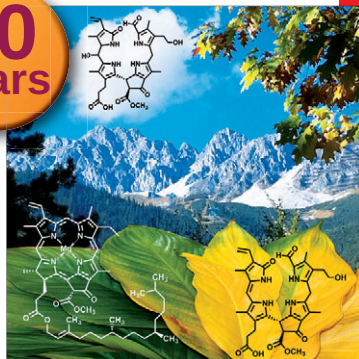
Let's celebrate leading society journals ...



CHEMISTRY
A **European** Journal

www.chemeurj.org

20
years



A Journal of

ChemPubSoc
Europe

2015-21/1



Supported by
ACES

WILEY-VCH



Palladium-Catalyzed Addition of Nucleophiles to Alkenes

Micro/Macromotors and the Environment

6539, Vol. 21, No. 1, 2015

CHEMISTRY
AN **ASIAN** JOURNAL

www.chemasianj.org

10th
volume

Special
Anniversary
Issue



1/10
2015

An **ACES** journal

A sister journal of *Angewandte Chemie*
and *Chemistry – A European Journal*

VOLUME
10
WILEY-VCH

ACES

5
years

**ChemistryViews**

... with
a piece
of cake

3:00 pm
Monday & Tuesday
March 23rd & 24th
Colorado Convention Center
Wiley Booth # 700

WILEY-VCH

WILEY

THE INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES &
THE AMERICAN CHEMICAL SOCIETY INVITE YOU TO

PACIFICHEM 2015

Chemical Networking: Building Bridges Across The Pacific



April 3: Abstract Submission Closes

Honolulu, Hawaii • December 15- 20, 2015

Housing Now Open | Registration Opens June 25, 2015

Become an exhibitor and reserve booth space now.

Contact expo@acs.org

- Gain access to scientists who work in the fields of chemical and life sciences
- Access the exclusive attendee advertising opportunities to promote your company and product exposure to our attendees
- Interact with our attendees and your colleagues during scientific and educational activities
- Network with attendees during social events where our attendees relax and recharge

Learn more at www.pacificchem.org



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 Denver. ACS encourages it's 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 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 to explore your specific interests.

ACS COUNCIL

The ACS Council meeting will begin at 8:00 AM, Wednesday, March 25, at the Hyatt Regency Denver at the Colorado. 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.



Colorado Convention Center PHOTO.UA / SHUTTERSTOCK.COM

ACS Committee on Science Emerging Frontiers in Science Symposium



Advanced Materials for Solar Energy Transitioning Between Academic Research into Practical Use

Monday, March 23

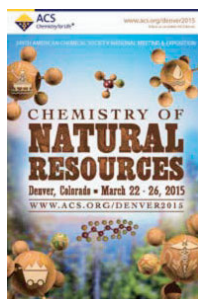
8:30 AM – 12:30 PM (Colorado Convention Center, Room 301)

Hear leading experts from:

Academia (Harry B. Gray-Caltech, James McCone-Cornell),
Government (John Turnel, NREL, Cheryl Martin, DOE ARPA-E) &
Industry (Anik R. Duggal, GE Global Research)

This distinguished panel will discuss key challenges and opportunities in advanced materials for solar energy and their commercial applications.

An ACS Presidential Event and Feature of the ACS Thematic Program (MPPG)
Cosponsored by the Division of Inorganic Chemistry



GOVERNANCE MEETINGS

For the complete list of committee meetings and agendas, please consult www.acs.org/denver2015.

BOARD & COUNCIL MEETINGS

ACS BOARD OF DIRECTORS. Board of Directors meeting, open to members who wish to participate, will be held in the Colorado Convention Center, Four Seasons Ballroom 4, from noon to 1:00 PM on Sunday, March 22. The guest speaker will be Deborah Blum, 2015 Grady Stack Award Recipient, and author of “The Poisoner’s Handbook.”

ACS COUNCIL. The ACS Council meeting will begin at 8:00 AM, Wednesday, March 25, at the Hyatt Regency Denver at Colorado Convention Center. 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.

COUNCIL POLICY COMMITTEE

The Council Policy Committee will open the floor during its meeting at 11:00 AM on Tuesday, March 24, 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. For more committee meeting details and agendas, please consult the meeting website at www.acs.org/denver2015 or the on-site program distributed during the meeting.

COUNCILOR CAUCUS MEETINGS

District II Councilor Caucus

Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall C

Middle Atlantic Councilor Caucus

Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall D

District IV Councilor Caucus

Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall E

District V Councilor Caucus

Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall F

District VI Councilor Caucus

Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall G

Division Officers/Councilors Caucus

Tuesday, March 24, 4:00 – 6:00 PM
Colorado Convention Center
Room 502

District I Councilor Caucus

Tuesday, March 24, 5:30 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall C

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 ex officio and elected councilors may attend; 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 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

Open Meeting

Saturday, March 21, 8:00 AM to noon
Hyatt Regency Denver at Colorado Convention Center, Centennial A

1. Report of the Chair
2. Report of the Treasurer & CFO:
 - a. Budgetary Performance Report for the Year Ended December 31, 2014
3. Reports from the B&F Subcommittees:
 - a. Financial Impact of Constitution & Bylaw Changes
 - b. Communications
 - c. Program Funding Requests
 - d. Program Review

GOVERNANCE & BUSINESS MEETINGS

CHEMICAL SAFETY

Elizabeth M. Howson, chair; safety@acs.org

Open Executive Session

Monday, March 23, 8:30 to 11:30 AM

Hyatt Regency Denver at Colorado Convention Center, Centennial F

1. Welcome
2. Minutes of August 11 Meeting
3. Reports of the Chair/Staff Liaison
4. Report of Subcommittees and Task Forces
5. Old and new business

CHEMISTRY & PUBLIC AFFAIRS

Susan B. Butts, chair; sbbuttsdc@gmail.com

Open Meeting

Saturday, March 21, 8:00 AM to 4:00 PM

Hyatt Regency Denver at Colorado Convention Center, Capitol 1/2

1. Welcome
2. Minutes of August 11 Meeting
3. Reports of the Chair/Staff Liaison
4. Report of Subcommittees and Task Forces
5. Old and new business

CHEMISTS WITH DISABILITIES

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

Combined Open and Executive Meeting

Sunday, March 22, 8:30 AM to 4:30 PM

Hyatt Regency Denver at Colorado Convention Center, Capitol 3

1. Welcome
2. Chair Report
 - a. Update of CWD Activities/Events, and Collaborative Opportunities
 - b. Diversity & Inclusion Advisory Group Report
 - c. Strategic Planning Retreat
 - d. Minutes from San Francisco, 2014
3. Staff Report
4. Future Event and Programming Planning
5. Subcommittee Progress Reports
 - a. CWD Poster Project
6. Reports of Liaisons to/from other committees
7. Ongoing Business
8. 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 23, 1:30 to 2:00 PM

Hyatt Regency Denver at Colorado Convention Center, Capitol 2

1. Welcome
2. Minutes of August 11-13, 2014
3. Reports of chair/staff liaison
4. Report of Subcommittees and Task Forces on:
 - a. Diversity
 - b. Leadership Development
5. Topics from floor

COMMUNITY ACTIVITIES

George L. Heard, chair; University of North Carolina, Asheville; glheard@gmail.com

Open Executive Session

Sunday, March 22, 7:45 AM to noon

The Curtis Hotel, Four Square B

CCA/LSAC Joint Open Meeting

Tuesday, March 24, 2:00 to 3:30 PM

The Curtis Hotel, Four Square Ballroom

1. Reports of chair, subcommittee chairs, staff liaison
2. Training materials for outreach
3. Reports of committee liaisons

CONSTITUTION & BYLAWS

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

Open Meetings

Sunday, March 22, 1:15 to 1:45 PM

Hyatt Regency Denver at Colorado Convention Center, Mineral F

Executive Session (Closed)

Sunday, March 22, 9:00 AM to noon

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

Executive Session

Sunday, March 22, 1:45 to 4:30 PM

Hyatt Regency Denver at Colorado Convention Center, Mineral F

1. Status of unit bylaws
2. Bylaw review process
3. Reports from liaisons from other committees
4. Petition on Member Expulsion
5. Petition on Preferential Voting
6. Open discussion

CORPORATION ASSOCIATES

Dawn Mason, chair; P.O. Box 431, Kingsport, TN 37662

Open Meeting

Monday, March 23, 8:00 AM to noon

Hyatt Regency Denver at Colorado Convention Center, Capitol 3

1. Welcome
2. Approval of Minutes
3. Reports of Chair/Staff Liaison
4. Report of Subcommittees
5. Open Discussion and New Business

COUNCIL POLICY

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

Open Meeting

Tuesday, March 24, 9:30 AM to noon

Hyatt Regency Denver at Colorado Convention Center, Capitol 1

1. Committee and Officer Reports
2. Report of CPC vice chair
3. Reports of Subcommittees and Task Forces on:
 - a. Petitions, Constitution and Bylaws
 - b. Long Range Planning
 - c. Task Forces: to review Councilor Travel Reimbursement Program; on Councilor and Member Duties and Conduct; on Divisor Communications
5. Schedule of business sessions, fall 2015
6. Review of Council agenda
7. Open forum
8. Old and new business

DIVISIONAL ACTIVITIES

Michael J. Morello, chair; mike.morello@pepsico.com

Open Session

Sunday, March 22, 8:00 AM to noon

Hyatt Regency Denver at Colorado Convention Center, Mineral E

1. Welcome
2. Review Denver Agenda
3. Minutes from 248th ACS National Meeting in San Francisco, CA
4. DAC Chair Report
5. Subcommittee Reports

ECONOMIC & PROFESSIONAL AFFAIRS

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

Executive Session

Saturday, March 21, 8:00 AM to 5:30 PM

Colorado Convention Center

Open Executive Session

Sunday, March 22, 8:00 AM to noon

Colorado Convention Center, Room 601

1. Opening Remarks/Introductions
2. Priorities and Strategic Plan
3. Subcommittee Meetings
4. Staff Reports
5. Wrap-Up and Process Check
6. Subcommittee Reports
 - a. Public Policy
 - b. Events, Volunteers and Employment Services
 - c. Marketing and Research
 - d. Standards and Ethics
7. Reports from Liaisons to and from CEPA
8. Old Business / New Business

EDUCATION

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

Open Meeting

Monday, March 23, 3:00 to 4:00 PM

Hyatt Regency Denver at Colorado Convention Center, Mineral D

Executive Session

Friday, March 20, 1:00 to 5:30 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial E

1. K-12 science topics, including ChemCom, ChemMatters, the American Association of Chemistry Teachers, High School Chemistry Clubs, Chemistry Olympiad, Science Coaches, and teacher professional development
 2. College/university topics, including two-year college chemistry, undergraduate programs, graduate and postdoctoral education, Chemistry in Context, and professional development
- Items 1-2 open to all Councilors with prior approval of the Chair

ENVIRONMENTAL IMPROVEMENT

Laura Pence, chair; lpence@hartford.edu

Open Executive Session

Saturday, March 21, 4:00 to 6:00 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial E

1. Chair's report and review of interim actions
2. Subcommittee on Member Involvement
3. Subcommittee on Programming and Education
4. Subcommittee on Public Policy
5. Staff reports from OPA and GCI
6. Reports of Other Working Groups and Liaisons
7. Committee Business
8. Open Discussion

GOVERNANCE & BUSINESS MEETINGS

ETHICS

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

Open Executive Session

Sunday, March 22, 9:00 AM to 4:30 PM

Hyatt Regency Denver at Colorado Convention Center, Capitol 5

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

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

Open Meeting

Saturday, March 21, 1:00 to 3:00 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial F/G

1. Welcome
2. Minutes of August 9, 2014
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

LOCAL SECTION ACTIVITIES

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

LSAC/CCA Joint Open Meeting

Tuesday, March 24, 2:00 to 3:30 PM

The Curtis Hotel, Four Square Ballroom

Open Executive Session

Sunday, March 22, 8:00 AM to noon

The Curtis Hotel, Four Square A

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

Open Executive Session

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

MEETINGS & EXPOSITIONS

Will E. Lynch, chair; Department of Chemistry & Physics, Armstrong Atlantic State University, 11935 Abercorn St., Savannah, GA 31419-1997

Open Executive Session

Sunday, March 22, 7:00 AM to noon

Colorado Convention Center, Room 207

1. Welcome
2. Minutes from San Francisco National Meeting
3. Chair's report
4. Subcommittee reports
5. Finance/Staff Liaison Report
6. Registration Fee Vote
7. New Business

MEMBERSHIP AFFAIRS

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

Open Session

Sunday, March 22, 2:00 to 3:00 PM

Hyatt Regency Denver at Colorado Convention Center, Capitol 1/2

1. Welcome
2. Minutes of August 11-12, 2014
3. Reports of Chair/Staff Liaison
4. Reports of Subcommittees
 - a. Categories & Dues
 - b. Retention, Benefits & Services
 - c. Recruitment & Admissions
5. Petition on Member Expulsion (For Consideration)
6. Topics from floor

MINORITY AFFAIRS

Madeleine Jacobs, chair; c/o ACS Office of Diversity Programs, 1155-16th St., N.W., Washington, DC 20036

Executive Session

Sunday, March 22, 8:00 AM to 12:30 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial D

1. Opening Remarks
2. Staff Report
3. Subcommittee Meetings

Open Session

Sunday, March 22, 12:30 to 2:00 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial D

1. Subcommittee Reports
2. Old Business
3. New Business
4. Open Discussion
5. Adjournment

NOMENCLATURE, TERMINOLOGY & SYMBOLS

Albert C. Censullo, chair; 1595 Cordova Dr., San Luis Obispo, CA 93405

Open Session

Monday, March 23, 2:00 to 5:00 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial H

1. Review minutes from San Francisco meeting
2. Chair/Staff Liaison reports
3. Reports from subcommittees
 - a. Communication/Outreach
 - b. Education
 - c. Committee Liaison
 - d. Long Range Planning
 4. IUPAC Reports
 5. Update to Kilogram, Amount of Substance and Mole Issues
 6. Task Force on new SI definitions

NOMINATIONS & ELECTIONS

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

Open Executive Session

Monday, March 23, 11:00 AM to noon

Hyatt Regency Denver at Colorado Convention Center, Mineral C

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

PATENTS & RELATED MATTERS

Sadiq Shah, chair; sadiq@utpa.edu

Open Meeting

Saturday, March 21, 9:00 AM to 5:00 PM

Hyatt Regency Denver at Colorado Convention Center, Capitol 4

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 22, noon to 1:00 PM

Marriott Denver City Center, Gold Coin

1. Implementation of New Guidelines for ACS Approval
2. Expectations for Polymer Chemistry
3. Supplements to the New Guidelines
4. Planning for Graduate Work in the Chemical Sciences
5. Survey of PhD Recipients
6. Directory of Undergraduate Research
7. 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 22, 9:30 to 10:30 AM

Hyatt Regency Denver at Colorado Convention Center, Agate B

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

Executive Session

Saturday, March 21, 10:30 AM to 5:00 PM

Hyatt Regency Denver at Colorado Convention Center, Mineral C

1. Subcommittee meetings 10:30 AM - noon
2. Minutes of August 9, 2014
3. Reports of Chair/Staff Liaison
4. Report of Subcommittees
5. Old and new business

PUBLICATIONS

Stephanie Brock, chair; Wayne State University, Chemistry, 5101 Cass Ave., Detroit, MI 48202-3929

Open Meeting

Friday, March 20, 4:30 to 5:00 PM

Hyatt Regency Denver at Colorado Convention Center, Mineral F/G

1. Updates from ACS Publications Division
2. Open Discussion

Executive Session

Friday, March 20, 1:00 to 5:00 PM

(Closed Executive Session until 4:30 PM)

Hyatt Regency Denver at Colorado Convention Center, Mineral F/G

(Closed Executive Session until 4:30 PM)

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

GOVERNANCE & BUSINESS MEETINGS

SCIENCE

Katherine Glasgow, chair; Nomacorc,
400 Vintage Park Dr., Zebulon, NC 27597-3803;

Open Meeting

Saturday, March 21, 8:00 AM to 4:30 PM

Hyatt Regency Denver at Colorado Convention
Center, Centennial B

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

George Heinze, chair; 30 Bunker Hill Run,
East Brunswick, NJ 08816-3317

Open Meeting

Monday, March 23, 8:00 AM to noon

Hyatt Regency Denver at Colorado Convention
Center, Mineral B

1. Welcome & Introductions
2. Discussion and approval of San Francisco Meeting Minutes
3. Reports of Chair & Staff Liaison
4. Subcommittee Reports
 - a. Newsletter
 - b. National Meeting Programming
 1. Denver
 2. Boston

c. Senior Activities in Local Sections

1. Mini Grant Awards
- d. Consulting & Mentoring
 1. Undergraduate Speed Networking Event
- e. Planning and Priorities
5. Old Business
 - a. Senior Chemists Breakfast
6. New Business
 - a. ChemLuminary Awards
7. Adjournment

TECHNICIAN AFFAIRS

Susan S. Marine, chair; CTA@acs.org

Closed Executive Session

Sunday, March 22, 8:30 AM to 2:00 PM

Hyatt Regency Denver at Colorado Convention
Center, Centennial A

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

Open Session

Sunday, March 22, 2:00 to 2:30 PM

Hyatt Regency Denver at Colorado Convention
Center, Centennial A

1. Welcome
2. Chair's Report
3. Subcommittee Reports
4. Topics from Floor
5. Adjourn

WOMEN CHEMISTS

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

Closed Executive Session

Saturday, March 21, 8:00 AM to 5:00 PM

Hyatt Regency Denver at Colorado Convention
Center, Centennial D

1. Welcome
2. Review of Fall Action Items & Minutes
3. Reports of Chair/Staff Liaison
4. Subcommittee Meetings
5. Report of Subcommittees and Task Forces:
 - a. Awards & Recognition
 - b. Communications & Technology
 - c. Professional Development
 - d. Programs & Events
6. New Business

YOUNGER CHEMISTS

Douglas B. Hausner, chair;

doug.hausner@gmail.com

Open and Executive Session

Sunday, March 22, 8:00 AM to noon

Hyatt Regency Denver at Colorado Convention
Center, Centennial C

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

Complimentary Exhibitor-Sponsored Workshops

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

- Introduce new products and services
- Build skills with specific tools and techniques
- Highlight innovative applications for existing instrumentation

ACS ATTENDEE WELCOME RECEPTION

Meet exhibitors and employers while networking and enjoying the reception!

Colorado Convention Center
Exhibit Halls A/F, Sunday
March 22, 6 - 8:30 PM

DAILY RAFFLE, BOOTH 339

Visit the Daily Prize Raffle area on Sunday through Tuesday for a chance to win a prize.

SPECIAL PRIZE GIVEAWAY

Get scanned by 20 exhibitors on Sunday through Tuesday and be entered into a raffle for a terrific prize.

ENJOY POSTERS ON EXPO FLOOR

Join us on Tuesday, inside the Colorado Convention Center Exhibit Halls A/F, for poster sessions on the show floor.

Please visit www.acs.org/denver2015 to register for their workshop(s)

Monday, March 23

Spectroscopy Simplified – How to Run a Research FT-IR System with the Touch of a Button

Sponsor: Thermo Scientific, 9:30 AM - 12:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Innovative Technologies to Engage Your Student's Learning Experience

Sponsor: McGraw Hill Higher Education, 9:30 AM - 12:00 PM
Colorado Convention Center, Room 103

SciFinder Training Session

Sponsor: CAS, 12:30 PM - 3:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Thermo Fisher Chromatography and Mass Spectrometry

Sponsor: Thermo Scientific, 12:30 PM - 3:00 PM
Colorado Convention Center, Exhibit Halls A/F
Exhibitor Workshop Room 2

Innovative Technologies to Engage Your Student's Learning Experience

Sponsor: McGraw Hill Higher Education, 12:30 PM - 3:00 PM
Colorado Convention Center, Room 103

Online Homework with Targeted Instructional Feedback Leads to Improved Student Learning Outcomes

Sponsor: Sapling Learning, 3:30 PM - 6:00 PM
Colorado Convention Center, Room 103

Tuesday, March 24

SciFinder Training Session

Sponsor: CAS, 9:30 AM - 12:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Tuesday, March 24, Cont'd

A Survey of Accelerated Materials Research Using Raman Microscopy and Imaging

Sponsor: Thermo Scientific, 9:30 AM - 12:00 PM
Colorado Convention Center, Room 103
Exhibit Halls A/F, Exhibitor Workshop Room 2

Compact Mass Spectrometry: A Swiss Army Knife Approach to Chemistry Challenges

Sponsor: Advion, 9:30 AM - 12:00 PM
Colorado Convention Center, Room 103

Intelligent Real-Time Reaction

Monitoring In The Fume Hood Using Benchtop NMR

Sponsor: Thermo Scientific, 12:30 PM - 3:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Analysis of Polymers by Vibrational

Spectroscopy and Microscopy

Sponsor: Bruker, 12:30 PM - 3:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 2

Advances in Atomic and Molecular Spectroscopy

Sponsor: Agilent Technologies, 12:30 PM - 3:00 PM
Colorado Convention Center, Room 103

Chromatography and Mass Spectrometry Tips, Tricks, and Advanced Techniques

Sponsor: Agilent Technologies, 3:30 PM - 6:00 PM
Colorado Convention Center, Room 103

Wednesday, March 25

Designing Inhibitors with MOE Structure-Based Drug Design Tools

Sponsor: Chemical Computing Group, 3:30 PM - 6:00 PM
Colorado Convention Center, Room 103

DIVISION MEETINGS & SOCIAL EVENTS

Division of Agricultural & Food Chemistry— AGFD

Membership Committee— Special Meeting	Sunday, March 22	12:00 PM - 1:00 PM	Room 113, Colorado Convention Center
Executive Committee Meeting	Sunday, March 22	5:00 PM - 8:00 PM	Mineral B Room, Hyatt Regency Denver
Future Programs Planning Meeting	Monday, March 23	12:00 PM - 1:00 PM	Room 701, Colorado Convention Center
AGFD Chair's Reception	Tuesday, March 24	6:00 PM - 8:00 PM	Crystal Ballroom B, Embassy Suites Denver Downtown

Division of Analytic Chemistry— ANYL

Sci-Mix	Monday, March 23	8:00 PM - 10:00 PM	Hall C, Colorado Convention Center
Analytical Posters	Tuesday, March 24	7:00 PM - 9:00 PM	Hall C, Colorado Convention Center

Division of Biological Chemistry— BIOL

Current Topics in Biological Chemistry	Sunday, March 22	8:15 PM - 9:45 PM	Hall B2, Colorado Convention Center
--	------------------	-------------------	-------------------------------------

Division of Biochemical Technology— BIOT

Company Seminar Luncheon	Sunday, March 22	12:30 PM - 2:00 PM	Capitol Peak B, Grand Hyatt Denver
Company Seminar Luncheon	Monday, March 23	12:30 PM - 2:00 PM	Capitol Peak B, Grand Hyatt Denver
Company Seminar Luncheon	Tuesday, March 24	12:30 PM - 2:00 PM	Capitol Peak B, Grand Hyatt Denver
Future Programming (Closed Meeting)	Tuesday, March 24	12:30 PM - 2:00 PM	Grays Peak, Grand Hyatt Denver
Program Chair Meeting (Closed Meeting)	Wednesday, March 25	11:30AM - 2:30 PM	Maroon Peak, Grand Hyatt Denver
Company Seminar Luncheon	Wednesday, March 25	12:30 PM - 2:00 PM	Capitol Peak B, Grand Hyatt Denver
Networking Session	Wednesday, March 25	6:00 PM - 8:00 PM	Capitol Peak B, Grand Hyatt Denver

Division of Business Development & Management— BMGT

BMGT Reception	Monday, March 23	5:30 PM - 7:30 PM	Crystal Ballroom B&C, Embassy Suites Denver Downtown
----------------	------------------	-------------------	--

Division of Carbohydrate Chemistry— CARB

2015 Carbohydrate Division Award Banquet (Ticketed Event)	Monday, March 23	7:00 PM - 10:00 PM	Appaloosa Grill
---	------------------	--------------------	-----------------

Division of Catalysis and Surface Science— CATL

Division Board/Leadership Meeting	Monday, March 23	6:00 PM - 8:00 PM	Room 108, Colorado Convention Center
Program Committee Meeting	Tuesday, March 24	6:00 PM - 8:00 PM	Room 605, Colorado Convention Center

Division of Cellulose and Renewable Materials— CELL

Anselme Payen Award Banquet (Ticketed Event)	Tuesday, March 24	6:30 PM - 10:00 PM	CooHills Restaurant
Business Meeting	Wednesday, March 25	5:00 PM - 6:00 PM	Room 404, Colorado Convention Center

Note: Due to space limitations, hotel abbreviations are used in these tables.

GOVERNANCE & BUSINESS MEETINGS

Division of Chemistry and Law— CHAL

CHAL Reception	Monday, March 23	5:00 PM - 8:00 PM	Crystal Peak A, Grand Hyatt Denver
----------------	------------------	-------------------	------------------------------------

Division of Chemical Health & Safety— CHAS

Laboratory Safety Workshop	Friday, March 20	7:30 AM - 5:30 PM	CCB 1, Embassy Suites Denver
Laboratory Waste Management Workshop	Friday, March 20	7:30 AM - 5:30 PM	CCB 2, Embassy Suites Denver
Chemical Reactivity Hazards: Laboratory-Scale Recognition & Control Workshop	Saturday, March 21	7:30 AM - 5:30 PM	CCB1, Embassy Suites Denver
Job Hazard Analysis Workshop	Saturday, March 21	7:30 AM - 5:30 PM	CCB 2, Embassy Suites Denver
How to be a More Effective Chemical Hygiene Officer Workshop	Saturday, March 21	7:30 AM - 5:30 PM	Silverton Ballroom 1, Embassy Suites Denver
NRCC Certification Exams	Sunday, March 22	8:00 AM - 12:00 PM	Rexford Room, Embassy Suites Denver
Executive Committee Meeting	Sunday, March 22	8:00 AM - 12:00 PM	Silverton Ballroom 3, Embassy Suites Denver

Division of Chemical Education— CHED

Chemical Education Research Committee	Sunday, March 22	7:00 AM - 9:00 AM	Plaza Court 6, Sheraton Denver Downtown
High School/College Interface Luncheon (Ticketed Event)	Sunday, March 22	12:00 PM - 1:00 PM	Silver Room, Sheraton Denver Downtown
Workshop 1	Sunday, March 22	8:00 AM - 12:00 PM	Plaza Court 3, Sheraton Denver Downtown
Workshop 2	Sunday, March 22	1:00 PM - 5:00 PM	Plaza Court 4, Sheraton Denver Downtown
Workshop 3	Monday, March 23	8:00 AM - 12:00 PM	Plaza Court 3, Sheraton Denver Downtown
Workshop 4	Monday, March 23	1:00 PM - 5:00 PM	Plaza Court 4, Sheraton Denver Downtown

Division of Chemical Information— CINF

Education Committee Meeting (Closed Meeting)	Saturday, March 21	1:00 PM - 3:00 PM	Room 604, Colorado Convention Center
Program Committee Meeting (Closed Meeting)	Saturday, March 21	1:00 PM - 3:00 PM	Room 606, Colorado Convention Center
Awards Committee Meeting (Closed Meeting)	Saturday, March 21	1:00 PM - 3:00 PM	Room 608, Colorado Convention Center
Executive Meeting (Closed Meeting)	Saturday, March 21	3:00 PM - 6:00 PM	Room 604, Colorado Convention Center
Open Business Meeting	Sunday, March 22	6:00 PM - 6:30 PM	Silverton Ballroom 3, Embassy Suites Denver
Welcoming Reception	Sunday, March 22	6:30 PM - 8:30 PM	Silverton Ballroom 3, Embassy Suites Denver
Luncheon (Ticketed Event)	Tuesday, March 24	12:00 PM - 1:30 PM	Silverton Ballroom 3, Embassy Suites Denver

Division of Colloid & Surface Chemistry— COLL

Open Business Meeting/Social Hour with Poster Session	Sunday, March 22	5:30 PM - 8:00 PM	Hall E, Colorado Convention Center
Luncheon	Tuesday, March 24	12:00 PM - 1:45 PM	Penrose Ballroom 1, Denver Marriott City Center

Division of Computers in Chemistry— COMP

Programming & Executive Board Meeting	Saturday, March 21	8:00 AM - 6:30 PM	Room 108, Colorado Convention Center
Poster and Awards Session	Tuesday, March 24	6:00 PM - 8:30 PM	Hall B2, Colorado Convention Center

Division of Energy & Fuel— ENFL

Division Dinner (Ticketed Event)	Tuesday, March 24	7:30 PM - 9:00 PM	Maggiano's Little Italy
----------------------------------	-------------------	-------------------	-------------------------

GOVERNANCE & BUSINESS MEETINGS

Division of Environmental Chemistry — ENVR

Program Planning Committee Meeting	Sunday, March 22	2:00 PM - 3:00 PM	Room 207, Colorado Convention Center
Long Range Planning Committee Meeting	Sunday, March 22	3:00 PM - 5:00 PM	Room 605, Colorado Convention Center
Executive Committee Meeting	Sunday, March 22	7:00 PM - 10:00 PM	Room 603, Colorado Convention Center
Reception (Ticketed Event)	Tuesday, March 24	6:00 PM - 7:30 PM	Wynkoop Brewing Company

Division of Geochemistry — GEOC

Business Committee Meeting	Tuesday, March 24	5:30 PM - 7:30 PM	Room 603, Colorado Convention Center
----------------------------	-------------------	-------------------	--------------------------------------

Division of Industrial & Engineering Chemistry — I&EC

Subcommittee Meeting (Closed Meeting)	Sunday, March 22	12:00 PM - 2:00 PM	Crystal Ballroom C, Embassy Suites Denver
General Posters Session	Tuesday, March 24	5:00 PM - 6:30 PM	Hall C, Colorado Convention Center

Division of Inorganic Chemistry — INOR

Dow Energy Water Nexus Reception	Tuesday, March 24	4:00 PM - 5:00 PM	Room 207, Colorado Convention Center
----------------------------------	-------------------	-------------------	--------------------------------------

Division of Medicinal Chemistry — MEDI

Business Meeting	Sunday, March 22	5:30 PM - 6:30 PM	Room 605, Colorado Convention Center
------------------	------------------	-------------------	--------------------------------------

Division of Nuclear Chemistry & Technology — NUCL

Social Hour	Monday, March 23	7:00 PM - 9:00 PM	Silverton Ballroom 2, Embassy Suites Denver
-------------	------------------	-------------------	---

Division of Organic Chemistry — ORGN

Executive Committee Meeting (Closed Meeting)	Sunday, March 22	1:00 PM - 5:00 PM	Room 603, Colorado Convention Center
--	------------------	-------------------	--------------------------------------

Division of Physical Science — PHYS

Poster Session	Wednesday, March 25	6:00 PM - 8:00 PM	Hall C, Colorado Convention Center
----------------	---------------------	-------------------	------------------------------------

Division of Polymer Chemistry — POLY

POLY/PMSE Awards Reception	Wednesday, March 25	5:30 PM - 8:30 PM	Plaza Ballroom A/B, Sheraton Denver Downtown
----------------------------	---------------------	-------------------	--

Division of Professional Relations — PROF

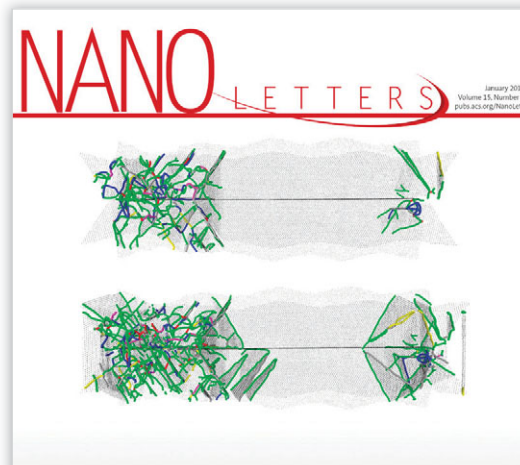
Professional Relations Executive Committee Meeting	Tuesday, March 24	3:00 PM - 5:00 PM	Capitol 3, Hyatt Regency Denver
--	-------------------	-------------------	---------------------------------

Division of Small Chemical Business — SCHB

SCHB & PROF Luncheon	Sunday, March 22	11:30 AM - 1:30 PM	Silverton Ballroom 2, Embassy Suites Denver
SCHB & HACH Award Luncheon	Monday, March 23	11:30 AM - 1:30 PM	Silverton Ballroom 2, Embassy Suites Denver
SCHB/HACH Award Reception	Monday, March 23	5:30 PM - 7:30 PM	Cactus Club

Nanoscience and Nanotechnology of Natural Resources

Symposium at the 2015 ACS Spring National Meeting



TUESDAY, MARCH 24 | 9:00 AM – 11:40 AM
Denver, CO | Colorado Convention Center | Mile High Ballroom 3A



Paul Weiss
 Editor-in-Chief, *ACS Nano*



Paul Alivisatos
 Co-Editor, *Nano Letters*

Join the Editors of *ACS Nano* and *Nano Letters* for the next joint session at the 2015 ACS Spring National Meeting Denver, CO. The session was specially designed for the National Meeting theme with world-renowned speakers presenting. All speakers are editors of *ACS Nano* or *Nano Letters*.

GUEST SPEAKERS

Naomi Halas, Rice University

Shuit-Tong Lee, Soochow University

Andrey Rogach, City University of Hong Kong

Uri Banin, The Hebrew University of Jerusalem

Paula T. Hammond, Massachusetts Institute of Technology

PRESENTATIONS

Your anion is my plasmonic nanostructure: Discovering molecular plasmonics

Silicon nanostructures for new energy applications

Design of colloidal heterostructures for photocatalytic hydrogen generation

Dimensionality matters: Dimensionality effects on optoelectronic behavior of semiconductor nanocrystals

Nanomaterials design for programmed multi- and staged release

SOCIAL & EDUCATIONAL EVENTS

PRESIDENTIAL EVENTS

DIANE GROB SCHMIDT, the 2015 ACS president, welcomes attendees to the 249th ACS National Meeting.

Schmidt's first presidential symposium, titled "Chemistry without Borders: The Transnational Practice of Chemistry & Allied Sciences & Engineering," will take place the morning of Sunday, March 22. This symposium will touch on the ever-increasing practice of researchers, students, and professionals working overseas and efforts to attract and build a workforce to benefit the worldwide success of chemistry.

The next presidential symposium begins later that afternoon on Sunday, March 22, and continues all day on Monday. "Nanotechnology: Delivering on the Promise" will highlight the fascinating research, development, and commercialization of nanochemistry and nanotechnology and will include 16 senior-level speakers from industry, academe, and government.

The third presidential symposium, "DOE Nanoscience Research Centers: National Resources for the Nanoscience Community," will feature the five heads of chemistry at U.S. national laboratories. This is the first symposium of its type to highlight these speakers collectively.

Always a highlight at the ACS national meetings are the Kavli lectures, which will take place on Monday, March 23, at the Colorado Convention Center. The first is The Kavli Foundation Emerging Leader in Chemistry Lecture given by Theodore Betley, a professor of chemistry and chemical biology at Harvard University, from 4:00 to 5:00 PM. Following shortly afterward, from 5:30 to 6:30 PM, is The Fred Kavli Innovations in Chemistry Lecture, given by Laura L. Kiessling, Steenbock Professor of Chemistry and Laurens Anderson Professor of Biochemistry at the University of Wisconsin, Madison, which will focus on how the features of carbohy-

drates on cell surfaces differ between mammals and microbes.

Details of presidential events and other recommended symposia can be found at www.acs.org/denver2015 and in the on-site program.

2015 NATIONAL AWARDS

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 24, at the Sheraton Denver Downtown Hotel, Ballroom. Dinner begins at 7:30 PM, and the general meeting begins at 8:30 PM. Jacqueline K. Barton will deliver the Priestley Medal Address at the general meeting. See Ticketed Events on page 71 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 250th ACS National Meeting in Boston in August.

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry, sponsored by Pearson Education, **Vickie M. Williamson**, Texas A&M University. Address to be presented before the Division of Chemical Education. March 23; Sheraton Denver Downtown Hotel; Gold Room; 3:35 PM.

ACS Award for Affordable Green Chemistry, sponsored by Dow Chemical and endowed by Rohm and Haas, **John Frye** and **Alan H. Zacher**, Pacific Northwest National Laboratory, and **Todd Werpy**, Archer Daniels Midland. Address to be presented before the Division of Cellulose & Renewable Materials. March 25; Colorado Convention Center; Room 403; 4:45 PM & 5:10 PM

ACS Award for Computers in Chemical & Pharmaceutical Research, sponsored by the ACS Division of Computers in Chemistry, **David A. Case**, Rutgers

University. Address to be presented before the Division of Computers in Chemistry. March 24; Colorado Convention Center; Mile High Ballroom 1D; 3:45 PM.

ACS Award for Creative Advances in Environmental Science & Technology, sponsored by the ACS Division of Environmental Chemistry, *Environmental Science & Technology*, and *Environmental Science & Technology Letters*, Paul B. Shepson, Purdue University. Address to be presented before the Division of Environmental Chemistry at the fall ACS national meeting in Boston.

ACS Award for Creative Invention, sponsored by ACS Corporation Associates, **Jotham W. Coe**, Pfizer. Address to be presented before the Division of Organic Chemistry. March 24; Colorado Convention Center; Four Seasons Ballroom 1; 11:10 AM.

ACS Award for Creative Research & Applications of Iodine Chemistry, sponsored by SQM S.A., **Karl O. Christe**, University of Southern California. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 10:00 AM.

ACS Award for Creative Work in Fluorine Chemistry, sponsored by the Juhua Group Technology Center (China), **Véronique Gouverneur**, University of Oxford. Address to be presented before the biennial Winter Fluorine Conference in January 2015 and the Division of Fluorine Chemistry. March 22; Embassy Suites Denver—Downtown Convention Center; Silverton Ballroom; 4:20 PM.

ACS Award for Creative Work in Synthetic Organic Chemistry, sponsored by Aldrich Chemical Co., **F. Dean Toste**, University of California, Berkeley. Address to be presented before the Division of Organic Chemistry. March 24; Colorado Convention Center; Four Seasons Ballroom 2&3; 11:05 AM.

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry, sponsored by Strem Chemicals, **Kim R. Dunbar**, Texas A&M University. Address to be presented before the Division

SOCIAL & EDUCATIONAL EVENTS

of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 10:45 AM.

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences, sponsored by the Camille & Henry Dreyfus Foundation, **Catherine H. Middlecamp**, University of Wisconsin, Madison. Address to be presented before the Division of Chemical Education. March 23; Sheraton Denver Downtown Hotel; Columbine Room; 1:50 PM.

ACS Award for Encouraging Women into Careers in the Chemical Sciences, sponsored by the Camille & Henry Dreyfus Foundation, **E. Ann Nalley**, Cameron University. Address to be presented before the Division of Professional Relations and the ACS Women Chemists Committee. March 24; Hyatt Regency Denver– Colorado Convention Center; Capitol Ballroom 6; 11:15 AM.

ACS Award for Research at an Undergraduate Institution, sponsored by Research Corporation for Science Advancement, **George C. Shields**, Bucknell University. Address to be presented before the Division of Computers in Chemistry. March 24; Colorado Convention Center; Mile High Ballroom 1E; 4:30 PM.

ACS Award for Team Innovation, sponsored by ACS Corporation Associates, **Ryan Gaston, James R. Keenihan, Abhijit A. Namjoshi, Stephen Pisklak,** and **Jason A. Reese**, Dow Chemical. Address to be presented before the Division of Energy & Fuels. March 24; Colorado Convention Center; Mile High Ballroom 4A; 8:05 AM.

ACS Award in Analytical Chemistry, sponsored by Battelle Memorial Institute, **John R. Yates III**, Scripps Research Institute, La Jolla, Calif. Address to be presented before the Division of Analytical Chemistry at the fall ACS national meeting in Boston.

ACS Award in Applied Polymer Science, sponsored by Eastman Chemical, **Geoffrey W. Coates**, Cornell University. Address to be presented before the Division of Polymeric Materials: Science & Engineering. March 22; Sheraton Denver Downtown Hotel; Governor's Square 16; 4:45 PM.

ACS Award in Chromatography, sponsored by Sigma-Aldrich/ Supelco, **Milton T. W. Hearn**, Monash University, in Australia. Address to be presented before the Division of Analytical Chemistry. March 23; Embassy Suites Denver– Downtown Convention Center; Aspen Room A; 8:05 AM.

ACS Award in Colloid & Surface Chemistry, sponsored by Colgate-Palmolive Co., **Paul S. Weiss**, University of California, Los Angeles. Address to be presented before the Division of Colloid & Surface Chemistry. March 24; Marriott City Center Denver; Colorado F; 3:40 PM.

ACS Award in Industrial Chemistry, sponsored by the ACS Division of Business Development & Management and the ACS Division of Industrial & Engineering Chemistry, **Thomas J. Colacot**, Johnson Matthey. Address to be presented before the Division of Business Development & Management and the Division of Industrial & Engineering Chemistry. March 23; Embassy Suites Denver– Downtown Convention Center; Crystal Ballroom B/C; 4:40 PM.

ACS Award in Inorganic Chemistry, sponsored by Aldrich Chemical Co., **John T. Groves**, Princeton University. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 9:30 AM.

ACS Award in Organometallic Chemistry, sponsored by the Dow Chemical Co. Foundation, **William J. Evans**, University of California, Irvine. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 9:00 AM.

ACS Award in Polymer Chemistry, sponsored by ExxonMobil Chemical, **Nikos Hadjichristidis**, King Abdullah University of Science & Technology, Thuwal, Saudi Arabia. Address to be presented before the Division of Polymeric Materials: Science & Engineering. March 25; Sheraton Denver Downtown Hotel; Governor's Square 15; 5:00 PM.

ACS Award in Pure Chemistry, sponsored by Alpha Chi Sigma Fraternity and Alpha Chi Sigma Educational Foundation, **Adam E. Cohen**, Harvard Univer-

sity, Howard Hughes Medical Institute. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 10:05 AM.

ACS Award in Separations Science & Technology, sponsored by Waters Corp., **Richard D. Noble**, University of Colorado, Boulder. Address to be presented before the Division of Industrial & Engineering Chemistry. March 22; Embassy Suites Denver– Downtown Convention Center; Crystal Ballroom A; 2:00 PM.

ACS Award in the Chemistry of Materials, sponsored by E. I. du Pont de Nemours & Co., **Mark E. Thompson**, University of Southern California. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 11:45 AM.

ACS Award in Theoretical Chemistry, sponsored by ACS, **Mark S. Gordon**, Iowa State University. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 9:35 AM.

Award for Volunteer Service to the American Chemical Society, sponsored by ACS, **Cynthia K. Larive**, University of California, Riverside. Address to be presented before the ACS ChemLuminary Awards at the ACS fall national meeting in Boston.

Roger Adams Award in Organic Chemistry, sponsored by Organic Reactions Inc. and Organic Syntheses Inc., **Larry E. Overman**, University of California, Irvine. Address to be presented before the biennial National Organic Chemistry Symposium of the ACS national meeting in July at the University of Maryland.

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry, sponsored by the Alfred R. Bader Fund, **Michael A. Marletta**, Scripps Research Institute, La Jolla, Calif. Address to be presented before the Division of Biological Chemistry. March 22; Hyatt Regency Denver– Colorado Convention Center; Capitol Ballroom 4; 7:00 PM.

Earle B. Barnes Award for Leadership in Chemical Research Management, sponsored by the Dow Chemical Co. Founda-

SOCIAL & EDUCATIONAL EVENTS

tion, **Christopher P. Austin**, National Institutes of Health. Address to be presented before the Division of Medicinal Chemistry. March 25; Colorado Convention Center; Mile High Ballroom 1A/1B; 4:15 PM.

Ronald Breslow Award for Achievement in Biomimetic Chemistry, sponsored by the Ronald Breslow Award Endowment, **Eric T. Kool**, Stanford University. Address to be presented before the Division of Organic Chemistry. March 22; Colorado Convention Center; Four Seasons Ballroom 2&3; 3:25 PM.

Herbert C. Brown Award for Creative Research in Synthetic Methods, sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment, **Gary A. Molander**, University of Pennsylvania. Address to be presented before the Division of Organic Chemistry. March 23; Colorado Convention Center; Four Seasons Ballroom 2&3; 4:10 PM.

James Bryant Conant Award in High School Chemistry Teaching, sponsored by Thermo Fisher Scientific, **Jenelle L. Ball**, Chico High School, California. Address to be presented before the Division of Chemical Education. March 22; Sheraton Denver Downtown Hotel; Silver Room; 1:00 PM.

Arthur C. Cope Award, sponsored by the Arthur C. Cope Fund, **Paul A. Wender**, Stanford University. Address to be presented before the Division of Organic Chemistry at the ACS fall national meeting in Boston.

Arthur C. Cope Scholar Awards, sponsored by the Arthur C. Cope Fund, **Michelle Chang**, University of California, Berkeley; **Debbie C. Crans**, Colorado State University, Fort Collins; **Antonio M. Echavarren**, Institute of Chemical Research of Catalonia, in Spain; **Ben L. Feringa**, University of Groningen, in the Netherlands; **Miguel A. Garcia-Garibay**, UC Los Angeles; **Neil K. Garg**, UC Los Angeles; **Chuan He**, University of Chicago; **Kenichiro Itami**, Nagoya University, in Japan; **Kenneth M. Nicholas**, University of Oklahoma; **Richmond Sarpong**, UC Berke-

ley. Address to be presented before the Division of Organic Chemistry at the ACS fall national meeting in Boston.

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator, sponsored by the Pfizer Endowment Fund, **Jin-Quan Yu**, Scripps Research Institute, La Jolla, Calif. Address to be presented before the Division of Organic Chemistry. March 23; Colorado Convention Center; Four Seasons Ballroom 2&3; 11:00 AM.

F. Albert Cotton Award in Synthetic Inorganic Chemistry, sponsored by the F. Albert Cotton Endowment Fund, **Jaqueline L. Kiplinger**, Los Alamos National Laboratory. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 8:30 AM.

Peter Debye Award in Physical Chemistry, sponsored by E. I. du Pont de Nemours & Co., **Xiaoliang Sunney Xie**, Harvard University. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 8:05 AM.

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry, sponsored by Waters Corp., **Hilkka I. Kenttämä**, Purdue University. Address to be presented before the Division of Analytical Chemistry. March 25; Embassy Suites Denver–Downtown Convention Center; Aspen Room A; 3:40 PM.

Francis P. Garvan-John M. Olin Medal, sponsored by the Francis P. Garvan-John M. Olin Medal Endowment, **Angela K. Wilson**, University of North Texas. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 9:05 AM.

James T. Grady-James H. Stack Award for Interpreting Chemistry for the Public, sponsored by ACS, **Deborah L. Blum**, University of Wisconsin, Madison. Address to be presented before the ACS Office of Public Affairs. March 22; Colorado Convention Center; Four Seasons Ballroom 4; 12:20 PM.

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator, sponsored by the Gray Award Endowment, **Emily A. Weiss**, Northwestern University. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 11:15 AM.

Ernest Guenther Award in the Chemistry of Natural Products, sponsored by Givaudan, **Thomas R. Hoye**, University of Minnesota. Address to be presented before the Division of Organic Chemistry. March 24; Colorado Convention Center; Four Seasons Ballroom 2&3; 3:45 PM.

Kathryn C. Hach Award for Entrepreneurial Success, sponsored by the Kathryn C. Hach Award Fund, **Terry L. Brewer**, Brewer Science Inc. Address to be presented before the Division of Small Chemical Businesses. March 23; Embassy Suites Denver–Colorado Convention Center; Cripple Creek Ballroom 2; 10:50 AM.

E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances, sponsored by Merck Research Laboratories, **Ruth R. Wexler**, Bristol-Myers Squibb. Address to be presented before the Division of Medicinal Chemistry. March 24; Colorado Convention Center; Mile High Ballroom 2A/2B; 11:20 AM.

Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids, sponsored by ExxonMobil Research & Engineering, **Mark Maroncelli**, Pennsylvania State University. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 8:35 AM.

E. V. Murphree Award in Industrial & Engineering Chemistry, sponsored by ExxonMobil Research & Engineering, **Joseph R. Zoeller**, Eastman Chemical. Address to be presented before the Division of Industrial & Engineering Chemistry. March 24; Embassy Suites Denver–Downtown Convention Center; Crystal Ballroom A; 4:00 PM.

Nakanishi Prize, sponsored by the Nakanishi Prize Endowment, **Fred W. McLafferty**, Cornell University. Address

SOCIAL & EDUCATIONAL EVENTS

to be presented before the Division of Analytical Chemistry. March 26; Embassy Suites Denver – Downtown Convention Center; Aspen Room A; 11:20 AM.

Nobel Laureate Signature Award for Graduate Education in Chemistry, sponsored by Avantor Performance Materials, **Denis Malyshev** (student), Synthorx, and **Floyd E. Romesberg** (preceptor), Scripps Research Institute, La Jolla, Calif. Address to be presented before the Division of Biological Chemistry. March 22; Hyatt Regency Denver – Colorado Convention Center; Capitol Ballroom 4; 8:30 AM & March 23; Hyatt Regency Denver – Colorado Convention Center; Capitol Ballroom 4; 10:45 AM.

James Flack Norris Award in Physical Organic Chemistry, sponsored by the ACS Northeastern Section, **Charles L. Perrin**, University of California, San Diego. Address to be presented before the Division of Organic Chemistry. March 24; Colorado Convention Center; Four Seasons Ballroom 1; 3:50 PM.

George A. Olah Award in Hydrocarbon or Petroleum Chemistry, sponsored by the George A. Olah Award Endowment, **Jingguang G. Chen**, Columbia University. Address to be presented before the Division of Catalysis Science & Technology. March 24; Colorado Convention Center; Room 108; 11:15 AM.

Charles Lathrop Parsons Award, sponsored by ACS, **Paul H. L. Walter**, Skidmore College. Address to be presented before the ACS Board of Directors. March 22; Hyatt Regency Denver – Colorado Convention Center; Centennial H; 1:30 PM.

George C. Pimentel Award in Chemical Education, sponsored by Cengage Learning and the ACS Division of Chemical Education, **I. Dwaine Eubanks**, Clemson University. Address to be presented before the Division of Chemical Education. March 24; Sheraton Denver Downtown Hotel; Columbine Room; 4:40 PM.

Priestley Medal, sponsored by ACS, **Jacqueline K. Barton**, California Institute of Technology. Address to be presented before the general meeting of

the American Chemical Society, Tuesday, March 24, at the Sheraton Denver Downtown Hotel, BCEF Ballroom.

Glenn T. Seaborg Award for Nuclear Chemistry, sponsored by the ACS Division of Nuclear Chemistry & Technology, **Heino Nitsche** (deceased), University of California, Berkeley. Address to be presented before the Division of Nuclear Chemistry & Technology. March 22; 8:30 AM & March 23; Embassy Suites Denver – Downtown Convention Center; Crestone Ballroom A; 8:10 AM.

Gabor A. Somorjai Award for Creative Research in Catalysis, sponsored by the Gabor A. & Judith K. Somorjai Endowment Fund, **Maurice Brookhart**, University of North Carolina, Chapel Hill. Address to be presented before the Division of Catalysis Science & Technology. March 23; Colorado Convention Center; Room 207; 4:50 PM.

George & Christine Sosnovsky Award for Cancer Research, sponsored by the George & Christine Sosnovsky Endowment Fund, **Christopher P. Leamon**, Endocyte, Inc.; **Philip Low**, Purdue University; **Joseph A. Reddy** and **Iontcho Vlahov**, Endocyte, Inc. Address to be presented before the Division of Medicinal Chemistry. March 25; Colorado Convention Center; Mile High Ballroom 1A/1B; 2:45 PM & 3:30 PM.

E. Bright Wilson Award in Spectroscopy, sponsored by the ACS Division of Physical Chemistry, **R. J. Dwayne Miller**, Max Planck Institute for the Structure & Dynamics of Matter, Hamburg, Germany, and University of Toronto. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 11:25 AM.

Ahmed Zewail Award in Ultrafast Science & Technology, sponsored by the Ahmed Zewail Endowment Fund established by Newport Corp., **Shaul Mukamel**, University of California, Irvine. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 10:55 AM.

National Fresenius Award, sponsored by Phi Lambda Upsilon, the National Chemistry Honor Society, **Abigail G.**

Doyle, Princeton University. Address to be presented before the Division of Organic Chemistry. March 25; Colorado Convention Center; Four Seasons Ballroom 2&3; 11:10 AM.

SOCIAL & TICKETED EVENTS

A VARIETY of social and special events will be held by event organizers during the meeting. Event participation is open to all interested registrants. View an updated listing of social and special events, including event locations, at www.acs.org/meetings.

The following social events require purchase of a ticket (event number in red), which can be purchased through Attendee Registration. Tickets will remain on sale until the evening prior to the event, if available. All tickets are sold on a first-come, first-served basis. Cancellations or refund requests must be made by March 8. No tickets will be refunded after that date.

FRIDAY, MARCH 20

CHAS Workshop: Laboratory Waste Management

7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Cripple Creek Ballroom 2

CHAS Workshop: Laboratory Safety

7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Cripple Creek Ballroom 1

SATURDAY, MARCH 21

CHAS Workshop: How to be a More Effective Chemical Hygiene Officer

7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 1

CHAS Workshop: Reactivity Hazards: Laboratory Scale Recognition & Control

7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Cripple Creek Ballroom 1

SOCIAL & EDUCATIONAL EVENTS

CHAS Workshop: Job Hazard Analysis

7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown
Convention Center
Cripple Creek Ballroom 2

COACH Workshop: COACHing Strong Women in the Art of Strategic Persuasion – Jr. Faculty

8:30 AM to 5:00 PM
Grand Hyatt Denver
Mt. Harvard

COACH Workshop: COACHing Strong Women in the Art of Strategic Persuasion – Sr. Faculty

8:30 AM to 5:00 PM
Grand Hyatt Denver
Mt. Princeton

Presidential Outreach Event – Exploring Our World Through Chemistry

Kids and families can learn more about the fascinating world of chemistry through hands-on, age-appropriate activities at the Denver Zoo.

10:00 AM to 2:00 PM
Denver Zoo
2300 Steele Street
Denver

COACH Reception

5:00 PM to 7:00 PM
Grand Hyatt Denver
Maroon Peak

SUNDAY, MARCH 22

CHAS Executive Committee Meeting

8:00 AM to 12:00 PM
Embassy Suites Denver - Downtown
Convention Center
Silverton Ballroom 3

CHED Workshop 1

8:00 AM – 12:00 PM
Sheraton Denver Downtown
Plaza Court 3

NRCC Certification Exams

8:00 AM to 12:00 PM
Embassy Suites Denver - Downtown
Convention Center
Rexford Room

ACS Career Fair Workshops: Career Pathways II

8:30 AM to 5:00 PM
Colorado Convention Center, Room 604

ACS Career Fair Workshops: Career Workshop

8:30 AM to 5:00 PM
Colorado Convention Center, Room 701

Undergraduate Hospitality Center

8:00 AM to 5:00 PM
Sheraton Denver Downtown,
Majestic Ballroom

Undergraduate Workshop: Making the Most of Your First National Meeting

9:00 AM to 9:45 AM
Sheraton Denver Downtown,
Majestic Ballroom

Society Communication Workshop: Improv Training

Room 1/SE03/SE03A/\$10
9:00 AM to 12:00 PM
The Curtis – a DoubleTree by Hilton,
Dodgeball Room

Undergraduate Workshop: Graduate School Reality Check: Getting In

10:00 AM to 11:15 AM
Sheraton Denver Downtown,
Plaza Ballroom AB

Harvey Mudd College Alumni & Friends Brunch

10:00 AM to 1:00 PM
Hotel Monaco – Panzano
1717 Champa Street
Denver

Chem Demo Exchange

11:00 AM to 12:30 PM
Colorado Convention Center, Hall B2

Undergraduate Workshop: Graduate School Reality Check: You're in-Now What?

11:15 AM to 12:30 PM
Sheraton Denver Downtown,
Plaza Ballroom AB

SCHB/PROF Luncheon

11:30 AM to 1:30 PM
Embassy Suites Denver - Downtown
Convention Center
Silverton Ballroom 2

ACS Board Open Session & Luncheon

(Open to staff and attendees)
12:00 PM to 1:00 PM
Colorado Convention Center,
Four Seasons Ballroom 4

ACS Career Fair Workshops: Career Pathways I

12:00 PM to 5:30 PM
Colorado Convention Center, Room 602

ACS Career Fair Workshops: Career Pathways III

12:00 PM to 5:30 PM
Colorado Convention Center, Room 606

CHED High School/College Interface Luncheon/SE05/\$0

(Included at no charge with high school teacher registration.)
12:00 PM to 1:00 PM
Sheraton Denver Downtown, Silver

Undergraduate Workshop: How to be a Successful ACS Student Chapter

1:00 PM to 2:30 PM
Sheraton Denver Downtown, Plaza
Ballroom DE

Undergraduate Workshop: Networking Social with Graduate School and Research Opportunity Representatives

1:00 PM to 5:00 PM
Sheraton Denver Downtown,
Grand Ballroom

CHED Workshop 2

1:00 PM to 5:00 PM
Sheraton Denver Downtown,
Plaza Court 4

Charles Lathrop Parsons Award, sponsored by ACS

Paul H. L. Walter, Skidmore College
Address to be presented before the
ACS Board of Directors
1:30 PM to 2:30 PM
Hyatt Regency Denver, Centennial H

Society Communication Workshop: Improv Training

Room 1/SE04/SE04A/\$10
1:30 PM to 4:30 PM
The Curtis – a DoubleTree by Hilton,
Keep Away Room

UPAB/CPC Strategy Cafe

(Co-sponsored by CPC)
2:45 PM to 4:00 PM
Hyatt Regency Denver at Colorado
Convention Center
Centennial B

Undergraduate Workshop: Can You Have a Life and Career

(Co-sponsored by WCC)
2:45 PM to 4:00 PM
Sheraton Denver Downtown,
Plaza Ballroom DE

Chemistry of Natural Resources Plenary

3:00 to 5:20 PM
Bellco Theater, Colorado Convention
Center

SOCIAL & EDUCATIONAL EVENTS

Characterizing Structure and Chemistry of Functional Nanomaterials

Sponsor: FEI Company
3:30 PM to 6:00 PM
Colorado Convention Center, Room 103

Undergraduate Workshop: Improving Scientific Communication Skills

4:00 PM to 5:30 PM
Sheraton Denver Downtown,
Plaza Ballroom AB

Undergraduate Workshop: Careers in Teaching Chemistry

4:00 PM to 5:30 PM
Sheraton Denver Downtown,
Plaza Ballroom DE

Nominees Town Hall Meeting

4:30 to 5:30 PM
Hyatt Regency Denver at Colorado
Convention Center
Centennial F/G

Grady-Stack Award Reception Honoring Deborah Blum

4:30 PM to 6:00 PM
Hyatt Regency Denver at Colorado
Convention Center
Centennial A

ACS Diversity Reception

5:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado
Convention Center
Centennial C

PNNL 50th Anniversary Reception

5:00 PM to 6:30 PM
Colorado Convention Center, Room 203

University of Wisconsin – Madison Alumni & Friends

5:00 PM to 7:00 PM
Marriott City Center Denver
Penrose Ballroom 1

Chemistry at Illinois Alumni & Friends Reception

5:00 PM to 8:00 PM
Marriott City Center Denver
Penrose Ballroom 2

CHED Social Reception

5:30 PM to 7:00 PM
Colorado Convention Center, Room 207

International Welcome Reception/ SE06/ \$No Fee

5:30 PM to 7:30 PM
Hyatt Regency Denver at Colorado
Convention Center
Centennial D

Research Corporation Reception in Honor of the Awardee for Research at an Undergraduate Institution

5:30 PM to 7:30 PM
Marriott City Center Denver,
Colorado Ballroom E

COLL Social Hour/ Poster Session/Open

Business Meeting
5:30 PM to 8:00 PM
Colorado Convention Center, Hall E

CINF Open Business Meeting

6:00 PM to 6:30 PM
Embassy Suites Denver - Downtown
Convention Center
Silverton Ballroom 3

Mid Atlantic Councilor Caucus

6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado
Convention Center
Mineral D

District IV Councilor Caucus

6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado
Convention Center
Mineral E

District V Councilor Caucus

6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado
Convention Center
Mineral F

District II Councilor Caucus

6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado
Convention Center
Mineral C

District VI Councilor Caucus

6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado
Convention Center
Mineral G

CELL & INOR Poster Session

6:00 to 8:00 PM
Colorado Convention Center, Hall C

Expo Attendee Welcome Reception

6:00 PM to 8:30 PM
Colorado Convention Center, Halls A/F

CINF Division Welcoming Reception

6:30 PM to 8:30 PM
Embassy Suites Denver - Downtown
Convention Center
Silverton Ballroom 3

CHED Posters Session

7:00 PM to 9:00 PM
Colorado Convention Center, Hall C

BIOL Poster Session

8:15 PM to 9:45 PM
Colorado Convention Center, Hall B2

MEDI & COLL Poster Session

7:00 to 9:00 PM
Colorado Convention Center, Hall E

ACS Student Chapter Awards Ceremony

7:00 PM to 8:30 PM
Colorado Convention Center,
Bellco Theater

ORGN Poster Session

8:00 to 10:00 PM
Colorado Convention Center, Hall C

Undergraduate Social

8:30 PM to 11:00 PM
Colorado Convention Center,
Four Seasons Ballroom

MONDAY, MARCH 23

WCC Women in the Chemical Enterprise Breakfast/SE01/\$40 (regular)/SE02/\$20 (student)

7:30 AM to 9:00 AM
(A limited number of student tickets are available. Students may purchase regular tickets if student tickets are sold out.)

Hyatt Regency Denver at Colorado
Convention Center
Centennial E

CHED Workshop 3

8:00 AM to 12:00 PM
Sheraton Denver Downtown,
Plaza Court 3

Undergraduate Hospitality Center

8:00 AM to 5:00 PM
Sheraton Denver Downtown,
Majestic Ballroom

ACS Career Fair Workshop: Career Pathways I

8:30 AM to 5:30 PM
Colorado Convention Center, Room 602

ACS Career Fair Workshop: Career Pathways II

8:30 AM to 5:30 PM
Colorado Convention Center, Room 604

ACS Career Fair Workshop: Career Pathways III

8:30 AM to 5:30 PM

SOCIAL & EDUCATIONAL EVENTS

Colorado Convention Center, Room 606

ACS Exposition

9:00 AM to 5:00 PM

Colorado Convention Center, Halls A/F

University of Wisconsin – Milwaukee Workshop: Scale Interventions for Lecture & Laboratory

9:00 AM to 12:00 PM

Sheraton Denver Downtown,
Plaza Court 2

Spectroscopy Simplified – How to Run a Research FT-IR

Sponsor: Thermo Scientific

9:30 AM to 12:00 PM

Colorado Convention Center, Exhibit
Halls A/F, Exhibitor Workshop Room 1

Innovative Technologies to Engage Your Student's Learning Experience

Sponsor: McGraw Hill Higher Education,
9:30 AM to 12:00 PM

Colorado Convention Center, Room 103

Driving Separations Success.

Sponsor: Waters Corporation

9:30 AM to 12:00 PM

Colorado Convention Center, Exhibit
Halls A/F, Exhibitor Workshop Room 2

Undergraduate Workshop: Networking 101

9:45 to 11:00 AM

Colorado Convention Center,
Rooms 601/603

Undergraduate Workshop: Chemists Celebrate Earth Day (Co-sponsored by Committee on Community Activities)

9:45 to 11:45 AM

Sheraton Denver Downtown,
Grand Ballroom II

Women Chemists of Color Social

10:00 AM to 11:30 AM

Hyatt Regency Denver at Colorado
Convention Center, Mineral D

Undergraduate Poster Session

12:00 PM to 2:00 PM

Colorado Convention Center, Hall C

Committee on Minority Affairs Luncheon/SE07/\$50

11:30 AM to 1:30 PM

Hyatt Regency Hotel at Colorado
Convention Center
Centennial E

SCHB/HACH Luncheon

11:30 AM to 1:30 PM

Embassy Suites Denver - Downtown
Convention Center
Silverton Ballroom 2

CHAL Luncheon/SE08/\$40

12:00 PM to 1:30 PM

Embassy Suites Denver - Downtown
Convention Center
Silverton Ballroom 3

SciFinder Training Session System with the Touch of a Button

Sponsor: CAS

12:30 PM – 3:00 PM

Colorado Convention Center, Exhibit
Hall A/F, Exhibitor Workshop Room 1

Protecting Our Natural Resources with GC-MS and LC-MS from Thermo Fisher Scientific

Sponsor: Thermo Scientific

12:30 PM to 3:00 PM

Colorado Convention Center, Exhibit
Halls A/F, Exhibitor Workshop Room 2

Innovative Technologies to Engage Your Student's Learning Experience

Sponsor: McGraw Hill Higher Education,
12:30 PM - 3:00 PM, Colorado
Convention Center, Room 103

CHED Workshop 4

1:00 PM to 5:00 PM

Sheraton Denver Downtown,
Plaza Court 4

College of Wooster Alumni, Students, Faculty & Friends of Helen Murray Free

2:30 to 4:30 PM

Colorado Convention Center, Room 701

CHED Younger Chemistry Education Scholars Social

3:00 PM to 5:00 PM

Sheraton Denver Downtown, Windows

WCC 'Just Cocktails'

3:30 PM to 4:30 PM

Hyatt Regency Denver at Colorado
Convention Center
Capitol 5

Online Homework with Targeted Instructional Feedback Leads to Improved Student Learning Outcomes

Sponsor: Sapling Learning

3:30 PM to 6:00 PM,

Colorado Convention Center, Room 103

Undergraduate Speed Networking with Chemistry Professionals

3:45 PM to 5:15 PM

Hyatt Regency Denver at Colorado
Convention Center

Centennial D/E

The Kavli Foundation Emerging Leader in Chemistry Lecture

4:00 PM to 5:05 PM

Colorado Convention Center,
Bellco Theater

CHAL Reception

5:00 PM to 8:00 PM

Grand Hyatt Denver, Capital Peak A

The Fred Kavli Innovations in Chemistry Lecture

5:30 PM to 6:30 PM

Colorado Convention Center,
Bellco Theater

Colorado State University Chemistry Alumni & Friends Reception

7:00 PM to 8:00 PM

CSU Denver Event Center
475 17th Street, Suite 200
Denver

Purdue Department of Chemistry Alumni Event/SE10/\$10

7:00 PM to 8:30 PM

The Curtis – a DoubleTree by Hilton,
Keep Away Room

ACS Graduate & Postdoctoral Scholars Reception

7:00 PM to 8:30 PM

Colorado Convention Center,
Four Seasons Ballroom 4

2015 CARB Award Banquet/SE09/\$60

7:00 PM to 10:00 PM

Appaloosa Grill – 535 16th Street,
Denver

NUCL Social Hour

7:00 PM to 9:00 PM

Embassy Suites Denver - Downtown
Convention Center
Silverton Ballroom 2

Sci-Mix Interdivisional Poster Session & Mixer

(Drink Ticket with registration)

8:00 PM to 10:00 PM

Colorado Convention Center, Hall C

TUESDAY, MARCH 24

Senior Chemists Breakfast/SE11/\$20

7:30 AM to 9:30 AM

Hyatt Regency Denver at Colorado
Convention Center
Centennial A/B

SOCIAL & EDUCATIONAL EVENTS

University of Minnesota Alumni & Friends Breakfast/SE20/\$5

7:30 AM to 9:30 AM
Colorado Convention Center, Room 207

ACS Career Fair Workshop: Career Pathways I

8:30 AM to 5:30 PM
Colorado Convention Center, Room 602

ACS Career Fair Workshop: Career Pathways II

8:30 AM to 5:30 PM
Colorado Convention Center, Room 604

ACS Career Fair Workshop: Career Pathways III

8:30 AM to 5:30 PM
Colorado Convention Center, Room 606

ACS Exposition

9:00 AM to 5:00 PM
Colorado Convention Center, Halls A/F

SciFinder Training Session

Sponsor: CAS
9:30 AM to 12:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1

A Survey of Accelerated Materials Research Using Raman Microscopy and Imaging

Sponsor: Thermo Scientific
9:30 AM to 12:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2

Compact Mass Spectrometry: A Swiss Army Knife Approach to Chemistry Challenges

Sponsor: Advion
9:30 AM to 12:00 PM
Colorado Convention Center, Room 103

Alpha Chi Sigma Fraternity Luncheon

11:00 AM to 1:30 PM
Bubba Gump Shrimp Co.
1437 California St., Denver

Eli Lilly Poster Session

11:00 AM to 12:00 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial A-C

CINF Division Luncheon/SE12/\$15 (students)/SE12A \$20 (regular)

12:00 PM to 1:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 3

WCC Eli Lilly Travel Award Poster Session & Luncheon/SE14/\$50 (regular)/SE15/\$25 (student)

12:00 PM to 1:30 PM
Hyatt Regency Denver at Colorado Convention Center
Centennial A – C

COLL Luncheon/SE13/\$40

12:00 PM to 1:45 PM
Marriott City Center Denver, Penrose Ballroom 1

Committee on Environmental (CEI) Film Series – Thin Ice: The Inside Story of Climate Science

12:00 PM to 2:00 PM
Sheraton Denver Downtown, Grand Ballroom I

PerkinElmer Workshop: Nano FFF & SP-ICP-MS

12:00 PM to 6:00 PM
Colorado School of Mines
1500 Illinois Street, Golden, CO

Intelligent Real-Time Reaction Monitoring In The Fume Hood Using Benchtop NMR

Sponsor: Thermo Scientific
12:30 PM to 3:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Analysis of Polymers by Vibrational Spectroscopy and Microscopy

Sponsor: Bruker
12:30 PM to 3:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2

Advances in Atomic and Molecular Spectroscopy

Sponsor: Agilent Technologies
12:30 PM to 3:00 PM
Colorado Convention Center, Room 103

ENFL Poster Session

2:00 to 4:00 PM
Colorado Convention Center, Halls A/F

Chromatography and Mass Spectrometry Tips, Tricks, and Advanced Techniques

Sponsor: Agilent Technologies
3:30 PM to 6:00 PM
Colorado Convention Center, Room 103

AGFD Poster Session

3:30 to 5:30 PM
Colorado Convention Center, Hall C

Dow Energy Water Nexus Reception

4:00 PM to 5:00 PM
Colorado Convention Center, Room 207

Division Councilors & Division Officers Caucus

4:00 PM to 6:00 PM
Colorado Convention Center, Room 502

I&EC Poster Session

5:00 to 6:30 PM
Colorado Convention Center, Hall C

VUV Analytics ACS Reception

5:00 PM to 7:30 PM
Colorado Convention Center, Mile High Ballroom 4D

District I Councilor Caucus

5:30 PM to 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral C

ENVR Reception/SE16/\$10

6:00 PM to 7:30 PM
Wynkoop Brewing Company
1634 18th Street, Denver

PMSE/POLY Joint Poster Session

6:00 to 8:00 PM
Colorado Convention Center, Hall E

CATL & INOR Poster Session

6:00 to 8:00 PM
Colorado Convention Center, Hall C

COMP Poster and Award Session

6:00 to 8:30 PM
Colorado Convention Center, Hall B2

BIOT Poster Session

6:00 to 9:00 PM
Grand Hyatt Denver, Imperial Ballroom

AGFD Chair's Reception

6:00 PM to 8:00 PM
Embassy Suites Denver - Downtown Convention Center
Crystal Ballroom B

Access meeting information
and the On-site Program at
www.acs.org/denver2015

SOCIAL & EDUCATIONAL EVENTS

ACS National Awards Reception, Banquet Ceremony & General Meeting of the Society/SE17/\$130

6:30 PM to 10:00 PM
Sheraton Denver Downtown Hotel,
Plaza Ballroom BCEF

CELL Anselme Payen Award Banquet/SE18/\$65

6:30 PM to 10:00 PM
CooHills Restaurant
1400 Wewatta St., Denver

CARB & ANYL Poster Session

7:00 to 9:00 PM
Colorado Convention Center, Hall C

ENFL Division Dinner/SE19/\$65

7:30 PM to 9:00 PM
Maggiano's Little Italy
500 16th St., Ste 150, Denver

ORGN Poster Session

8:00 to 10:00 PM
Colorado Convention Center, Hall C

WEDNESDAY, MARCH 25

ACS Career Fair Workshop: Career Pathways I

8:30 AM to 5:30 PM
Colorado Convention Center, Room 602

ACS Career Fair Workshop: Career Pathways II

8:30 AM to 5:30 PM
Colorado Convention Center, Room 604

ACS Career Fair Workshop: Career Pathways III

8:30 AM to 5:30 PM
Colorado Convention Center, Room 606

New Developments in Isothermal Titration Calorimetry from MicroCal

Sponsor: Malvern Instruments
9:30 AM to 12:00 PM
Colorado Convention Center, Room 103

PerkinElmer Workshop: Nano FFF & SP-ICP-MS

12:00 PM to 6:00 PM
Colorado School of Mines
1500 Illinois Street, Golden, CO

Designing Inhibitors with MOE Structure-Based Drug Design Tools

Sponsor: Chemical Computing Group
3:30 PM to 6:00 PM
Colorado Convention Center, Room 103

POLY/PMSE Awards Reception

5:30 PM to 8:30 PM
Sheraton Denver Downtown Hotel,
Plaza Ballroom A/B

PHYS & ENVR Poster Session

6:00 PM to 8:00 PM
Colorado Convention Center, Hall C

Joint MEDI & ORGN Poster Session

7:00 PM to 10:00 PM
Colorado Convention Center,
Four Seasons Ballroom

STUDENT & TEACHER ACTIVITIES

EDUCATION-FOCUSED programs and specialty activities are being held for undergraduate students, graduate students, high school teachers, and chemical professionals. Explore these opportunities in depth at www.acs.org/denver2015.

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 Henry Kohlbrand from Dow Chemical will discuss sustainability from a research and industrial point of view.

SUNDAY, MARCH 22

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

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

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

**Graduate School Reality Check, Step I:
Getting In,** 10:00 to 11:15 AM

**Graduate School Reality Check, Step
II: You're In—Now What?** 11:15 AM to
12:30 PM

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

**Networking Social with Graduate
School Recruiters,** 1:00 to 5:00 PM

**Networking Social with Graduate
School and Research Opportunity
Representatives,** 1:00 to 2:30 PM

Can You Have a Life and Career?
(cosponsored by WCC), 2:45 to
4:00 PM

**Workshop: Careers in Teaching
Chemistry,** 4:00 to 5:30 PM

**Workshop: Improving Scientific Com-
munication Skills,** 4:00 to 5:30 PM

Student Chapter Awards Ceremony,
7:00 to 8:30 PM

Undergraduate Social, 8:30 to
11:00 PM

MONDAY, MARCH 23

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

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

**Technical Symposium: NREL Biomass
to Fuel & Products** (cosponsored by
CELL and ENFL), 9:00 to 10:30 AM

Workshop: Networking 101, 9:45 to
11:00 AM

**Workshop: Chemists Celebrate Earth
Day,** (cosponsored by CCA) 9:45 to
11:45 AM

**Technical Symposium: Forensic Toxi-
cology of Marijuana** (cosponsored by
BMGT and TOXI), 10:45 to 11:45 AM

**Undergraduate Research Poster
Session** (sponsored by CHED), noon to
2:00 PM

**Eminent Scientist Lecture: "Sustain-
ability in the 21st Century: Optimizing
Complex Interdependent Systems,"
with Henry Kohlbrand, Dow Chemical**
(cosponsored by CELL and ENFL), 2:30
to 3:30 PM

**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 24

Chemistry and 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: Matthew Mio, University of Detroit, Mercy. Program Chair: Daniel Swartling, Tennessee Technological University, Cookeville. For more information, go to 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 Colorado Convention Center.

MONDAY, MARCH 23

Graduate & Postdoctoral Scholars Reception, 7:00 to 8:30 PM.

For more information about this reception and other ACS programs offered to graduate students and postdocs, visit www.acs.org/grad or contact the ACS Graduate & Postdoctoral Scholars Office at 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, "Chemistry of Natural Resources." 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 22

High School Teachers Program, 8:30 AM to 4:30 PM; Sheraton Denver Downtown Hotel.

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

WORKSHOPS

THE FOLLOWING workshops require a separate registration process and/or entry fee to participate in the event, as indicated in this listing. Participation is open to all interested registrants.

Division of Chemical Health & Safety (CHAS)-sponsored workshop fees (unless otherwise indicated). CHAS member: \$300; non-CHAS member: \$350. Registration is required for all CHAS workshops. Register online at dchas.org.

Laboratory Waste Management. Friday, March 20, 7:30 AM to 5:30 PM, Embassy Suites Denver, Cripple Creek Ballroom 2. **Sponsored by CHAS.** Presenter: Russ Phifer. This comprehensive course will identify various regulatory requirements that apply to laboratories that generate hazardous waste, as well as provide insight on the options for on-site management and off-site disposal. The focus will include discussion of recycling/reclamation techniques, economical handling of waste, and liability issues.

Laboratory Safety. Friday, March 20, 7:30 AM to 5:30 PM, Embassy Suites Denver, Cripple Creek Ballroom 1. **Sponsored by CHAS.** Presenters: James Kaufman and/or Jack Breazeale. This presentation on laboratory safety by the Laboratory Safety Institute has been attended by thousands of safety professionals. With experience in both industrial and academic laboratories, the presenters take a real-world

approach to safety issues in the lab. Interactive demonstrations will teach you about issues such as creative wiring in the lab and how to work with administrators to keep a safe working environment. This workshop provides an excellent forum to speak openly about safety in the workplace.

How To Be a More Effective Chemical Hygiene Officer. Saturday, March 21, 7:30 AM to 5:30 PM, Embassy Suites Denver, Silverton Ballroom 1. **Sponsored by CHAS.** Presenter: Russ Phifer. Take a close look at the Chemical Hygiene Officer (CHO) position, and prepare at the same time for the CHO Certification exam, which will be held on Sunday, March 22, through the National Registry of Certified Chemists. This workshop will focus on what you do and how you can do it better. The course covers all of the content areas of the certification exam and includes a sample test in the same format as the real one. Request an application packet for the CHO Certification examination at www.acs.org/dchas.

Chemical Reactivity Hazards: Laboratory-Scale Recognition & Control. Saturday, March 21, 7:30 AM to 5:30 PM, Embassy Suites Denver, Cripple Creek Ballroom 1. **Sponsored by CHAS.** Presenter: Neal Langerman. This workshop addresses the risks associated with chemicals such as *t*-butyllithium and processes such as thermal distillations. The objective is to provide participants with the knowledge and skills to screen processes for potential hazards, to recognize when reactive hazards are present, and to implement appropriate controls to reduce the risk of an incident associated with the hazards. Workshop attendees will review case studies of actual incidents and do screening 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. Preregistration for this event is required.

Job Hazard Analysis Workshop. Saturday, March 21, 7:30 AM to 5:30 PM, Embassy Suites Denver, Cripple Creek Ballroom 2. **Sponsored by CHAS.**

CHEMISTRY OF NATURAL RESOURCES

Denver, CO • March 22–26, 2015

Organized by Robert S. Weber, Senior Scientist and Operating Officer, Institute for Integrated Catalysis, Pacific Northwest National Laboratory; Associate Editor, Energy & Fuels.



Chemistry of Natural Resources Plenary Session

Colorado Convention Center, Belco Theater

Sunday, March 22, 2015, 3:00 – 5:00 PM



Dr. Carolyn A. Koh

Department of Chemical & Biological Engineering
Colorado School of Mines

Fundamentals of Gas Hydrates and Their Role in Energy Transportation and Storage

Understanding of the economic and environmental components of gas hydrates.



Dr. Peter Kareiva

Chief Scientist for The Nature Conservancy

Water in the Anthropocene: Too Much, Too Little, Too Dirty

Understanding water as it relates to science, policy and financial incentives.



Dr. Paul F. Bryan

Department of Chemical & Biomolecular Engineering
University of California, Berkeley

The Four Horsemen of the Advanced Biofuels Apocalypse – Sustainability, Technology, Profitability, and Politics

Understanding Advanced Biofuels (ABF), government funding, their technology, and development.

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 American Chemical Society gratefully acknowledges The Kavli Foundation's generous support for The Fred Kavli Innovations in Chemistry Lecture and The Kavli Foundation Emerging Leader in Chemistry Lecture.

The Kavli Foundation Emerging Leader in Chemistry Lecture

Colorado Convention Center, Belco Theatre

Monday, March 23, 2015

4:00 – 5:00 PM



Dr. Theodore Betley

Professor of Chemistry and Chemical Biology
Harvard University

Radical Frontiers in Catalysis

Understanding of factors contributing to the promotion of productive small molecule activation processes.

The Fred Kavli Innovations in Chemistry Lecture

Colorado Convention Center, Belco Theatre

Monday, March 23, 2015

5:30 – 6:30 PM



Dr. Laura L. Kiessling

Steenbock Professor of Chemistry
Laurens Anderson Professor of Biochemistry
University of Wisconsin-Madison

Us Versus Them: Distinguishing Humans from Microbes with Carbohydrates

How the features of carbohydrates on the cell surfaces differ between mammals and microbes.



ACS

Chemistry for Life®

Theme-Related Technical Symposia & Programming

Full Program information is available online at www.acs.org/denver2015

Division of Agricultural and Food Chemistry (AGFD)

- Water Our Most Critical Resource

Division of Biochemical Technology (BIOT)

- Biofuels & Sustainable Energy: Engineering Microbes to Utilize Next Generation Feedstocks
- Biofuels & Sustainable Energy: Development of Sustainable & Low-cost Feedstocks for Biofuels & Bioproducts
- Biofuels & Sustainable Energy: Biomass Pretreatment & Hydrolysis
- Biofuels & Sustainable Energy: Biological Fuel & Energy Production Using Photons & Electrons
- Downstream Processing: Downstream Processing for the Biobased Industries

Division of Catalysis Science & Technology (CATL)

- Catalytic Materials and Technologies for Upgrading of CO_x and Natural Gas
- Electrocatalysis and Photocatalysis
- Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis
- Novel Catalytic Materials for Renewable Fuels/Chemicals

Division of Cellulose & Renewable Materials (CELL)

- Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser
- Cellulose Dissolution: New Solvents and Mechanisms
- Cellulose in Solid State and Solution: Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau
- Conservation Science of Cellulosic Materials: Recent Developments
- Frontiers in Glycoscience
- Functional Lignocellulosics and Nanotechnology
- CELL General Posters
- Lignin Biosynthesis, Characterization and Modifications
- Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America
- Application of Computational Chemistry to Biomass Chemistry and Utilization
- Research on Renewable Materials: US and EU Perspectives
- Smart and Responsive Composites from Renewable Building Blocks

Division of Chemical Education (CHED)

- Citizens First: Communicating Climate Science to the Public

Division of Chemical Information (CINF)

- Information Sources on Natural Resources

Division of Computers in Chemistry (COMP)

- Computational Pyrolysis & Upgrading of Bio-Oils

Division of Energy & Fuels (ENFL)

- 12th International Symposium on Heavy Oil Upgrading, Production & Characterization
- Catalysis for Un-conventional Energy Sources
- Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR and Novel Approaches
- Nanomaterials for Solar Energy Conversion & Storage

Division of Environmental Chemistry (ENVR)

- Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment
- Assessing Toxicity of Environmental Contaminants
- Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment
- Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs
- Chemical Processes at Environmental Interfaces
- Chemistry in the Marine Boundary Layer
- Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter
- Environmental Chemistry: Pedagogical Models and Practices

Division of Environmental Chemistry (ENVR)

- Environmental Reactivity of Organic Micropollutants and their Transformation Products in Receiving Waters
- Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment
- Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment
- Hydraulic Fracturing Impacts on Water, Soil and Air Quality
- Solutions to Metals Contamination of Water
- Surface Physicochemical Processes in Engineered and Natural Systems
- Trace Materials in Air, Soil, and Water
- Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use
- Water Sustainability in Oil and Gas Exploration: Treatment Issues

Division of Geochemistry (GEOC)

- Coupled Cycling of Biogeochemical Critical Elements and Contaminants
- Geochemistry and Reactive Transport in Nano-Pore Geomaterials
- How Do Geologic Processes Drive the Structure and Function of Aquatic and Riparian Ecosystems?
- Iron Oxides: Formation, Structure, Reactivity and Applications
- Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces
- Understanding the Geochemical Interactions of Organic Compounds in the Subsurface

Division of the History of Chemistry (HIST)

- Chemical Technology in Antiquity

Division of Industrial & Engineering Chemistry (I&EC)

- Uranium in Seawater

Division of Inorganic Chemistry (INOR)

- Earth-Abundant Materials for Sustainable Hydrogen Production and Storage
- Environmental and Energy-Related Inorganic Chemistry
- Chemistry of the Energy Water Nexus: Focus on Fracking

Multidisciplinary Program Planning Group (MPPG)

- Chemistry of Natural Resources Plenary
- The Kavli Foundation Lecture Series
- Nanoscience and Nanotechnology of Natural Resources

Division of Organic Chemistry (ORGN)

- Chemistry of Natural Resources

Division of Small Chemical Businesses (SCHB)

- Water is the Next Oil: Small Businesses Percolating to the Top

Society Committee on Education (SOCED)

- Sustainability in the 21st Century: Optimizing Complex Interdependent Systems
- Biomass to Fuel and Products
- Forensic Toxicology of Marijuana

Presenter: Sammuella Sigmann. Job Hazard Analysis (JHA) is one method to consider hazards associated with lab research and guide the control of those hazards. JHA can assist a researcher in uncovering potential hazards in synthesis, instrumental studies, physical manipulations, and more. Identified hazards can then be mitigated or eliminated. In this workshop, participants will learn the basic principles, required elements, and format of the common JHA. Examples of completed tools, such as nitric acid digestion of metal samples, cryogenic work, and HPLC with THF/DCM/Water, will be utilized to examine the technique. Each participant will create a ready-to-use JHA based on some task applicable to their lab, so attendees should come with a specific idea of a chemical or process they would like to investigate.

COACH-the-COACHes. Saturday, March 21, 8:30 AM to 5:00 PM, Grand Hyatt Denver, Mt. Wilson. **Sponsored by COACH.** This workshop is designed for women faculty who are interested in being trained to offer COACH workshops to graduate students and post-doctoral associates at their academic institution and/or regional professional meetings and who have attended COACH workshops in the past. This session will be a refresher of the negotiation and communication skills taught in faculty COACH workshops and also cover interview techniques, CV and website building, and effective scientific presentation. Participants will need to attend the full day of activities from 8:00 AM to 4:00 PM. The traditional COACH reception will follow the day's activities. Participants must have attended a COACH workshop previously. Apply at: coach.uoregon.edu. For more information, contact Priscilla Lewis: coach@uoregon.edu; phone: 541-346-0116. Fee: Free.

COACHing Strong Women in the Art of Strategic Persuasion—Senior Faculty. Saturday, March 21, 8:30 AM to 4:30 PM, Grand Hyatt Denver, Mt. Princeton.

COACHing Strong Women in the Art of Strategic Persuasion—Junior Faculty. Saturday, March 21, 8:30 AM to 5:00

PM, Grand Hyatt Denver, Mt. Harvard. **Sponsored by COACH.** These workshops will help professional women be more effective when leading or participating in discussions, meetings, or group negotiations. Learn about strategic rather than reactive behaviors and effective speaking voices while tuning out stress and tension, which will allow you to be heard. The workshops combine presentation, leadership training, and faculty development in an interactive format that encourages highly personal learning. Topics include communication styles effective for women; projecting confidence and credibility through voice, image, and body language; dealing with difficult conversations; and using powerful rather than weak words. Preregistration is required; visit coach.uoregon.edu. For more information, contact Priscilla Lewis at coach@uoregon.edu or (541) 346-0116. Fee: Free.

Improv Training. Sunday, March 22, 9:00 AM to noon and 1:30 to 4:00 PM, The Curtis Hotel, Training Rooms 1 thru 4. **Sponsored by Society Communications.** \$10 per session. Catalyze your communication skills at this improv session with trainers from the acclaimed Alan Alda Center for Communicating Science. You'll learn how to connect with the audience and create effective delivery that will captivate and inform. Whether you're new to communicating or want to pick up some new tips, this workshop is for you.

"Scale Interventions for Lecture & Laboratory" Monday, March 23, 9:00 AM to noon, Sheraton Denver Downtown, Plaza Court 2. **Sponsored by the University of Wisconsin, Milwaukee.** According to AAAS and NRC, an important component of a student's science literacy is scale and concepts relating to scale. We have created both lecture and laboratory instructional materials, which can easily be incorporated into any general chemistry course, on the subject of scale and the skills related to understanding quantity within chemistry concepts. At this workshop, we will present the continuing results of our experiments on scale, share how we measure the scale knowledge of our students, introduce and describe

several of the activities we have incorporated into our curriculum, and provide resources for educators who wish to incorporate our activities into their own courses.

Nano FFF & SP-ICP-MS. Tuesday, March 24, noon to 6:00 PM, and Wednesday, March 25, noon to 6:00 PM, Colorado School of Mines. **Sponsored by PerkinElmer and Colorado School of Mines.** This hands-on workshop will allow researchers to learn from the experts on single particle-ICP-MS and field flow fractionation (FFF) technologies in a working laboratory setup. Learn more and register at acsnanoworkshop.eventbrite.com.



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 Denver 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 Systems 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 Denver.

ACS PROFESSIONAL EDUCATIONAL SHORT COURSES

REFRESH YOUR SKILLS or branch into new areas with an ACS short course. Held in conjunction with ACS national meeting in Denver, 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 Denver or to register, visit www.proed.acs.org/denver. If you have questions, call 202-872-4508, fax 202-872-6336, or e-mail proed@acs.org.

NRCC CERTIFICATION EXAMS

- WHAT:** Certification exams of the National Registry of Certified Chemists
- WHEN:** Sunday, March 22, 8:00 AM to noon
- WHERE:** Embassy Suites Denver Downtown, Rexford Room
- HOW:** Advance registration and completion (with approval) of application must be done before March 2. Applications may be downloaded from www.nrcc6.org.

ANALYTICAL

1-D & 2-D NMR Spectroscopy: Structure Determination of Small-Molecule Organic Compounds, March 20–21

Practical & Applied Gas Chromatography, March 20–21

COMPUTERS/STATISTICS/ENGINEERING

Experimental Design for Productivity & Quality in Research & Development, March 20–22

ORGANIC/PHYSICAL CHEMISTRY

1-D & 2-D NMR Spectroscopy: Structure Determination of Small-Molecule Organic Compounds, March 20–21

Dispersions in Liquids: Suspensions, Emulsions & Foams, March 22–23

POLYMER CHEMISTRY

Polymer Science & Technology, March 20–21

Surfactants & Block Copolymers, March 22

PROFESSIONAL DEVELOPMENT

Effective Supervision of Scientists & the Technical Staff, March 20–21

Effective Technical Writing, March 20–21

Project Management for Technical Professionals, March 20–21

Write Your Own Patent Applications, half-day course, March 22

Intellectual Property Strategies for Technical Professions, half-day course, March 22

REGULATORY/ENVIRONMENTAL

Methods Development, Validation Procedures & Regulatory Compliance Issues, March 20–21

2015 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 Systems 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.

Leading Without Authority. Sunday, March 22, 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 23, 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.

Coaching & Feedback. Monday, March 23, 1:00 to 5:00 PM. 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 24, 8:00 AM to noon. Of the various 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 that aligns with the ACS Board of Directors' strategic goals.

Fostering Innovation. Tuesday, March 24, 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.

ACS CAREER FAIR ON-SITE AND ONLINE

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 22, 9:00 AM to 5:30 PM; Monday, March 23, 9:00 AM to 5:00 PM; Tuesday, March 24, 9:00 AM to 5:00 PM; and Wednesday, March 25, 8:30 AM to 12:30 PM (workshops only) in the Colorado Convention Center. The Virtual Career Fair will be held on March 23 and 24, 8:00 AM to 6:00 PM (central time). Whether on-site or online, 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 30 career-related workshops
- Keynote speakers presented live and via webcast
- Request live and virtual interviews

On-site job seekers must be ACS members, be registered for the national meeting, and complete career fair registration at www.acs.org/careers (pick up a career fair registration badge beginning Sunday, March 22).

GET ONLINE AND OPTIMIZE YOUR JOB SEARCH! The virtual portion of the ACS Career Fair eliminates geographical barriers, enabling job seekers and employers to connect with each other from their home, from their office, or from the dedicated computer stations at the meeting. Interviews and informal discussions will take place in virtual booths via text or video chat. Additionally, job seekers can schedule time with ACS career consultants for one-on-one consultations and attend live events via webcast. In today's tough economy, it makes good sense to enhance your job search by participating fully in both the on-site and online ACS career fairs. Register at www.acs.org/vcf.

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

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 and virtual 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 and online 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 and online networking forums.
- Extend your presence for 30 days after the career fair via the ACS jobs database and your virtual booth.

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 Garretta Rollins at 800-227-5558 ext. 6209 (U.S./Canada only), 202-872-6209 (international), or e-mail g_rollins@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 www.acs.org/careerfair. You can also contact Garretta Rollins at 800-227-5558 ext. 6209 (U.S./Canada only), 202-872-6209 (international), or e-mail g_rollins@acs.org.

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 9:00 AM on Sunday, March 22, on a first-come, first-served basis.

CAREER AND PROFESSIONAL DEVELOPMENT WORKSHOPS. More than 30 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 www.acs.org/careerfair for location.

SUNDAY, MARCH 22

Acing the Interview, 8:30 AM to 12:30 PM; 1:30 to 5:30 PM

New Technology To Find Jobs & Manage Your Career, 10:00 to 11:30 AM

Soups to Nuts of Entrepreneurship, noon to 1:30 PM

Foreign National Scientist Obtaining a Job in the U.S., 1:30 to 3:00 PM

Finding your Path, 1:30 to 5:30 PM

Working in Industry, 1:30 to 5:30 PM

Writing Excellent Proposals, 3:30 to 5:00 PM

MONDAY, MARCH 23

Working for Yourself, 8:30 AM to 12:30 PM

Working in Government, 8:30 AM to 12:30 PM

Working in Higher Education, 8:30 AM to 12:30 PM

Acing the Interview, 1:30 to 5:30 PM

Finding Your Path, 1:30 to 5:30 PM

Working in Industry, 1:30 to 5:30 PM

TUESDAY, MARCH 24

Acing the Interview, 8:30 AM to 12:30 PM

Finding Your Path, 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

Working for Yourself, 1:30 to 5:30 PM

WEDNESDAY, MARCH 25

Acing the Interview, 8:30 AM to 12:30 PM

Finding Your Path, 8:30 AM to 12:30 PM

Working in Industry, 8:30 AM to 12:30 PM

EXPOSITION

SEE WHAT'S NEW INSIDE THE EXPOSITION. Visit the ACS National Exposition at the Colorado Convention Center, Halls A/F, from Sunday, March 22, through Tuesday, March 24. 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 be available to give demonstrations, answer questions, and discuss your specific 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 units 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/denver2015 to learn more about exhibiting companies and to 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 Colorado 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. Exhibitor workshop registration is now available at www.acs.org/denver2015.

Presentations, Prizes & Special Events. Visit the Daily Prize Raffle area on Sunday through Tuesday for a chance to win a prize. Then automatically be entered in our special prize giveaway Sunday through Tuesday after being scanned by 20 exhibitors. Don't forget to join us on Sunday from 6:00 to 8:30 PM for the Attendee Welcome Reception. Also, visit the Networking Lounge inside the exposition for poster sessions and to connect with colleagues.

Internet & Technology. Use free Internet access and leave messages for one another at the Meeting Mail terminals located inside the Networking Lounge. Enjoy free Wi-Fi service at designated areas in the Colorado 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, by mail, or in person at ACS Attendee Registration, Colorado Convention Center, Lobby A/F.

EXHIBITOR SPONSORED WORKSHOPS

EXHIBITING COMPANIES will host free education sessions for attendees that will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications for existing instrumentation. Visit www.acs.org/denver2015 to register for workshops.

SUNDAY, MARCH 22**Characterizing Structure & Chemistry of Functional Nanomaterials. Sponsor:**

FEI Co., 3:30 to 6:00 PM, Colorado Convention Center, Room 103. The development of technologies for efficient resource usage, energy conversion, transportation, or environmental protection relies heavily on advances in developing new and improved nanostructures and nanomaterials. Characterization on length scales down to subnanometer and focus on structural evolution with the link to the nanomaterial's performance play a crucial role in obtaining detailed knowledge about the relationship between structure, unique property, and function in these systems of reduced dimensions. In this workshop, we will profile use cases in catalyst development and polymer engineering and take you through different electron microscopy characterization methods and routines that will enable you to get more insights into structure and chemistry of your functional nanomaterials.

MONDAY, MARCH 23**Spectroscopy Simplified: How To Run a Research FTIR. Sponsor:**

Thermo Scientific, 9:30 AM to noon, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1. This workshop will demonstrate the power and flexibility of the Thermo Scientific Nicolet iS50 FTIR spectrometer system and its unique capabilities to simplify its operation down to the touch of a button. The Nicolet iS50 research FTIR spectrometer system was designed to meet the needs of a dynamic research laboratory, providing the capability to configure the system with a number of spectral ranges, beam paths, and accessories. With this versatility, most users will assume the software will then be complicated to operate, requiring dedicated operators to maximize the productivity of the system. Yet with the unique touchpoint operation of the iS50, most system capabilities can be used with just the push of a button.

Innovative Technologies To Engage Your Student's Learning Experience. Sponsor:

McGraw-Hill Higher Education, 9:30 AM to noon, Colorado Convention Center, Room 103.

9:30 AM— **Flipping the Classroom.** Presenter: Danaë Quirk Dorr, Minnesota State University, Mankato. The flipped classroom model has become one of the hottest topics in the higher education space in recent years thanks to a real improvement in technology and an overall change in scholarly mind-set. Learn about strategies and tools available to help you flip.

11:00 AM— **Teaching Organic Chemistry in the 21st Century: The Rewards of Technology.** Presenters: Philip A. Janowicz, California State University, Fullerton, and Michael Lewis, St. Louis University. Organic chemistry students are performing better using online homework. Janowicz will talk more in depth about his study on ACS exam scores for students who completed online homework versus those who completed written homework. Lewis will discuss how to flip an organic chemistry classroom.

Driving Separations Success. Sponsor:

Waters Corp., 9:30 AM to noon, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2.

9:45 AM— **Part 1: Meeting the Challenges of Food Quality Control Using UPLC.** Focusing on UPLC for food testing using optical (non-MS) detectors and MS detectors, this session will cover applications including quality and nutrition: sweeteners, soft drink additives, amino acids, dairy (whey proteins, sugars, vitamins, preservatives), and safety: PAHs and aflatoxins.

11:00 AM— **Part 2: Driving LC Success: Technical Seminar: Systematic Protocol.** This technical seminar will teach a systematic protocol that can alleviate challenges in method development. This generic protocol will lead you toward successful and robust chromatographic separations.

SciFinder Training Session System with the Touch of a Button. Sponsor:

CAS, 12:30 to 3:00 PM, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1. Come learn about how SciFinder brings data

to your lab, as well as details and tips for refining and using your results with powerful features such as relevance ranking, experimental procedure information, and SciPlanner.

Protecting Our Natural Resources with GC/MS & LC/MS from Thermo Fisher Scientific. Sponsor:

Thermo Scientific, 12:30 to 3:00 PM, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2. Our natural resources are a precious commodity, and keeping them clean and pure can be a daunting task. This workshop will highlight two technologies from Thermo Fisher that are used to help ensure that the world is a cleaner, safer, and healthier place.

12:30 PM— Learn how you can access the next evolution of GC/MS/MS technology to achieve more at faster speeds. This means more capacity, more information, more compounds, and more results per unit time for higher levels of productivity and efficiency in analytical workflows.

1:45 PM— Significant advances in triple-quadrupole technologies have resulted in two state-of-the-art, next-generation instruments. See details of the groundbreaking advances “from an ion's view,” and hear about transformations in your targeted quantitative workflows.

Innovative Technologies To Engage Your Students' Learning Experience. Sponsor:

McGraw-Hill Higher Education, 12:30 to 3:00 PM, Colorado Convention Center, Room 103.

1:00 PM— **Moving Beyond Traditional Homework with ALEKS.** Presenter: Tracy McGill, Emory University. Are you struggling to find which adaptive online learning system is right for you? McGill will share why ALEKS for Chemistry is the perfect choice for her and her students. ALEKS uses adaptive questioning to quickly and accurately determine exactly what a student knows and doesn't know in a course.

2:30 PM— Revolutionizing the Lab Experience: LearnSmart Labs for General Chemistry. Presenters:

Deborah Exton, University of Oregon, and Jimmy Reeves, University of North Carolina, Wilmington. LearnSmart Labs provides an adaptive, interactive, and personal-

ized 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.

Online Homework with Targeted Instructional Feedback Leads to Improved Student Learning Outcomes.

Sponsor: Sapling Learning, 3:30 to 6:00 PM, Colorado Convention Center, Room 103. Sapling Learning delivers online homework that engages students and empowers educators. Still, homework is only one piece of a full course solution. In this workshop, hear about the various ways that Sapling Learning provides or enables educators to select the best course materials for them. Whether you use a printed textbook, lecture slides, open educational resources, or some combination thereof, you can learn how to provide a unified learning experience for your students. You'll learn about the suite of options from Sapling Learning and our partners and how to incorporate them into a seamless learning experience. Our discussion will include used textbooks and instructor-generated content, and you will hear from faculty who are successfully implementing these varied resources. Each attendee will receive a free copy of the eTextbook "Chemistry," by John Olmsted and Greg Williams.

TUESDAY, MARCH 24

SciFinder Training Session System with the Touch of a Button. **Sponsor:** CAS, 9:30 AM to noon, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1. See SciFinder Training for Monday, 12:30 to 3:00 PM.

A Survey of Accelerated Materials Research Using Raman Microscopy & Imaging. **Sponsor:** Thermo Scientific, 9:30 AM to noon, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2. Raman spectroscopy is essential to competitive academic research in many applied scientific disciplines, including materials science, life sciences research, and chemical and biological engineering. Advances in Raman microscopy

and imaging have made the technique accessible to a wide variety of researchers, regardless of expertise or field of study.

A case study showing how one leading research university has transformed its approach to research, including obtaining results faster, increasing the number and quality of publications, and improving funding successes, will be shared. See examples of current research using advanced Raman microscopy, which has been designed for greater accessibility and significantly enhanced productivity than previously possible.

Analysis of Polymers by Vibrational Spectroscopy & Microscopy.

Sponsor: Bruker, 12:30 to 3:00 PM, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2. The latest advances in FTIR and Raman instrumentation and applications will be reviewed, with a thorough discussion of the following topics: polymers identification and classification, additives and contaminations, fast reaction monitoring, defects analysis using vibrational microscopy, chemical imaging, and depth profiling.

Compact Mass Spectrometry: A Swiss Army Knife Approach to Chemistry Challenges.

Sponsor: Advion, 9:30 AM to noon, Colorado Convention Center, Room 103. Chemists ask many questions that each require a different approach. Advion offers a compact mass spectrometer that couples to any range of techniques to provide chemists with a complete answer to the questions they ask. This workshop will show examples using a direct sample analysis approach valuable to reaction monitoring, compound identification, natural product analysis, and food safety. Attendees who wish to learn more about an affordable mass spectrometer that does not require sample prep, has an easy user interface (including TLC and Direct Sample Analysis Probe), and offers answers in less than a minute are encouraged to attend.

Intelligent Real-Time Reaction Monitoring in the Fume Hood Using Benchtop NMR.

Sponsor: Thermo Scientific, 12:30 to 3:00 PM, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1. Teaching

reaction kinetics, thermodynamics, and pathways is a standard part of any undergraduate organic chemistry curriculum. Having hands-on access for the student to measure reaction mechanics in real time in the laboratory may give them insights not previously available in the classroom alone. This workshop will demonstrate a new capability of the Thermo Scientific picoSpin NMR spectrometer to intelligently measure reaction pathways from a reactor in real time. Watch products form in increasing concentration, right next to the apparatus.

Advances in Atomic & Molecular Spectroscopy.

Sponsor: Agilent Technologies, 12:30 to 3:00 PM, Colorado Convention Center, Room 103. Recent innovation in FTIR, atomic spectroscopy, and elemental analysis (including ICP/MS) technology has allowed for more sensitive, accurate, and flexible measurements of organic and inorganic materials. This workshop will focus on two main techniques, FTIR and atomic spectroscopy/spectrometry.

12:30 to 1:30 PM — **Innovations in FTIR: How New Technology Is Changing Infrared Analysis**

1:45 to 2:45 PM — **New Elemental Analysis Solutions and Advanced Applications Using Next-Generation MP/AES, ICP/OES, ICP/MS, and ICP/QQQ**

Chromatography & Mass Spectrometry Tips, Tricks & Advanced Techniques.

Sponsor: Agilent Technologies, 3:30 to 6:00 PM, Colorado Convention Center, Room 103. Stay up to date on the latest technology and applications using HPLC, LC/MS, GC, and GC/MS. This workshop will focus on implementing 2-D HPLC and other advanced HPLC techniques in your lab, ion mobility qTOF for advanced molecular analysis, and improving GC/MS capability using some new tips and tricks.

3:30 to 4:15 PM — **Demystifying 2-D HPLC: Techniques You Can Use Tomorrow**

4:15 to 5:00 PM — **Advantages of Ion Mobility qTOF for Characterization of Large Biological Molecules**

5:00 to 5:45 PM — **GC/MS: Advanced Topics and Helpful Tips & Tricks**

WEDNESDAY, MARCH 25

New Developments in Isothermal Titration Calorimetry from MicroCal.

Sponsor: Malvern Instruments, 9:30 AM to noon, Colorado Convention Center, Room 103. Measurements and characterization of binding interactions between proteins and low-molecular-weight (LMW) ligands are fundamental for drug discovery. Among the most recognized challenges in characterizing binding interactions are the need to (1) accurately assess a wide span of binding affinities (K_d) and (2) accurately rank and characterize LMW ligands based on affinity, mechanism of action, and energetics of interaction. Reliable interpretation of binding data can be complicated by the presence of inactive protein fractions or inaccurate assessment of protein concentration. Assessment of these data can be further hampered by inherent uncertainty in the concentration of compound stocks.

This uncertainty results from inaccurate measurement, limited solubility, or potential chemical heterogeneity of the compounds, such as the presence of enantiomers and isomers. Isothermal titration calorimetry (ITC) directly measures heat released or absorbed in a binding event, providing means for studying protein-small molecule interactions in solution without the need for labeling or immobilization.

This workshop will present the new developments in highly sensitive MicroCal ITC instrumentation and data analysis. We will discuss the improvements in data quality that enable increased confidence when analyzing challenging data with low heats when sample is precious or low concentrations are required to accurately quantitate low-nanomolar-affinity interactions. We will present the new developments in MicroCal ITC software that allow automated data analysis, minimizing analysis time and user subjectivity in

assessing data quality.

Designing Inhibitors with MOE Structure-Based Drug Design Tools.

Sponsor: Chemical Computing Group, 3:30 to 6 PM, Colorado Convention Center, Room 103. This workshop covers the application of in silico structure-based drug design (SBDD) tools for the rational design of Tarceva-based EGFR kinase inhibitors. Starting with raw PDB protein-ligand 3-D structures, all the steps required to initiate and advance an SBDD study are covered: preparing PDB structures for modeling, binding pocket visualization, protein-ligand contact analysis, and the use of SAR for in situ modeling (modifying and optimizing ligands in the binding pocket) to design new compounds. Advanced topics such as pharmacophore query generation, protein-ligand docking, protein alignments for binding-site comparison, and in situ combinatorial synthesis will also be covered.

ACS EXCELLENCE

Spring 2015

The ACS Publications Magazine

**HOW ACS HELPS
AUTHORS MEET
OPEN ACCESS
REQUIREMENTS** PAGE 14

**3 WAYS
RESEARCHERS CAN
BOOST THEIR SOCIAL
MEDIA SAVVY** PAGE 16

**Carolyn Bertozzi and
ACS Central Science:
READY TO MAKE HISTORY**

PAGE 9

**MEET THE
NEW EDITORS**

PAGE 3



ACS Publications
Most Trusted. Most Cited. Most Read.

3 Q&A

Meet the newest ACS EICs

Check out some brief Q&As with these new Editors at 6 ACS journals.

6

C&EN's new Editor looks ahead

"We're already doing excellent work," says Dr. Bibiana Campos-Seijo. "But we can do even better."

9

Taking center stage

Dr. Carolyn Bertozzi and *ACS Central Science* are ready to rock the world of science.



14

out

Feeling out of compliance?

ACS has the programs to help authors meet funders' open access requirements.

16

Learn 3 ways

to tweet and post your way to greater success for your research.

18

Most cited journals

The most recent citation data on the journals of the ACS.

22

It's all about the resources

Resources today's students and scientists need are at the ACS booth.



ACS Publications
Most Trusted. Most Cited. Most Read.

CO-EDITORS

Joe Graham & Selenah Njoloma

DESIGN

Surface2 Design

ACS PUBLICATIONS MARKETING TEAM

J'Nai Baylor, Melissa Blaney, Andrew Clinton, Shayla Jackson, Renee John, Jamie Liu, Kelley Maddox, Annie Reed, Liesa Ross, Freddy Tellez, Angela Walker, Erin Wiringi, Mike Woodruff, Wendy Wise

Questions or comments for the Editor

j_graham@acs.org

Meet the new Editors-in-Chief



Thomas F. Hofmann, Ph.D.

JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY

Thomas F. Hofmann is professor and chair of Food Chemistry and Molecular Sensory Science and Vice President for Research & Innovation at the Technische Universität München in Germany.

Q: How does research in your journal's area affect people's everyday lives?

TH: Primary agriculture and food production are facing limiting factors for key resources like land, water, energy, and inputs. On the other hand, the world faces a double burden of undernutrition and obesity. New procedures and products originating from sustainable agriculture to be used as food, feed, green biomaterials, or biofuel as well as new energy-efficient engineering solutions designed to deliver affordable, safe, nutritional, and tasty foods and beverages will have to be developed to better serve the coming needs of society and to create economic impact along the value chain. New knowledge on the chemistry and biochemistry involved is key for success and that's why the *Journal of Agricultural and Food Chemistry* is on the spot! I will do my very best to maintain *JAFC* as the premier journal publishing these scientific innovations.

Go to pubs.acs.org/jafc for more information



Sharon Hammes-Schiffer, Ph.D.

CHEMICAL REVIEWS

Sharon Hammes-Schiffer is Swanlund Professor of Chemistry at the University of Illinois at Urbana-Champaign.

Q: What are you most looking forward to about this new position?

SHS: I am looking forward to enhancing the topical diversity, visibility, and educational impact, while also retaining the comprehensive and accessible nature of the review articles in this journal. I plan to pursue several initiatives that will help achieve these goals. From a personal perspective, I am looking forward to interacting with chemists from all disciplines and learning about exciting new areas of chemistry.

Q: How does research in your journal's area affect people's everyday lives?

SHS: This journal serves as an educational tool for students and scientists entering new fields. The articles have both short-term and long-term impact. My own son, who is a junior chemical engineering major at Princeton, just told me that he used a *Chemical Review* from 1997 as the main source for his presentation on phage display for a course. My students have also used *Chemical Reviews* to learn about new topics.

Go to pubs.acs.org/cr for more information



Paul J. Chirik, Ph.D.

ORGANOMETALLICS

Paul J. Chirik is the Edward S. Sanford Professor at Princeton University.

Q: How did you first become interested in your journal's area of focus?

PC: My interest in organometallic chemistry began during my freshman year at Virginia Tech. I was fascinated by Professor Joseph Merola's work on iridium compounds that seemed to be able to activate and break some of the strongest bonds in chemistry. Despite my inexperience, he allowed me to work in his lab, gave me my own project, and the rest is history.

Q: What are you most looking forward to about this new position?

PC: I am looking forward to having *Organometallics* serve as the focal point for a vibrant, diverse, and collegial community. As Editor-in-Chief, I hope to meet new organometallic chemists from around the globe, learn about their science, and capture the best of it in the journal. I am also looking forward to maintaining the great tradition of excellence established by my predecessors, Dietmar Seyferth and John Gladysz.

Q: What's something about your journal's focus area that most people don't understand?

PC: Most people don't realize that organometallic compounds operate "behind the scenes" to enable our quality of life. In addition to helping discover new medicines, organometallic compounds are responsible for making plastics that are ubiquitous in our daily lives, serve as precursors for electronics, and are even found in the body, such as vitamin B-12.

Go to pubs.acs.org/organometallics for more information



David L. Sedlak, Ph.D.



David L. Sedlak is Malozemoff Professor in Mineral Engineering, Co-director of Berkeley Water Center, and Director of the Institute for Environmental Science and Engineering at the University of California, Berkeley.

Q: How did you first become interested in your journal's area of focus?

DS: I first became aware of the field of environmental chemistry as I became interested in addressing problems associated with contamination of groundwater and soil at hazardous waste sites. As my awareness of the topic grew, I became aware of *Environmental Science & Technology* and its role as the leading journal in the field. *ES&T* was the journal where I published my first paper in 1990 and I have been publishing there ever since.

Q: What are your goals as Editor-in-Chief?

DS: We are proud of our reputation as the most read and most cited journal covering the environment. But bibliographic indicators will not save the planet. As Editor-in-Chief, I will work with the editorial team to leverage our standing as the leading environmental research journal to become the authoritative voice for advancing solutions to the environmental challenges facing society.

Go to pubs.acs.org/est and pubs.acs.org/estlett for more information



Kai Rossen, Ph.D.

Organic Process Research & Development

Kai Rossen is group leader at Sanofi in Germany.

Q: How does research in your journal's area affect people's everyday lives?

KR: *Organic Process Research & Development* has a very concrete and relevant influence on the lives of people. Unfortunately, this is seen only when things go wrong and an accident at a plant injures people or waste from a plant is polluting the environment. This context makes it very difficult to have a discussion with the public, as a perception is created that is simply wrong: the physician is saving the life of the patient, while the chemist in the pharmaceutical industry that gives the physicians the tools to do so is not seen as positive. I am aware that technical journals speak primarily to a closed audience and don't tend to reach the public, but it is important to tell the positive and relevant examples of our work to get the message of our positive contributions for the well-being of mankind across also to the general public.

Q: What are your goals as Editor-in-Chief?

KR: This is very simple: try to convey the excitement for the type of work ongoing in the pharmaceutical, agrochemical, flavor and fragrance, and fine-chemical and chemical industries, and its relationship with exciting new developments in various fields of science and engineering, to a new and younger generation of scientists from all over the world.

Go to pubs.acs.org/oprd for more information



Francoise Winnik, Ph.D.

Langmuir

Francoise Winnik is Professor, Faculty of Pharmacy and Department of Chemistry at the University of Montreal, Canada; Principal Investigator, International Center for Materials Nanoarchitectonics at the National Institute for Materials Science in Tsukuba, Japan; and Finnish Distinguished Professor at the University of Helsinki, Finland.

Q: What are your goals as Editor-in-Chief?

DS: *Langmuir* is a multidisciplinary journal. Its authors and readers are spread throughout the world. It is time to strengthen the ties of *Langmuir* with its readers, particularly outside North America, by increasing the number of non-North American members of the Board and by selecting Senior Editors worldwide. In addition, it is important to recognize outstanding research as it appears in *Langmuir*. Immediacy is key. Instant recognition by a journal creates a permanent bond between the author and the journal. Excellent articles published in *Langmuir* must be promoted among ACS readers and beyond. A related objective, probably even more important, will be to reach out to scientists who are no longer submitting their manuscripts to *Langmuir* and to those who have not published in *Langmuir* so far.

Go to pubs.acs.org/langmuir for more information

New Editor-in-Chief looks ahead

Bibiana Campos-Seijo seeks to make the best even better

When asked what challenges she faces for the upcoming year, Bibiana Campos-Seijo, Ph.D., admits that it will be a challenge to improve upon the number-one magazine in the chemical sciences. “We’re already doing excellent work,” she says. “But we can do even better.”

Campos-Seijo took the helm in December 2014 as editor-in-chief of *Chemical & Engineering News* (C&EN) and VP of C&EN Media Group. She plans to continue and expand the magazine’s outreach in the year ahead.

First, she’s hoping to lead the redesign of both the print and web magazine. Both projects are in their early stages. She also wants to improve C&EN’s impact on social media and develop more high-quality multimedia content, including videos, webinars, and Google Hangouts.

“Researchers depend on us to curate science from around the world and deliver it in an intuitive, user-friendly way.”

—Dr. Bibiana Campos-Seijo

She wants to create a cohesive “family of products” among all C&EN content. “Many of our members read our print magazine, but don’t know about our digital channels,” Campos-Seijo says. “Others may read us online, but don’t know how our different products relate. We want to take a close look at all of our content and make sure products complement one another and share a consistent look and feel.”

Campos-Seijo also champions what she calls an “entrepreneurial” approach to journalism. “Researchers depend on us to curate science from around the world and deliver it in an intuitive, user-friendly way.” This means listening and adapting not just to the types of content readers want to see, but how they want it presented. A priority for the website redesign will be to implement responsive design, which will ensure a good experience across all devices.

All of this is part of C&EN’s “digital-first” approach designed to keep readers informed on the latest research news. Although C&EN’s print magazine is published weekly, new content hits its website (cen.acs.org) every day. Campos-Seijo says that while there’s no typical day at C&EN, daily editorial meetings are what make always-current web content possible.



Bibiana Campos-Seijo, Ph.D.

Making chemistry more accessible to all

Campos-Seijo also recognizes that she is leading C&EN at a critical time. Science awareness and interest are entering the mainstream in new and surprising ways: go to a restaurant, and you might see a dish inspired by molecular gastronomy. Turn on the television and watch entertainers like Bill Nye the Science Guy make science fun. Actor Alan Alda is helping researchers better communicate their work to the public. And traveling science festivals and workshops are teaching kids about everything from climate science to computer code.

“In other words, science is quite hot right now,” Campos-Seijo says.

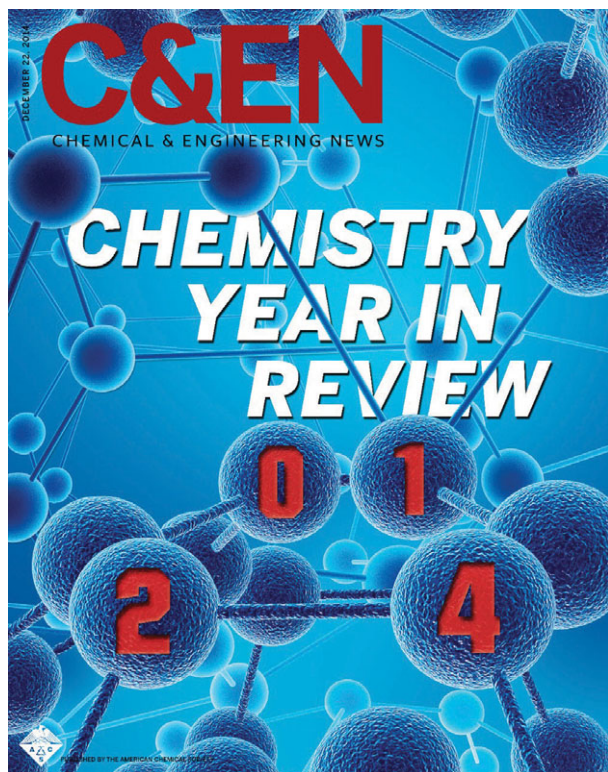
Quenching the world’s thirst for science is part of C&EN’s mission, and part of her role as editor-in-chief, Campos-Seijo says. “It’s important for us to communicate not just with ACS members, but also nonmembers. We’re ambassadors for

“Chemistry and science are not geographically limited. They’re universal.”

—Dr. Bibiana Campos-Seijo

“Working for C&EN is an ambition I’ve had for a long time.”

—Dr. Bibiana Campos-Seijo



chemistry. So we need to be out there talking to people and finding out what issues people care about and what support they need.”

To wit: in 2014, C&EN produced “From the SCENEs,” weekly stories based on papers in ACS journals; a webinar on the chemistry of cocktails; and the “Chemistry in Pictures” blog, all designed to reach people with different levels of chemistry knowledge. While C&EN’s primary audience remains the chemical sciences community, new and upcoming initiatives are designed for accessibility and broad appeal.

A perfect fit

Campos-Seijo (who goes by “Bibi”) was raised in Galicia, in northwest Spain. She holds a B.Sc. in chemistry from Spain’s University of Santiago de Compostela and England’s Manchester Metropolitan University and a Ph.D. in chemistry from Manchester Metropolitan.

She worked as a technical editor and in scientific publishing after earning her degree. In 2009, she became editor of *Chemistry World*, the magazine of the UK’s Royal Society of Chemistry. “This was sort of a natural progression for me,” Campos-Seijo says. “I’ve known and admired ACS and C&EN

for many years. Working for C&EN is an ambition I’ve had for a long time.”

Campos-Seijo replaces Rudy Baum. Her experience makes her a perfect match for the new position. Having worked for both societies and commercial organizations, she understands the importance of building relationships with members and advertisers alike.

Campos-Seijo, along with her husband and children, relocated to ACS’ Washington, D.C. headquarters in November 2014. One challenge the family faces in their new home, she says, has been the switch to American English. “I think it was George Bernard Shaw who said that the U.S. and Britain are two countries divided by a common language,” she laughs. “We’re definitely finding that to be true.”

“It’s important for us to communicate not just with ACS members, but also nonmembers. We’re ambassadors for chemistry.”

—Dr. Bibiana Campos-Seijo

The language of science

While words and phrases may differ, Campos-Seijo points out that the issues facing scientists across countries and cultures are more alike than different.

“We live in a global industry,” she says. “Scientists can collaborate more easily than ever before. As a publication, I think there’s a lot we can learn from this.” She looks forward to helping C&EN remain a bridge for science enthusiasts of all kinds—members and non-members, professionals and the public—all around the world.

“Chemistry and science are not geographically limited,” Campos-Seijo says. “They’re universal.”

C&EN
CHEMICAL & ENGINEERING NEWS


Go to cen.acs.org

INTRODUCING THE CLASS OF 2015



ACS Publications
Most Trusted. Most Cited. Most Read.

SCIENCE ROCK STAR

A woman with short brown hair, wearing a light blue button-down shirt and tan pants, is playing a red and black electric guitar. She is positioned in the center of the frame, slightly to the left, and is looking down at her instrument. In front of her is a black microphone on a stand. The background is a vibrant, swirling galaxy or nebula with shades of orange, yellow, and red, set against a dark, starry space. The overall scene is lit with a warm, golden glow.

Seeks your greatest hits in research

Exceptional research

ACS Central Science takes center stage—while giving your exceptional research limitless possibilities to influence and inspire.

In December, ACS Publications began accepting submissions for *ACS Central Science*, a groundbreaking new journal that promises to elevate the prominence of chemistry as the discipline to which all other areas of science are linked.

ACS
central
science

This open access, multidisciplinary journal will showcase ultra-high-quality primary research in chemistry and allied fields, including biomedicine, energy science, nanotechnology, materials science, and earth and planetary science. Every month, issues will include a complement of thought-provoking review and opinion articles, commentaries, and interviews. Only 100–200 articles will be published each year, making the journal fiercely selective.

“With *ACS Central Science*, we have an opportunity to create a journal that not only offers exciting primary research articles, but that can also reach out and deliver the message that chemistry is the central science to the public at large,” says journal

Editor-in-Chief Carolyn Bertozzi, Ph.D. “We want to get people thinking about the connections between chemistry and other fields.”

As ACS Publications’ first completely open access journal, *ACS Central Science* is the centerpiece of the Society’s efforts to redefine how the most innovative research is shared with the world. But this isn’t just about improving access



< First, let’s set the record straight.

Carolyn Bertozzi did not play guitar in the hard-rock-rap band “Rage Against the Machine.” However, she did play keyboards in a band called “Bored of Education” while at Harvard with Tom Morello, who later went on to form and play guitar in “Rage Against the Machine,” one of the most popular and influential bands of the 1990s. In the tweet above, the two former bandmates were reunited, raising hopes that the band might re-form at a future ACS National Meeting! All of us at ACS Publications are glad Dr. Bertozzi chose to rock our new journal, *ACS Central Science*.

should have no limits

to research. ACS Publications is also planning a host of supporting activities to elevate chemistry's visibility with the general public.

Improving access to research

Accessibility for the public is a key goal for *ACS Central Science*. The editorial team hopes to accomplish this through the journal's open access status and engaging front-end material.

As Bertozzi notes, "This is beneficial to the research community, but think about what it means to the general public.

"What if you're a high school science teacher and you want to assign high-level research to your students? Now you can."

The journal will also have a substantive front section, such as the news and views included in the cleverly titled "First Re-

Removing barriers to publishing open access

As a key component to ACS Publications' open access initiatives, *ACS Central Science* does not levy any article processing fees on authors. Authors whose papers are selected for publication in *ACS Central Science* receive an ACS AuthorChoice license for immediate open availability at no charge.

"We want to get people thinking about the connections between chemistry and other fields."

—Dr. Carolyn Bertozzi

As an open access journal, all *ACS Central Science* content will be accessible by anyone at any time, free of subscription charges. Yet the publication will still offer the same exceptionally high quality standards and rigorous peer review that are a signature of all ACS Publications journals.

"We want to help readers 'get behind the scenes' of research and hear from other scientists in the field about what it means."

—Dr. Kevin Davies

actions," that will include feature stories, reviews, commentary, interviews, and more, all designed to complement the original research. The aim is to create readable, engaging content that puts the research in context.

"With First Reactions, we will provide succinct, accessible analysis of the research," says Kevin Davies, Ph.D., Vice President of Business Development for ACS Publications. "We want to help readers 'get behind the scenes' of research and hear from other scientists in the field about what it means. It will have a magazine-like format that accompanies the journal's research matter."

ACS Central Science will tap C&EN writers and social media platforms, including Twitter, Reddit, and Google+, to promote content and to showcase researchers. Publishing in *ACS Central Science* will give authors the visibility and prestige of publishing in a world-class, open access research journal, while offering access to the promotional powerhouse of the world's largest scientific society.

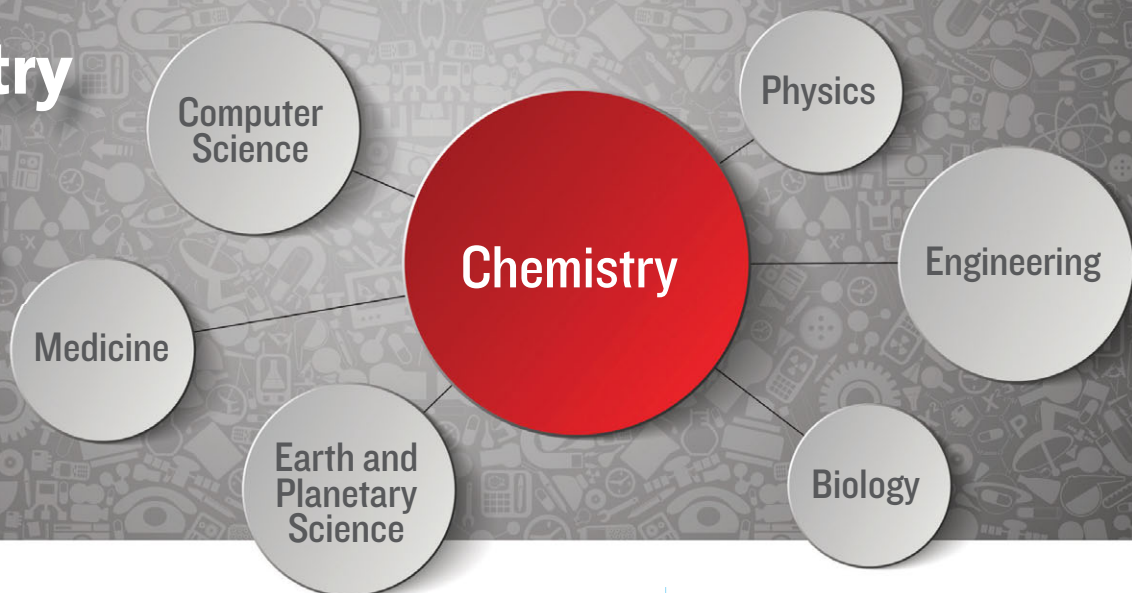
The editorial staff is also committed to creating a positive experience for authors.

"We are committed to fast decision-making and turnaround," says Bertozzi. "We are all active researchers who understand the frustrations that can come with the peer-review process. We are going to provide constructive peer reviews, limit the number of reviews, and make decisions quickly and decisively. That's not unique to *ACS Central Science*. ACS Publications as a whole is committed to this."

"We are committed to fast decision-making and turnaround."

—Dr. Carolyn Bertozzi

Chemistry is the Central Science



“We envision *ACS Central Science* as the primary venue for reporting the most important advances in chemistry and in allied fields wherein chemical concepts and tools play a major role.”

—Dr. Carolyn Bertozzi

Engaging the global community

The multidisciplinary nature of the journal demands an editorial team that has a global perspective, both in terms of research interests and geographical location. The selection of Bertozzi as Editor-in-Chief is instrumental to fulfilling this vision, Davies says.

“Carolyn is passionate about the interaction of chemistry and other research disciplines and understands the importance of open access,” observes Davies. “She’s going to be a dynamic leader for the journal. She wants to build a journal of great international reputation, to make it a must-read journal of not just research but also of engaging, accessible material.”

Initially, five Senior Editors will help Bertozzi guide the direction of *ACS Central Science*. All active researchers, the Senior Editors represent an impressive array of research backgrounds and achievements.

“I wanted people who are very broad in their expertise and research activities and are highly respected in the community,” notes Bertozzi. “Because they will

“I wanted people who are very broad in their expertise and research activities and are highly respected in the community.”

—Dr. Carolyn Bertozzi

shape the journal’s contents, I wanted people who would be good stewards of the whole enterprise. We also needed global diversity. We wanted people who are in regions that are rich with top-notch science.”

The journal’s editorial advisory board is a globally diverse group of active researchers who are top scientists in their fields. The board’s international and scientific diversity reflects the broad range of sciences that will be covered in the journal, which will ensure a fair and expeditious review of all material.

“World-class chemistry and related sciences are happening all over the globe,” Davies notes. “Our intention is that the board will reflect the geographic strength of science around the world.”

Coming soon...

ACS Central Science opened for submissions in December, and the initial response has been extremely positive. Articles will be published on the journal’s website shortly after they are accepted. The first issue is expected to be published in Q1 2015.

For updates, visit the *ACS Central Science* website and follow the journal on Twitter at @ACSCentSci.

Bertozzi’s vision for the journal, as well as submission procedures and a profile of the Senior Editors, can also be found on the *ACS Central Science* website.

Go to pubs.acs.org/centralscience

MEET THE EDITORIAL TEAM



EDITOR-IN-CHIEF

Carolyn Bertozzi

Howard Hughes Medical Institute
University of California, Berkeley
Departments of Chemistry and
Molecular and Cell Biology

Dr. Bertozzi's work spans a wide range of technologies and approaches at the interface of chemistry and biology. Her research focuses on creating new platform technologies for the development of medicines and diagnostics that will improve human health; for probing natural biology; and to develop road maps for creating synthetic life forms to serve human needs.

She is the T. Z. and Irmgard Chu Distinguished Professor of Chemistry, and Professor of Chemistry and Molecular and Cell Biology at University of California, Berkeley; Professor of Molecular and Cellular Pharmacology at University of California, San Francisco; Senior Faculty Scientist at Lawrence Berkeley National Laboratory; and a Howard Hughes Medical Institute Investigator.

She has served as Co-Director of the Berkeley Nanosciences and Nanoengineering Institute (BNNI) since 2011 and as Co-Director of the UC Berkeley Chemical Biology Graduate Program since 2001. She is co-founder and Chair of the Scientific Advisory Board of Redwood Bioscience and serves in a variety of other advisory roles, including the Research Advisory Board for GlaxoSmithKline and the Broad Institute Board of Scientific Counselors.

In April, Dr. Bertozzi will move her lab to Stanford University, where she will be Professor of Chemistry and, by courtesy, of Chemical and Systems Biology. Dr. Bertozzi will be a founding scientist of Stanford ChEM-H (Chemistry, Engineering & Medicine for Human Health), a new initiative chaired by Chaitan Khosla, which draws together faculty from diverse disciplines with the goal of improving lives.

SENIOR EDITORS



Christopher Chang

Howard Hughes Medical Institute
University of California Berkeley
Departments of Chemistry and
Molecular and Cell Biology

Dr. Chang's research is at the interface of inorganic chemistry, organic chemistry, and chemical and molecular biology. His research interests include molecular imaging and catalysis applied to neuroscience, stem cells, cancer, infectious diseases, renewable energy, and green chemistry.



Ben G. Davis

University of Oxford
Chemistry Research Laboratory

Dr. Davis' research covers organic chemistry and several disciplines within biology. His interests include synthesis and methodology, inhibitor/probe/substrate design, biocatalysis, enzymology, biosynthetic pathway determination, protein engineering, drug delivery, glycobiology, and molecular imaging.



Monica Olvera de la Cruz

Northwestern University
Department of Materials Science
and Engineering

In Dr. Olvera de la Cruz's research, she has developed theoretical models to determine the thermodynamics, statistics, and dynamics of macromolecules in complex environments including multicomponent solutions of heterogeneous synthetic and biological molecules, and molecular electrolytes.



David A. Tirrell

California Institute of Technology
Chemistry and Chemical Engineering

Dr. Tirrell's research covers biopolymers and polymers. Specifically, his research uses organic, biological, and materials chemistry to make new macromolecular systems of controlled architecture and novel function.



Dongyuan Zhao

Fudan University
Laboratory of Advanced Materials
Department of Chemistry

Dr. Zhao's research covers materials science generally, with a focus on the design, synthesis, assembly, growth, and properties of materials, including MOFs and nanomaterials.

Are you **out** of compliance

Here's how ACS Publications helps you go open access and meet funder requirements with our expanded ACS AuthorChoice and innovative ACS Author Rewards programs

Your research is groundbreaking. Your article has been accepted by your journal of choice. So, your work as an author is done, right? Not quite.

Does your article need to be open access? Requirements for open access are not uniform across funding agencies and institutions. That's why today's authors need to know the rules, not just for their funders and institutions, but also for their co-authors.

The world is embracing open access, putting more published, peer-reviewed research articles within the public's reach. While this is a positive development, it also means authors are often tasked with additional responsibilities to ensure they are in compliance with their funders' open access requirements.

As of January 2014, ACS has moved to

the forefront of the open access world by offering new options to help authors negotiate this changing landscape. ACS AuthorChoice and ACS Author Rewards are designed to help authors efficiently and affordably satisfy the open access requirements of their funders and institutions.

ACS AuthorChoice: Your fast and affordable way to make articles open access

With the expanded ACS AuthorChoice program, ACS Publications helps authors meet open access requirements by offering more flexible options, money-saving discounts, and timesaving services that simplify compliance.

For a one-time fixed fee, the ACS AuthorChoice program enables authors to make the final published article freely

accessible and can choose:

- **Immediate open availability upon publication**
- **Open availability 12 months after publication (ACS AuthorChoice+12)**
- **Creative Commons licenses**

Significant discounts are available for ACS members and authors at subscribing institutions.

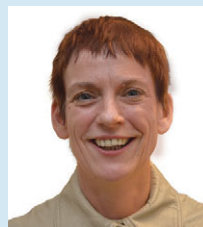
Authors always have the option of self-depositing the accepted manuscript (the post-peer review version, accepted by the journal, prior to additional editing and production enhancement by ACS Publications) to meet open access requirements. The accepted manuscript is available through the ACS Paragon Plus system and there is no cost or fee for this option.

ACS in harmony with CHORUS initiative

CHORUS, the Clearinghouse for the Open Research of the United States, offers a suite of services and best practices that provide a sustainable solution for agencies and publishers to deliver public access to published articles reporting on funded research in the United States. The first initiative of CHOR, Inc., a US 501(c)(3) non-profit organization, CHORUS leverages widely used technology to facilitate a simple compliance process, optimized search and dashboard services, and multi-party archiving and preservation capabilities.

Susan King, Ph.D., Senior Vice President of the Journals Publishing Group at ACS, is helping to lead the effort as the Chair of the CHOR, Inc. Board of Directors. In addition, Dan O'Brien, Assistant Director of Publishing Technology, and Dave Martinsen, Ph.D., Senior Scientist, Digital Strategy at ACS, participate in the CHORUS Technical Working Group. Once again, ACS Publications is at the forefront, working with publishers and agencies to create a sustainable solution for researchers to publish their work.

Utilized by the U.S. Department of Energy (DOE) in their PAGES (Public Access Gateway for Energy & Science) discovery



Susan King, Ph.D.

service, CHORUS links users to published research on participating publishers' websites. ACS Authors have options to use ACS Author Rewards and ACS AuthorChoice to enable public availability of their final published article on the ACS Publications platform with related essential context, tools, and information, either immediately or

12 months after publication.

"Our participation in CHORUS is just one more way that ACS strives to make open access compliance as easy and streamlined as possible, while helping authors broaden their exposure in the scientific and public communities," says Dr. King.

CHORUS

with your funders?

ACS AuthorChoice makes the final published article, also known as the Version of Record, freely available. This is the professionally edited and typeset version of the article, with enhanced functionality, as it appeared in the ACS journal. Authors who choose ACS AuthorChoice also gain the advantages of ACS Certified Deposit.

ACS Certified Deposit: Assisting authors with managing deposits

ACS Certified Deposit is a program designed to help authors manage deposits of ACS AuthorChoice articles into repositories. Authors who participate in ACS AuthorChoice and ACS AuthorChoice+12, or who are selected for publication in *ACS Central Science* or ACS Editors' Choice, are eligible to receive ACS Certified Deposit at no charge. ACS also maintains long-term records verifying the deposit of an article in a repository, and will make those records available to the authors of an article published with ACS upon request.

For more information about ACS Certified Deposit or to submit a request, visit http://pubs.acs.org/page/certified_deposit.html or email certifieddeposit@services.acs.org.

ACS Author Rewards: Helping the scientific community transition to open access, while also thanking authors for their contributions

The ACS Author Rewards program is another of the four open access initiatives introduced by ACS Publications in January 2014. This \$60 million direct-to-author open access stimulus program is designed to encourage authors to publish open access. Under this program, every corresponding author of a peer-reviewed article that was published in an ACS journal during 2014 received two ACS Author Rewards worth \$750 each.

The rewards, provided as promotional codes, can be applied toward any ACS AuthorChoice license. They can be used individually on separate articles, combined, or transferred to a colleague.

Deposited into authors' ACS ChemWorx accounts in December 2014, the rewards are redeemable from January 1, 2015, to December 31, 2017.

Two free apps are available through ACS ChemWorx to help authors manage their open access options. The ACS AuthorChoice app guides authors through the process of making their

articles open access. The ACS Author Rewards app allows authors to manage their rewards. Visit ACS ChemWorx at <https://hp.acschemworx.acs.org/>.

Four pillars of ACS Open Access



ACS AuthorChoice

< Expanded open access publishing options for authors and their sponsors.



ACS Author Rewards

< Credits to fund open access publishing options from ACS.



ACS Editors' Choice

< Free public access to research of interest to the global community.



ACS Central Science

< A new journal that's free to both readers and authors.

RESOURCES AVAILABLE FOR ADDITIONAL SUPPORT

ACS has an established reputation for supporting researchers with the publication process and has resources in place to assist with navigating these new open access options.

ACS Help Desk—The ACS Help Desk offers the extensive Knowledge Base, a compendium of more than 1,000 support references on a variety of topics. The Help Desk also offers 24x7, global support via live chat over the web, with Skype, and by telephone. To get support, call **1-800-227-9919** (toll free) or **1-202-872-4357** (international), or visit <https://help.acs.org>

ACS AuthorChoice—The ACS AuthorChoice webpages provide an informative overview of the program, helpful FAQs, pricing information, decision trees for selecting the best AuthorChoice option, and more. Go to <http://pubs.acs.org/page/4authors/authorchoice/index.html>

ACS Author Rewards—Visit the ACS Author Rewards webpages for more information about the program, helpful FAQs, and a guide to using the ACS Author Rewards app. Go to <http://pubs.acs.org/page/4authors/authorrewards/index.html>



3 Ways Researchers Can Boost Their Social Media Savvy

Social networks have become far more than just a way to stay close to family and friends. These digital communities are now a commonplace tool for scientists and publishers alike to collaborate, evaluate, and gain exposure to goings-on in their scientific communities.

How has social media transitioned from a fun distraction to a professional asset? For one, it gives researchers a channel they can use to engage with a range of stakeholders they may not have previously had direct access to, including editors, publishers, colleagues, professors, and lab mates. It is also an excellent way to network, as such platforms provide marketplaces in which even the most niche communities can be built; and in this environment, feedback can happen fast.

While consumption of research findings was once limited to the subscribers of a journal, digital networks now allow articles to achieve a broader reach at a faster pace. There are limitless opportunities for an article to go viral, and with open access becoming more and more prevalent throughout the scientific publishing landscape, the value and impact of social media is even more important.

So whether you're a researcher, author, or editor, a bit of social media savvy can pay off. Keep these tips in mind as you're building—or refining—your online presence.

1. Be present and participate

Whether gathering peer-reviewed articles or looking up a simple piece of information, most of today's research

happens online. That's why you and your research need to be discoverable. Social media is an effective tool for optimizing this search engine visibility.

Your online presence—or lack thereof—affects how prominently your research appears in search results, which could limit your reach in the scientific community and beyond. Make sure you have an online profile and that your bio is updated and accurate on any associated academic institutions' websites. Good places to start are Google Scholar, Google+ (think SEO!), and LinkedIn.

Similarly, publishers often maintain social profiles to generate interest in their publications, share submission deadlines, and highlight emerging research.

“It can be too easy to get lost in a stream of technical jargon.”

—Dr. Jillian Buriak

Twitter is a great resource for exposing people to your work, and a great channel to use to keep up with industry developments and your colleagues' latest research. Take advantage of Twitter's "list" functionality; create one that covers all relevant journals and publishers for your work. In turn, share your Twitter list with your own network, thus making yourself a resource for others in your field.

2. Be creative

Think beyond just posting links as you develop and engage with social media content. If you've just published a new article, use social media not only to promote the publication, but also to generate further discussion with fellow scientists, authors, and researchers. Engaging posts and interesting visuals will keep your profile fresh and those interested in your research intrigued.

Posts should:

- **Provide information**
- **Include a call to action**
- **Be grammatically correct**
- **Keep things positive**
- **Provide a link**
- **Include images or visuals**
- **Be mobile friendly**
- **Demonstrate that you are present**
- **Alternate formats**
- **Be customized**

Use Facebook posts to promote appearances at conferences and events, then tweet from the event to share updates and start conversations. By engaging in social media, you can meet new people and grow your network. Many events are now facilitating such interactions, with Meetups, event-specific hashtags, and even conference-specific apps.

Reddit is also a valuable resource for the scientist, but be careful not to post solely about your own content. This

social media channel is a community in the strongest sense, and users expect true thought leadership. A great balance is Reddit's "Ask Me Anything (AMA)" format, which is an excellent way to respond to questions about your work. The community has an opportunity to get their questions answered, and you have the opportunity to go more in-depth.

3. Be methodical

Decide what you want to share, then determine the best way to share it. New social media tools are emerging on a daily basis, and old tools are constantly evolving. What does this mean for you? Always keep one eye on the bigger picture. Ask yourself: Who am I trying to reach? Is this platform the right fit for what I'm trying to communicate?

Twitter is a good forum to communicate opinions, post updates for conferences and meetings, and quickly disseminate information and easily digestible news. Conversely, a blogging platform, like WordPress, is more suited for longer articles and collections of links to published content.

Another advantage of social media is that it yields data you can use to make better decisions about your content. Consider signing up for free management systems like Tweetdeck or HootSuite, which will give you a bird's eye view of what is happening online. Do people respond more favorably to certain platforms or formats than others? Stay informed on new ways to engage and explore mediums that make sense for you.

Remember, you don't always have to reinvent the wheel. As many researchers have discovered, the LinkedIn for scientists is... LinkedIn.

[Go to pubs.acs.org/page/follow.html](http://pubs.acs.org/page/follow.html)

SOCIAL MEDIA IS NOT IMMATERIAL TO YOUR SUCCESS: TIPS FROM AN EDITOR



Dr. Jillian Buriak

“With only 140 characters, it's a challenge to express science in a way that is creative and attracts attention,” says Jillian Buriak, Editor-in-Chief of *Chemistry of Materials* and a popular presence on social media.

“It can be too easy to get lost in a stream of technical jargon. Try thinking carefully about condensing your meaning into 5 to 10 words, and harness the power of commonly used hashtags (#graphene, #solar, #nano, #OA, #materials, for instance). If you want to catch the attention of someone in particular, top off the tweet with the Twitter handle of a scientist and/or their institutions. This encourages retweeting to further spread your message.”

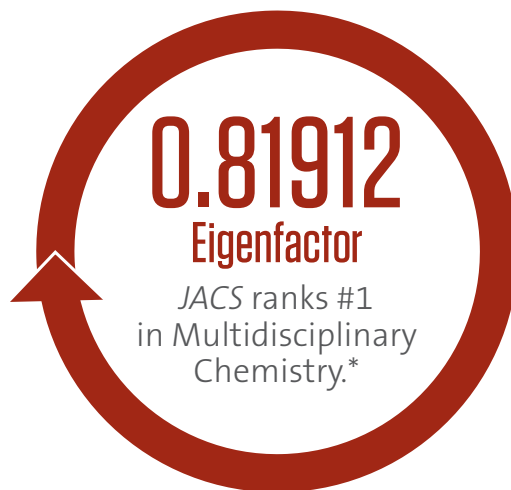
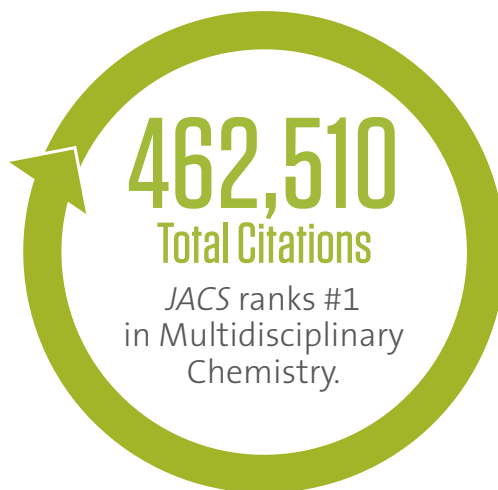
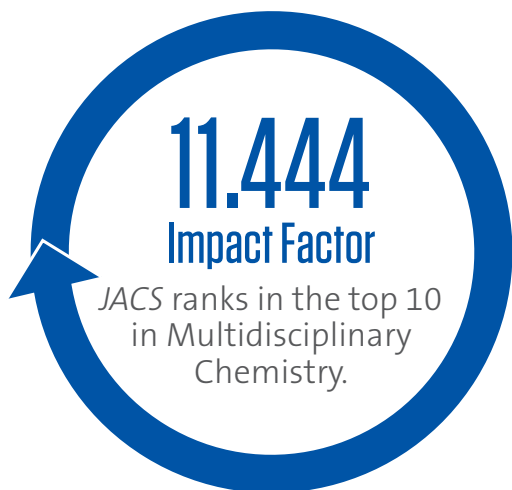
The Most Cited Journals

ACS Publications is a Leader in Chemistry & Related Areas of Science, as reported in the 2013 Journal Citation Reports® from ThomsonReuters

Journal Title	Total Citations	Impact Factor	Current Articles
Accounts of Chemical Research	47,005	24.348	279
ACS Applied Materials & Interfaces	16,373	5.900	1,781
ACS Catalysis	4,446	7.572	378
ACS Chemical Biology	4,711	5.356	314
ACS Chemical Neuroscience	1,259	4.210	153
ACS Combinatorial Science	685	3.401	87
ACS Macro Letters	1,847	5.242	231
ACS Medicinal Chemistry Letters	1,737	3.073	214
ACS Nano	58,446	12.033	1,178
Analytical Chemistry	102,654	5.825	1,638
Biochemistry	88,295	3.194	920
Bioconjugate Chemistry	14,074	4.821	209
Biomacromolecules	27,578	5.788	501
Chemical Research in Toxicology	11,018	4.19	191
Chemical Reviews	124,463	45.661	207
Chemistry of Materials	79,744	8.535	604
Crystal Growth & Design	24,937	4.558	664
Energy & Fuels	21,961	2.733	840
Environmental Science & Technology	105,646	5.481	1,689
Industrial & Engineering Chemistry Research	43,808	2.235	1,910
Inorganic Chemistry	90,888	4.794	1,646
Journal of Agricultural and Food Chemistry	82,432	3.107	1,506
Journal of Chemical & Engineering Data	16,833	2.045	460
Journal of Chemical Education*	7,338	1.001	359
Journal of Chemical Information and Modeling	11,630	4.068	296
Journal of Chemical Theory and Computation	14,415	5.310	553
Journal of Medicinal Chemistry	61,787	5.480	797
Journal of Natural Products*	20,791	3.947	336
The Journal of Organic Chemistry	98,978	4.638	1,397
Journal of Physical Chemistry A	57,303	2.775	1,470
Journal of Physical Chemistry B	121,463	3.377	1,720
Journal of Physical Chemistry C	96,606	4.835	3,113
Journal of Physical Chemistry Letters	13,562	6.687	677
Journal of Proteome Research	19,028	5.001	527
Journal of the American Chemical Society	462,510	11.444	2,840
Langmuir	113,157	4.384	1,887
Macromolecules	101,162	5.927	1,049
Molecular Pharmaceutics	8,173	4.787	450
Nano Letters	103,399	12.940	996
Organic Letters	80,234	6.324	1,584
Organic Process Research & Development	4,201	2.549	170
Organometallics	41,998	4.253	898

*co-publications

There are many ways to measure a journal...

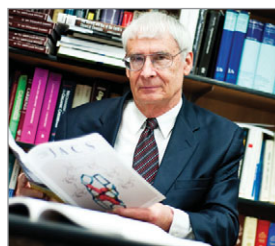


Here's another way: Look at its editors. >>>

JACS editors: distinguished

Unlike journals with editors who are full-time publishing professionals, *JACS* offers you the benefit of having your manuscript submission handled by scientists who are engaged in cutting-edge research and still publishing their own papers. That's why *JACS* editors have a better idea of what is important to the science, where a field is headed, and what is important to you as an author.

At *JACS*, serving the scientific community is what matters most. That's the real measure of our success.



EDITOR
Peter J. Stang
Distinguished Professor
David P. Gardner
Presidential Chair
University of Utah

ASSOCIATE EDITORS



Eric V. Anslyn
University Distinguished Teaching
Professor and Norman Hackerman
Professorship in Chemistry
The University of Texas at Austin



Weston Thatcher Borden
Distinguished University Research
Professor and Welch Chair
University of North Texas



Kara L. Bren
Professor of Chemistry
University of Rochester



Benjamin F. Cravatt
Professor and Chair, Department
of Chemical Physiology,
The Scripps Research Institute,
Scripps California



Paul S. Cremer
J. Lloyd Huck Chair in
Natural Sciences
The Pennsylvania State
University



Lyndon Emsley
Professor of Chemistry
Université de Lyon, France



Jean M. J. Fréchet
Vice President for Research
and Distinguished Professor
of Chemistry, King Abdullah
University of Science and
Technology, Saudi Arabia



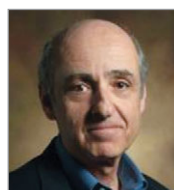
Gregory C. Fu
Altair Professor of Chemistry
California Institute of Technology



Miguel A. García-Garibay
Professor and Chair,
Department of Chemistry
and Biochemistry
University of California,
Los Angeles



Martin Gruebele
James R. Eiszner Endowed Chair
in Chemistry, Professor of Physics
and Center for Biophysics and
Computational Biology
University of Illinois at
Urbana-Champaign



Sidney M. Hecht
Director, Center for
BioEnergetics,
Biodesign Institute, and
Professor of Chemistry
Arizona State University



Taeghwan Hyeon
Distinguished University
Professor and Director, Center for
Nanoparticle Research, Institute
for Basic Science
Seoul National University, Korea

and active researchers



William D. Jones
C. F. Houghton Professor
of Chemistry
University of Rochester



Thomas E. Mallouk
Evan Pugh Professor,
Associate Director, Penn State
MRSEC, Director, Center for
Solar Nanomaterials
The Pennsylvania State
University



Chad A. Mirkin
Director of the International
Institute for Nanotechnology,
the George B. Rathmann Prof. of
Chemistry, Prof. of Chemical and
Biological Engineering, Prof. of
Materials Science & Engineering,
and Prof. of Medicine
Northwestern University



Klaus Müllen
Professor and Director,
Max Planck Institute for
Polymer Research, Mainz,
Germany



Eiichi Nakamura
Professor of Physical
Organic Chemistry
The University of Tokyo,
Japan



William R. Roush
Professor of Chemistry,
Associate Dean of
Graduate Studies,
The Scripps Research
Institute, Florida



Melanie S. Sanford
Moses Gombert Collegiate
Professor of Chemistry,
Arthur F. Thurnau Professor
of Chemistry
University of Michigan



Alanna Schepartz
Milton Harris '29 Ph.D.
Professor of Chemistry,
Professor of Molecular, Cellular,
and Developmental Biology
Yale University



Matthew S. Sigman
Presidential Endowed Chair
of Chemistry
University of Utah



Donald G. Truhlar
Regents Professor
University of Minnesota



Li-Jun Wan
Professor and Director,
CAS Key Laboratory of
Molecular Nanostructure and
Nanotechnology, Director,
Beijing National Laboratory for
Molecular Sciences,
Institute of Chemistry,
Chinese Academy of Sciences



Henry S. White
Distinguished Professor
University of Utah



Karen L. Wooley
W. T. Doherty-Welch
Chair and University
Distinguished Professor
Professor of Chemistry,
Chemical Engineering,
and Materials Science &
Engineering
Director, TAMU Laboratory for
Synthetic-Biologic Interactions
Texas A&M University



Omar M. Yaghi
The James and Neeltje
Tretter Professor of
Chemistry
University of California,
Berkeley



Peidong Yang
S.K. and Angela Chan
Distinguished Professor
of Energy,
Professor of Chemistry
University of California,
Berkeley



ACS Publications
Most Trusted. Most Cited. Most Read.

Submit your best research to *JACS* at pubs.acs.org/jacs



ACS is ready with the resources

The American Chemical Society (ACS) 249th National Meeting and Exposition is entitled “The Chemistry of Natural Resources.” The name is appropriate, since ACS is all about providing resources to chemists around the world. The 5-day meeting is a resource in itself to expose you to exciting advances in science. We invite you to come to the ACS booth to learn about the programs, products, and services that ACS offers as resources to its members. If you will not be in attendance, please read on to learn about how ACS helps scientists excel in their careers and their research.

C&EN

To start, *Chemical & Engineering News* (C&EN) is the weekly resource chemists count on to deliver the latest chemistry news from the worlds of research, business, education, government, and beyond. C&EN’s online resources include C&EN Archives, a growing collection of full, cover-to-cover C&EN issues, with the previous year’s issues added on a rolling basis each year. In addition, with C&EN Mobile, members of the ACS can

now access all of the issues for no charge by entering their ACS ID. If you are not a member, individual issues of C&EN are available for purchase within the app.

ACS Publications

ACS Publications will introduce its newest journal, *ACS Central Science*, along with its Editor-in-Chief, Dr. Carolyn Bertozzi, at the ACS booth. *ACS Central Science* is the first completely open access journal from the ACS. This groundbreaking, highly selective journal, publishing only 100-200 papers in its first year, is now accepting submissions. Find out more at the ACS Publications booth or go to pubs.acs.org/centralscience. Stop by also to learn about *ACS Infectious Diseases* and *ACS Biomaterials Science & Engineering*, two new journals

publishing their first issues in 2015.

On Monday, March 23rd at 12:00 noon MT, you can take part in an exciting live ACS Publications webinar at the booth’s main stage. “Mastering the Art of Scientific Publication,” the popular, new webinar series, will feature a panel of distinguished ACS journal editors giving tips and advice to help authors, with a Q&A period at the end of the event.





CAS

CAS, the world's authority for chemical information, will have a strong presence at the ACS booth where you will discover the many resources CAS offers to scientists around the world. You will see how the authoritative and in-depth databases from CAS can meet your most challenging research needs when combined with the advanced search and analysis technologies of SciFinder® and STN®. Ask the CAS staff for a demonstration of SciFinder®, learn about the exciting new product features, and take part in promotions for chances at exciting prizes!

- **SciFinder®**, the choice for chemistry research, is a powerful discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances, and reactions. SciFinder offers you the tools to enhance your research efforts every step of the way, including access to CAS REGISTRYSM—the gold standard for chemical substance information.
- **STN®**, the choice of patent experts, offers access to trusted scientific and technical information. Intellectual property professionals and patent examiners at the world's major patent offices and research organizations rely on STN for their information needs.

Learn more about CAS and all of its powerful solutions today at www.cas.org

www.acs.org

As one of the most valuable ACS resources, the ACS Web site at

www.acs.org is becoming more personalized, so we can deliver the most relevant ACS content, programs, products and services—all tailored for you! When you visit the ACS Web kiosk, you will see what we've personalized so far, share your interests, and help us take ACS Web



personalization to the next level. From changes in "My Account" to the www.acs.org home page, we are striving to develop the best personalized ACS web experience for you. Those who come to provide input will not only influence the site, but also receive a thank you gift.

ACS Career Navigator®

The ACS Career Navigator® is your home for career services, leadership development, in-person and online professional education courses, and market intelligence resources. The team will be on hand to explain how the services ACS Career Navigator® offers will help you achieve your career goals

with opportunities to refresh your skills and branch into new areas of emerging science and advanced applications. Use the interactive recommendation tool on the iPad to get a list of training courses or career services available for your specific needs. All who use the tool onsite are automatically entered to win an iPad mini.

ACS Member Insurance

The Member Insurance Program provides resources to encourage you to fall in step with a healthier lifestyle. A special interactive challenge will energize you to improve your own health and that of the entire planet. Speak with representatives to explore the plans available exclusively to ACS members such as Life & Disability Insurance, International Term Life Insurance, Auto & Homeowners, Professional Liability, Pet Insurance, and more.

ACS members get a shirt for sharing their story at www.my.acs.org or onsite at the National Meeting at the My ACS Story kiosk. Let us know how you connect, share, discover, and advance with ACS.

Of course, the Member Benefits kiosk will be onsite at the National Meeting to answer any questions you have about the benefits of ACS membership. You will also receive a gift to thank you for your membership.

Questions?

If you have questions about ACS membership before or after the ACS National Meeting, please call 800-333-9511 or +1-614-447-3776 (from outside of the US), M-F, 8:30 a.m.-5:00 p.m. Eastern Time or email us at service@acs.org.

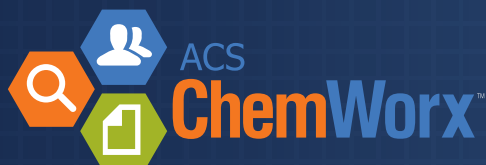


*“One of the members of our lab left, and we’re having a difficult time finding his **data**, **files**, and **references**.”*

Does this problem sound familiar?

Everyone in your lab group can store their files and references in ACS ChemWorx, and share them with whom they want.

Register free at www.acschemworx.org! (even for non-ACS members)



 @ACSChemWorx



ACS Publications
Most Trusted. Most Cited. Most Read.

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 (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 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.

SPEAKER READY ROOMS & AUDIO-VISUAL SERVICE CENTERS.

Presenters may use the speaker ready rooms to preview their presentation, ensure compatibility with our LCD projectors, or fulfill last-minute audiovisual equipment orders. We strongly recommend that all presenters come to the

speaker ready room the day before their presentation to check for connectivity and resolution. The hours of operation will be from 3:00 to 5:00 PM Saturday and 7:00 AM to 6:00 PM Sunday through Thursday. Visit the ACS Operations Office at any ACS property for speaker ready room locations. Speaker ready rooms are not equipped with copy machines. There is a UPS Store located in Concourse A of the convention center that provides a range of services including computer access and copying, faxing, printing, and shipping.

POSTER SESSIONS. All materials must be confined to a 4-foot-high by 8-foot-wide display board in the convention center and 4-foot-high by 6-foot-wide display board in hotels. Presenters must mount their poster one hour before the scheduled session start time. Poster numbers supplied by ACS will be in the upper corner of each poster board, and this number corresponds with the number assigned to each poster in the technical program. Pushpins will be available at the poster session. Presenters must remain with their posters for the duration of their scheduled session as indicated in the technical program. All posters must remain up until the session ends and then must be removed within one hour. ACS cannot assume responsibility for materials beyond these time limits.

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 249th national meeting is now available at www.acs.org/denver2015. You can search by divisions or committees, symposia, speakers, or keywords from abstracts as well as presidential events and the multidisciplinary theme of "Chemistry of Natural Resources."

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. 30 or on-site in Denver from March 22 to 26. 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 Colorado Convention Center. You can have a USB flash drive shipped to you if you place your order by Jan. 30, 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.

Polymer Chemistry.

Kathy Mitchem, e-mail: kathy@vt.edu

Polymeric Materials: Science & Engineering Inc.

Visit pmse.sites.acs.org/pmsepreams.htm.

Denver 2015

Interdivisional Poster Session & Mixer

Monday, March 23
Colorado Convention Center
Hall C from 8PM – 10PM

SCI-MIX

Sci-Mix is a national meeting wide social event with colleagues meeting each other in a relaxed atmosphere combined with serious scientific poster discussions. Speak informally with presenters as they represent the best of what their division has to offer in terms of science and presentation. It is free and all attendees are welcomed.

You can now access the [Sci-Mix](#) sessions on the free meeting mobile app. Download it today!

TECHNICAL PROGRAM SUMMARY

Presidential Events

PRES

Diane Grob Schmidt, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders**	A				
Nanotechnology: Delivering on the Promise**	P	D			
DOE Nanoscience Research Centers			A		
Particles at Fluid Interfaces* (COLL)	D	A			
Functionalization of Complex Nanosurfaces* (COLL)	D	D	A		
Basic Research in Colloids, Surfactants & Nanomaterials* (COLL)	D			A	D
Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion* (COLL)	DE	D	A	D	
Department, University & National Models for Faculty Development To Support Adoption of Evidence-Based Teaching* (CHED)	P				
Plasmonic Catalysis & Sensing* (COLL)	E	D	A	D	
Nanoscience* (INOR)	E		E	D	D
Fundamental Research in Colloids, Surfaces & Nanomaterials* (COLL)	E				
Transitioning between Academic Research into Practical Use: Solar Energy & Advanced Materials* (COMSCI)	A				
Electrical, Thermal & Mass Transport in Polymer Nanocomposites & Alloys* (POLY)		D	E		
Excellence in Graduate Polymer Research* (POLY)		D	E		
Advances in Formulations Science & Technology* (COLL)		P			
Nanoscience & Nanotechnology of Natural Resources* (MPPG)			A		
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Presidential Events (continued)

PRES

Diane Grob Schmidt, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
The Interface of Chemical & Biological Sciences International Disarmament Efforts* (IAC)			D		
Applied Nanotechnology for Food & Agriculture* (AGFD)			P	A	
Ask Dr. Safety: EH&S Support of Nanotechnology R&D* (CHAS)			A		

Multidisciplinary Program Planning Group

MPPG

R. Weber, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Chemistry of Natural Resources Plenary <i>CNR</i>	P				
The Fred Kavli Innovations in Chemistry Lecture <i>CNR</i>		P			
The Kavli Foundation Emerging Leader in Chemistry Lecture		P			
Nanoscience & Nanotechnology of Natural Resources** <i>CNR</i>			A		
Green Chemistry & the Environment* (ENVR)	D	A		E	
Catalysis for Unconventional Energy Sources* (ENFL)	D	A			
Nanomaterials for Solar Energy Conversion & Storage* (ENFL)	D	D	D	D	A
Uranium in Seawater* (I&EC)	D	D			
Environmental Reactivity of Organic Micropollutants & Their Transformation Products in Receiving Waters* (ENVR)	D			E	
Assessing Toxicity of Environmental Contaminants* (ENVR)	D			E	
Biogenically Enhanced Recovery & Bioremediation in Fossil Fuel Reservoirs* (ENVR)	D			E	
Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)* (ENFL)	D				

PROGRAM SUMMARY

Multidisciplinary Program Planning Group (continued)

MPPG

R. Weber, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Understanding the Geochemical Interactions of Organic Compounds in the Subsurface* (GEOC)	D				
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Environmental Chemistry & Health Impacts of Fine & Ultrafine Particulate Matter* (ENVR)		A		E	
Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR & Novel Approaches* (ENFL)		A			
Biomass to Fuel & Products* (SOCED)		A			
Geochemistry & Reactive Transport in Nano-Pore Geomaterials* (GEOC)		A			
Transitioning between Academic Research into Practical Use: Solar Energy & Advanced Materials* (COMSCI)		A			
Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment* (ENVR)	D	A	E		
Hydraulic Fracturing Impacts on Water, Soil & Air Quality* (ENVR)	D	D			
Chemical Technology in Antiquity* (HIST)	D				
Solutions to Metals Contamination of Water* (ENVR)	P	D	E		
Chemistry in the Marine Boundary Layer* (ENVR)	P		E		
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community* (PRES)			A		
C1 Chemistry* (ENFL)			D	D	A
Iron Oxides: Formation, Structure, Reactivity & Applications* (GEOC)			D	D	
Molecular Catalyst for Solar Fuels* (INOR)			DE	A	
Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment* (ENVR)			D	E	

Multidisciplinary Program Planning Group (continued)

MPPG

R. Weber, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Chemistry of the Energy Water Nexus: Focus on Fracking* (INOR)			D		
12th International Symposium on Heavy Oil Upgrading, Production & Characterization* (ENFL)				D	A
Surface Physicochemical Processes in Engineered & Natural Systems* (ENVR)				D	A
Computational Pyrolysis & Upgrading of Bio-Oils* (COMP)				D	
Analytical Chemistry of Natural Resources* (ANYL)				D	
Trace Materials in Air, Soil & Water* (ENVR)				D	
Water Sustainability in Oil & Gas Exploration: Treatment Issues* (ENVR)				DE	
Water Our Most Critical Resource* (AGFD)				P	A
ACS Award for Affordable Green Chemistry: Honoring John Frye, Todd Werpy & Alan Zacher* (CELL)				P	
Water Recycling in Domestic Use, Energy Extraction & Agricultural Use* (ENVR)				E	A
Bioavailability & Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment* (ENVR)				E	A
Environmental Chemistry: Pedagogical Models & Practices* (ENVR)				E	A

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

PROGRAM SUMMARY

Division of Agricultural & Food Chemistry

AGFD

K. Deibler, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Undergraduate Symposium**	A				
Vitamin D: Past, Present & Future for Animals & Humans	P				
Graduate Student Symposium**	P				
Agricultural & Food Chemistry General Papers		D	A	P	
Medicinal & Aromatic Crops: Production, Phytochemistry & Utilization**		D			
Sci-Mix		E			
Phenolic & Polyphenolic Chemistry in Food Processing**			D		
Applied Nanotechnology for Food & Agriculture**			P	A	
Agricultural & Food Chemistry General Posters			P		
Water Our Most Critical Resource** <small>CNR</small>				P	A
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Undergraduate Research Posters* (CHED)		P			
Ask Dr. Safety: EH&S Support of Nanotechnology R&D* (CHAS)			A		

Division of Agrochemicals

AGRO

P. Rice, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Environmental Reactivity of Organic Micropollutants & Their Transformation Products in Receiving Waters* (ENVR)	D			E	
Assessing Toxicity of Environmental Contaminants* (ENVR)	D			E	
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Medicinal & Aromatic Crops: Production, Phytochemistry & Utilization* (AGFD)		D			
Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment* (ENVR)			D	E	
Phenolic & Polyphenolic Chemistry in Food Processing* (AGFD)			D		

Division of Agrochemicals (continued)

AGRO

P. Rice, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Surface Physicochemical Processes in Engineered & Natural Systems* (ENVR)				D	A
Microalgae: A Renewable Energy Source & a Sustainable Solution for the Environment* (ENVR)				D	
Water Recycling in Domestic Use, Energy Extraction & Agricultural Use* (ENVR)				E	A

Division of Analytical Chemistry

ANYL

D. Duckworth, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Environmental Analytical Chemistry: A Tool for Introducing Research	P				
Advances in Bioanalytical Chemistry		D	D		
Advances in Analytical Separations		D			
Sci-Mix		E			
Advances in Mass Spectrometry			A		
Active Learning in the Undergraduate Analytical Chemistry Curriculum			P		
General Analytical Posters			E		
Advances in Electrochemistry				A	
Analytical Chemistry of Natural Resources**				D	
Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Honoring Hilka I. Kenttämaa**				P	
Nakanishi Prize: Honoring Fred W. McLafferty					A
Advances in Analytical Spectroscopy					P
Macromolecular & Nanoparticle Separation Science* (POLY)	D	D	DE		
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment* (ENVR)		D	A	E	
Undergraduate Research Posters* (CHED)	P				

PROGRAM SUMMARY

Division of Analytical Chemistry (continued)

ANYL

D. Duckworth, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
DOE Nanoscience Research Centers: National Resources for Nanoscience Community* (PRES)			A		
Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment* (ENVR)			D	E	
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		
The Interface of Chemical & Biological Sciences International Disarmament Efforts* (IAC)			D		

Division of Biochemical Technology

BIOT

M. Lazzara, A. Kantardjieff, Program Chairs

Grand Hyatt Denver	S	M	Tu	W	Th
David Perlman Memorial Lectureship	A				
Downstream Processes <i>CNR</i>	D	D	D	D	D
Upstream Processes	D	D	D	D	D
Biomolecular & Biophysical Processes	D	D	D	D	D
Emerging Technologies	D	D	D		
Colorado Biotechnology <i>CNR</i>	D	P			
Biosimilars & Follow-On Biologics		A	A		
Marvin J. Johnson Award in Microbial & Biochemical Technology		A			
Sci-Mix		E			
BIOT Young Investigator Award			A		
Biofuels & Sustainable Energy <i>CNR</i>			P	D	D
Alan S. Michaels Award in the Recovery of Biological Products			P		
Poster Session			E		
Biotechnology & Bioengineering Awards Presentation & Gaden Award				A	
Quality-by-Design for Biopharmaceuticals				D	
Biotechnology & Bioengineering Daniel I. C. Wang Award				P	

Division of Biochemical Technology (continued)

BIOT

M. Lazzara, A. Kantardjieff, Program Chairs

Grand Hyatt Denver	S	M	Tu	W	Th
WCC Rising Stars Awards Symposium* (WCC)		D			
Undergraduate Research Posters* (CHED)		P			
Phenolic & Polyphenolic Chemistry in Food Processing* (AGFD)			D		

Division of Biological Chemistry

BIOL

C. Crews, V. Bandarian, Program Chairs

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Young Investigators in Biological Chemistry	A				
Complex Enzymatic Transformations	P				
Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Honoring Michael A. Marletta	E				
Current Topics in Biological Chemistry	E				
The Chemistry & Biology of Non-Natural Nucleic Acids		A			
New Approaches to Investigating Chromatin Modifying Enzymes: Structure & Function		P			
Putting Chemical Biology in Context			A		
ACS Chemical Biology Award Symposium			P		
In Vivo We Trust: Small Molecule Phenotypic Screening in Animals				A	
Graduate Student & Postdoctoral Symposium				P	
Interfacial Biomolecular Recognition* (COLL)	E		A	D	D

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

PROGRAM SUMMARY

**Division of Biological Chemistry
(continued)**

BIOL

C. Crews, V. Bandarian, Program Chairs

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Undergraduate Research Posters* (CHED)		P			
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Division of Carbohydrate Chemistry (continued)

CARB

E. Rozners, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
General Posters* (CELL)	E				
Frontiers in Glycoscience* (CELL)		D	D		

Division of Business Development & Management

BMGT

K. Allen, J. Bryant, Program Chairs

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
ACS Award in Industrial Chemistry: Honoring Thomas J. Colacot**		D			
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders* (PRES)	A				
Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations* (PROF)	P				
Forensic Toxicology of Marijuana* (SOCED)		A			
Innovations in Macromolecular Network Chemistry* (POLY)		P	E	P	D

Division of Catalysis Science & Technology

CATL

V. Schwartz, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Theoretical & Experimental Synergies at the Frontiers of Renewable Energy Catalysis <i>CNR</i>	D	A	P	A	A
Electrocatalysis & Photocatalysis <i>CNR</i>	D	D			
Honoring Jens Rostrup-Nielsen	D	P	D		
New Catalysis through Ligand Design	D				
George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Honoring Jingguang G. Chen		D	A		
Surface Chemistry & Catalysis on Oxides		D	D	D	
Gabor A. Somorjai Award for Creative Research in Catalysis: Honoring Maurice Brookhart		P			
Sci-Mix		E			
Catalytic Materials & Technologies for Upgrading of CO _x & Natural Gas <i>CNR</i>			D	D	D
General Poster Session			E		
Novel Catalytic Materials for Renewable Fuels/Chemicals <i>CNR</i>				D	D
General Papers				P	D
Catalysis for Unconventional Energy Sources* (ENFL)	D	A			
E.V. Murphree Award in Industrial & Engineering Chemistry: Honoring Joseph R. Zoeller* (I&EC)			D		
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		
Elucidation of Mechanisms & Kinetics on Surfaces* (COLL)				D	

Division of Carbohydrate Chemistry

CARB

E. Rozners, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Wolfrom Award Symposium	A				
Isbell Award & Gin New Investigator Award Symposium	P				
Glycomimetic Compounds: An Untapped Source of Novel Therapeutics		D			
Sci-Mix		E			
Protein Glycosylation: Simulation, Synthesis, Characterization & Application			D		
General Posters			E		

PROGRAM SUMMARY

Division of Cellulose & Renewable Materials

CELL

C. Frazier, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Functional Lignocellulosics & Nanotechnology <i>CNR</i>	D	D	A	D	
Cellulose in Solid State & Solution: Structure, Chemistry & Reaction Mechanisms: Anselme Payen Award Honoring Thomas Rosenau <i>CNR</i>	D	D	D	A	
Lignin Biosynthesis, Characterization & Modifications <i>CNR</i>	D	D			
Application of Computational Chemistry to Biomass Chemistry & Utilization <i>CNR</i>	D	P			
Advances in Lignocellulosic Materials & Chemistry: A Tribute to W.G. Glasser <i>CNR</i>	DE	A			
General Posters** <i>CNR</i>	E				
Frontiers in Glycoscience** <i>CNR</i>		D	D		
Sci-Mix		E			
Renewable Resources for Materials & Energy: Recent Research & Developments in Ibero-America <i>CNR</i>			A	D	A
Smart & Responsive Composites from Renewable Building Blocks** <i>CNR</i>			A	D	
Cellulose Dissolution: New Solvents & Mechanisms <i>CNR</i>				D	A
ACS Award for Affordable Green Chemistry: Honoring John Frye, Todd Werpy & Alan Zacher** <i>CNR</i>				P	
Research on Renewable Materials: US & EU Perspectives <i>CNR</i>					D
Conservation Science of Cellulosic Materials: Recent Developments <i>CNR</i>					D
Biomass to Fuel & Products* (SOCED)		A			
Polymeric Biomaterials* (PMSE)		P	D	D	A
Sustainability in the 21st Century: Optimizing Complex Interdependent Systems* (SOCED)		P			

Division of Chemical Education

CHED

W. Jones, I. Levy, A. Marsh, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Current Practice & Research Using ACS Exams	A				
Undergraduate Research Papers**	D	D			
Chemistry Education Research	D		P	D	
NMR Spectroscopy in the Undergraduate Curriculum	D				
From Cornerstone to Capstone: Culminating Experiences in the Undergraduate Chemistry Curriculum that Foster Integration & Application of Foundational Knowledge	D				
High School Program**	D				
Department, University & National Models for Faculty Development to Support Adoption of Evidence-Based Teaching**	P				
General Posters	E				
Integrating Chemistry & Polymer Science Research into the Classroom**		A			
Research at Community Colleges: Strategies for Enhancing Student Transfer & Success		A			
Experiments for Physical Chemistry Laboratory		D			
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Honoring Vickie M. Williamson**		D			
Chemistry Education: International & Multi-Cultural Perspectives		D			
Undergraduate Research Posters**		P			
ACS Award for Encouraging Disadvantaged Students in Chemistry: Honoring Catherine H. Middlecamp**		P			
Online Course Development & the Effects on the On-Campus Classroom		P			
Sci-Mix		E			

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM

E = EVE DE = AM/PM/EVE PE = PM/EVE

PROGRAM SUMMARY

Division of Chemical Education (continued)

CHED

W. Jones, I. Levy, A. Marsh, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum**		E			
Successful Student Chapters		E			
Chemistry Education Research: Graduate Student Research Forum			A		
ACS-CEI Award for Incorporating Sustainability into Chemistry Education**			A		
Citizens First: Communicating Climate Science to the Public** <small>CNR</small>			A		
George C. Pimentel Award in Chemical Education: Honoring I. Dwaine Eubanks**			D		
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis**			D		
NSF Programs that Support Undergraduate Education			D		
Overcoming Obstacles in Student Learning in Physical Chemistry			P		
Perspectives on Climate Change Literacy & Education: Local to International			P		
General Papers			E		A
Instructors & Researchers: Advancing Graduate Education in Chemistry				A	
Process-Oriented Guided Inquiry Learning (POGIL)				A	
Using Technology in the Undergraduate Laboratory				A	
Computational Chemistry in the Undergraduate Curriculum: What Is Working & How Do We Assess It?**				D	
Green Chemistry: Theory & Practice**				D	
Undergraduate Research in Chemistry: Expanding Opportunities & Broadening Participation				P	
Nanotechnology in Undergraduate Education & Research				P	
Research on Learning in the Laboratory				P	
Undergraduate Symposium* (AGFD)	A				

Division of Chemical Education (continued)

CHED

W. Jones, I. Levy, A. Marsh, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Graduate Student Symposium* (AGFD)	P				
Diversifying STEM: Uniting through Our Differences for a Brighter Scientific Future* (CMA)		A			
Environmental Chemistry: Pedagogical Models & Practices* (ENVR)				E	A

Division of Chemical Health & Safety

CHAS

D. Decker, F. Wood-Black, J. Pickel, Program Chairs

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Legalized Marijuana & Health & Safety**		P			
Sci-Mix		E			
Safety in Undergraduate Teaching**			P		
Ask Dr. Safety: EH&S Support of Nanotechnology R&D**			A		
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

Division of Chemical Information

CINF

E. Bolstad, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Getting to the Best Reaction: Tools for Finding a Needle in a Haystack	A				
Defining "Value" in Scholarly Communications: Evolving Ways of Evaluating Impact on Science	P				
Research Results: Reproducibility, Reporting, Sharing & Plagiarism		D	A		
Sci-Mix		E			
Molecular & Structural 2D & 3D Chemical Fingerprinting: Computational Storing, Searching & Comparing Molecular & Chemical Structures			P		

PROGRAM SUMMARY

Division of Chemical Information (continued)

C I N F

E. Bolstad, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Development & Use of Data Format Standards for Cheminformatics				D	
Drug Discovery* (COMP)	D	D	D	D	

Division of Chemical Toxicology

T O X I

A. C. Bryant-Friedrich, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Forensic Toxicology of Marijuana* (SOCED)		A			

Division of Chemistry & the Law

C H A L

K. Bianco, J. Hasford, Program Chairs

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions	A				
Hot Topics in Chemical and Pharmaceutical Patent Law	P				
A Patent Litigation Primer		A			
Anti-Doping: A Unique Combination of Chemistry and the Law		P			
Sci-Mix		E			
Fundamental Concepts in Protecting Chemical Technologies			A		
Legal and Business Considerations for Chemical Technologies			P		
Patenting Chemical Inventions				A	
Intellectual Property and Natural Resources: What Can I Protect and How?				P	
The Many Faces of CHAL: Where Chemistry Meets the Law					A
The Interface of Chemical & Biological Sciences International Disarmament Efforts* (IAC)			D		

Division of Colloid & Surface Chemistry

C O L L

R. Nagarajan, Program Chair

Marriott City Center Denver	S	M	Tu	W	Th
Particles at Fluid Interfaces**	D	A			
Biomembrane Synthesis, Structure, Mechanics & Dynamics	D	D	A	D	
Molecular Engineering of Peptide Assembly	D	D	A		
Functionalization of Complex Nanosurfaces**	D	D	A		
Basic Research in Colloids, Surfactants & Nanomaterials**	D			A	D
Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion**	DE	D	A	D	
ACS Award in Colloid & Surface Chemistry: Honoring Paul S. Weiss	P	D	D		
Plasmonic Catalysis & Sensing	E	D	A	D	
Interfacial Biomolecular Recognition**	E		A	D	D
Fundamental Research in Colloids, Surfaces & Nanomaterials**	E				
Advances in Formulations Science & Technology**		P			
Sci-Mix		E			
Natural Resource Capture, Storage & Energy Conversion				D	D
Elucidation of Mechanisms & Kinetics on Surfaces**				D	
Chemical Processes at Environmental Interfaces* (ENVR)	D	A		E	
Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease* (PHYS)	D	D	P		
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
WCC Rising Stars Awards Symposium* (WCC)		D			
Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces* (GEOC)			D	D	

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

PROGRAM SUMMARY

Division of Computers in Chemistry

COMP

E. Esposito, S. Wildman, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
Molecular Mechanics**	D	A		A	
Computational Design, Discovery & Optimization of Organic Semiconductor Materials**	D	A			
Drug Discovery**	D	D	D	D	
Electronic Structure Methods for Highly Polarizable Systems**	D	D			
Quantum Chemistry**	P	P	P	D	
ACS Award for Research at an Undergraduate Institution: Honoring George C. Shields		P	D		
ACS Award for Computers in Chemical & Pharmaceutical Research: Honoring David A. Case**		P	D		
Sci-Mix		E			
Computational Study of Water			A	A	
Materials Science			D		
The Chemical Computing Group Excellence Award for Graduate Students			E		
The OpenEye Outstanding Junior Faculty Award			E		
Poster Session			E		
NVIDIA GPU Award			E		
Computational Pyrolysis & Upgrading of Bio-Oils** <small>CNR</small>				D	
Symposium Organizer Selections				P	
Membranes				P	
Modeling Excited States of Complex Systems* (PHYS)	D	D	P	D	A
Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease* (PHYS)	D	D	P		
Computational Chemical Dynamics: Advancing Our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems* (PHYS)	D	D		D	A
Modeling Complex Biomolecules: From Structure to Dynamics & Function* (PHYS)	D	D		D	A
Undergraduate Research Posters* (CHED)		P			
Phenolic & Polyphenolic Chemistry in Food Processing* (AGFD)			D		

Division of Energy & Fuels

ENFL

A. Park, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Catalysis for Unconventional Energy Sources** <small>CNR</small>	D	A			
Nanomaterials for Solar Energy Conversion & Storage** <small>CNR</small>	D	D	D	D	A
Materials & Interfaces in Lithium Batteries & Beyond	D	D	D	D	A
Hybrid Functional Porous Materials for Sustainable Energy: Carbon, MOF & Conductive Polymers	D	D			
Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)** <small>CNR</small>	D				
Chemistry of Energy & Fuels	D				
Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR & Novel Approaches** <small>CNR</small>		A			
ENFL Distinguished Researcher Award: Honoring James Burrington		D	A		
Two-Dimensional Materials for Energy & Fuel		P	D	D	A
Sci-Mix		E			
C1 Chemistry**			D	D	A
Advances in the Chemistry of Energy & Fuels			P		
12th International Symposium on Heavy Oil Upgrading, Production & Characterization** <small>CNR</small>				D	A
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Biomass to Fuel & Products* (SOCED)		A			
Sustainability in the 21st Century: Optimizing Complex Interdependent Systems* (SOCED)		P			
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community* (PRES)			A		
Energy & Materials* (POLY)			DE	D	D
Computational Pyrolysis & Upgrading of Bio-Oils* (COMP)				D	

PROGRAM SUMMARY

Division of Environmental Chemistry

ENVR

S. Al-Abed, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Chemical Processes at Environmental Interfaces** <small>CNR</small>	D	A		E	
Green Chemistry & the Environment** <small>CNR</small>	D	A		E	
Environmental Reactivity of Organic Micropollutants & Their Transformation Products in Receiving Waters** <small>CNR</small>	D			E	
Assessing Toxicity of Environmental Contaminants** <small>CNR</small>	D			E	
Biogenically Enhanced Recovery & Bioremediation in Fossil Fuel Reservoirs** <small>CNR</small>	D			E	
Environmental Chemistry & Health Impacts of Fine & Ultrafine Particulate Matter** <small>CNR</small>		A		E	
Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment** <small>CNR</small>		D	A	E	
Hydraulic Fracturing Impacts on Water, Soil & Air Quality** <small>CNR</small>		D	D		
Solutions to Metals Contamination of Water** <small>CNR</small>		P	D	E	
Dispersion of Nanoparticles & Its Implication for Interfacial, Biological & Environmental Processes		P	D		
Chemistry in the Marine Boundary Layer** <small>CNR</small>		P		E	
Sci-Mix		E			
Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment** <small>CNR</small>			D	E	
Environmental Implications of Nano: Release from Consumer Products & Advances in Nanometrology				AE	
Surface Physicochemical Processes in Engineered & Natural Systems** <small>CNR</small>				D	A
Microalgae: A Renewable Energy Source & a Sustainable Solution for the Environment** <small>CNR</small>				D	
Trace Materials in Air, Soil & Water** <small>CNR</small>				D	
Water Sustainability in Oil & Gas Exploration: Treatment Issues** <small>CNR</small>				DE	
Water Recycling in Domestic Use, Energy Extraction & Agricultural Use** <small>CNR</small>				E	A

Division of Environmental Chemistry (continued)

ENVR

S. Al-Abed, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment** <small>CNR</small>				E	A
Environmental Chemistry: Pedagogical Models & Practices** <small>CNR</small>				E	A
General Posters				E	
Undergraduate Research Posters* (CHED)		P			
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		
Elucidation of Mechanisms & Kinetics on Surfaces* (COLL)				D	

Division of Fluorine Chemistry

FLUO

V. Petrov, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
ACS Award for Creative Work in Fluorine Chemistry: Honoring Véronique Gouverneur**	D				
Sci-Mix		E			
ACS Award for Creative Research & Applications of Iodine Chemistry: Honoring Karl O. Christe**			D		

Division of Geochemistry

GEOC

S. Kerisit, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Coupled Cycling of Biogeochemical Critical Elements & Contaminants <small>CNR</small>	D	A			

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

PROGRAM SUMMARY

Division of Geochemistry (continued)

GEOC

S. Kerisit, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Understanding the Geochemical Interactions of Organic Compounds in the Subsurface** <small>CNR</small>	D				
Geochemistry & Reactive Transport in Nano-Pore Geomaterials** <small>CNR</small>		A			
2015 Geochemistry Division Medal Symposium		P			
Sci-Mix		E			
Iron Oxides: Formation, Structure, Reactivity & Applications** <small>CNR</small>			D	D	
Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces** <small>CNR</small>			D	D	
Honoring Donald Sparks, 2015 Geochemistry Medal Recipient			P	D	D
Precipitation, Dissolution & Adsorption under Confinement					D
WCC Rising Stars Awards Symposium* (WCC)		D			
Undergraduate Research Posters* (CHED)		P			

Division of Industrial & Engineering Chemistry

I & EC

P. Smith, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Uranium in Seawater** <small>CNR</small>	D	D			
ACS Award in Separations Science & Technology: Honoring Richard D. Noble	D				
Sci-Mix		E			
E.V. Murphree Award in Industrial & Engineering Chemistry: Honoring Joseph R. Zoeller**			D		
General Posters			E		
General Papers				D	
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
ACS Award in Industrial Chemistry: Honoring Thomas J. Colacot* (BMGT)		D			
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Division of History of Chemistry

HIST

S. Rasmussen, Program Chair

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
HIST Tutorial & General Papers	P				
Chemical Technology in Antiquity** <small>CNR</small>		D			
Sci-Mix		E			
Modern Chemical Warfare: History, Chemistry, Toxicology, Morality			D		
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
George C. Pimentel Award in Chemical Education: Honoring I. Dwaine Eubanks* (CHED)			D		

Division of Inorganic Chemistry

INOR

S. Koch, N. Radu, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
Environmental & Energy-Related Inorganic Chemistry <small>CNR</small>	A		E	P	
Organometallic Chemistry	AE		E	D	A
Chemistry of Materials	AE			P	D
Chemical Approaches to Spintronics Research	D	P	A		
ACS Award in Organometallic Chemistry: Honoring William J. Evans	D	P	A		
ACS Award in Inorganic Chemistry: Honoring John T. Groves	D	P			
Earth-Abundant Materials for Sustainable Hydrogen Production & Storage <small>CNR</small>	D		E		
Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Honoring Emily A. Weiss**	D				
Undergraduate Research at the Frontiers of Inorganic Chemistry	DE	P	D		
2015 Priestley Medalist: Honoring Jacqueline K. Barton	DE	P	D		

PROGRAM SUMMARY

Division of Inorganic Chemistry (continued)

I N O R

S. Koch, N. Radu, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
ACS Award in the Chemistry of Materials: Honoring Mark E. Thompson	P				
Division of Inorganic Chemistry Celebration of the Gabor A. Somorjai Award: Honoring Maurice Brookhart	P				
Lanthanide & Actinide Chemistry	PE			P	P
ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Honoring Kim R. Dunbar**	E	P	D	A	
Bioinorganic Chemistry	E	P	E		A
Coordination Chemistry	E		E	A	D
Nanoscience**	E		E	D	D
Inorganic Spectroscopy	E			P	
ACS National Awards in Inorganic Chemistry: Plenary Session	A				
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Honoring Jaqueline L. Kiplinger**	P	D			
Interactions of Metal Complexes with Proteins or Nucleic Acids		P	DE	A	
Division of Inorganic Chemistry Celebration of the Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Honoring Michael A. Marletta		P			
Sci-Mix		E			
Chemistry of the Energy Water Nexus: Focus on Fracking** <small>CNR</small>			D		P
Molecular Catalysts for Solar Fuels**			DE	A	
Soluble Inorganic Semiconductors: Synthesis, Properties & Applications			DE		
Solid-State Inorganic Chemistry			PE	A	
Inorganic Catalysts			PE	P	A
Electrochemistry			E	P	
Main Group Chemistry			E		A
Department, University & National Models for Faculty Development To Support Adoption of Evidence-Based Teaching* (CHED)	P				

Division of Inorganic Chemistry (continued)

I N O R

S. Koch, N. Radu, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
WCC Rising Stars Awards Symposium* (WCC)		D			
Undergraduate Research Posters* (CHED)		P			
ACS Award for Creative Research & Applications of Iodine Chemistry: Honoring Karl O. Christe* (FLUO)			D		

Division of Medicinal Chemistry

M E D I

W. Young, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Applications of Positron Emission Tomography in Drug Discovery	A				
Targeting the Microbiome	A				
General Oral Session	D			D	
Young Investigators in Medicinal Chemistry**	P				
Biased Agonism: An Emerging Paradigm in GPCR Drug Discovery	P				
General Poster Session	E			E	
Approaches To Targeting RNA with Small Molecules		A			
Innate Potential: Advances in Non-Biologic Modulation of Innate Immune Targets		A			
Recent Advances in Targeting the Nav1.7 Sodium Channels		A			
Honoring Richard Gibbs		P			
Modulators of the Nuclear Receptor RORc		P			
New Models for Drug Discovery: Public, Private & Non-Profit		P			
Sci-Mix		E			
E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Honoring Ruth R. Wexler**			A		

PROGRAM SUMMARY

Division of Medicinal Chemistry (continued)

MEDI

W. Young, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Observations from Recent Drug Launches: The Rules of Today May Not Apply Tomorrow			A		
Why You Should Have Paid Attention in P-Chem: Thermodynamics in Drug Discovery			A		
Smissman Award: Honoring Dennis Liotta			P		
The Role of Rings in Drug Design			P		
Advances in the Treatment of Fibrotic Diseases				A	
Small Molecule Approaches to Autism Spectrum Disorder Therapy				A	
First Time Disclosures				P	
MEDI Award Symposium				P	
Drug Discovery* (COMP)	D	D	D	D	
Medicinal & Aromatic Crops: Production, Phytochemistry & Utilization* (AGFD)		D			
Undergraduate Research Posters* (CHED)		P			
Phenolic & Polyphenolic Chemistry in Food Processing* (AGFD)			D		
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Division of Nuclear Chemistry & Technology

NUCL

J. Braley, D. Hobart, Program Chairs

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Glenn T. Seaborg Award for Nuclear Chemistry: Honoring Heino Nitsche	D	D			
Nuclear Forensics	P	D			
50th Anniversary of the NUCL Division			D	D	
Convergence of Theory & Experiment in Heavy Element Chemistry				D	A
Uranium in Seawater* (I&EC)	D	D			
Chemical Tales of Success: Helpful Tips for Younger Chemists* (YCC)			A		

Division of Organic Chemistry

ORGN

M. McIntosh, R. Broene, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
Materials, Devices & Switches	A				
New Reactions & Methodology	D	D	A	A	
Asymmetric Reactions & Syntheses	D				
Nanomaterials	P				
Development of Direct C-H Functionalization Processes towards the Synthesis of Biologically Active Compounds	P				
Ronald Breslow Award for Achievement in Biomimetic Chemistry: Honoring Eric T. Kool	P				
Asymmetric Reactions & Syntheses; Chemistry of Fullerenes, Carbon Nanotubes & Graphene; Materials, Devices & Switches; Nanomaterials; Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species; Total Synthesis of Complex Molecules	E				
Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Honoring Jin-Quan Yu		A			
Miniaturization in Chemistry: Sub-Nanoscale Synthesis, Analysis & Application		A			
Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species		D	A		
Molecular Recognition & Self-Assembly		D			
Synthetic Biology Applied to Natural & Unnatural Product Pathways		P			
Herbert C. Brown Award for Creative Research in Synthetic Methods: Honoring Gary A. Molander		P			
Sci-Mix		E			
ACS Award for Creative Invention: Honoring Jotham W. Coe			A		
ACS Award for Creative Work in Synthetic Organic Chemistry: Honoring F. Dean Toste			A		
Biologically-Related Molecules & Processes			D		

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM

E = EVE DE = AM/PM/EVE PE = PM/EVE

PROGRAM SUMMARY

**Division of Organic Chemistry
(continued)**

ORGN

M. McIntosh, R. Broene, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
Metal-Mediated Reactions & Syntheses			P	D	
Green Chemistry: Reactions in Alternative Media			P		
James Flack Norris Award in Physical Organic Chemistry: Honoring Charles L. Perrin			P		
Ernest Guenther Award in the Chemistry of Natural Products: Honoring Thomas R. Hoye			P		
Biologically Related Molecules & Processes; Chemistry of Natural Resources; Metal-Mediated Reactions & Syntheses; Molecular Recognition & Self-Assembly; Peptides, Proteins & Amino Acids <i>CNR</i>			E		
National Fresenius Award: Honoring Abigail G. Doyle**				A	
Total Synthesis of Complex Molecules				A	
Heterocycles & Aromatics				D	
ACS Award for Creative Invention: Honoring Jotham W. Coe				P	
Peptides, Proteins & Amino Acids				P	
Heterocycles & Aromatics; New Reactions & Methodology				E	
Department, University & National Models for Faculty Development To Support Adoption of Evidence-Based Teaching* (CHED)	P				
WCC Rising Stars Awards Symposium* (WCC)		D			
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Division of Physical Chemistry

PHYS

E. Sibert, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Atmospheric Chemistry: Transformations of Matter in the Troposphere	D	D	P	D	A
Modeling Excited States of Complex Systems**	D	D	P	D	A
Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease**	D	D	P		
Computational Chemical Dynamics: Advancing Our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems**	D	D		D	A
Modeling Complex Biomolecules: From Structure to Dynamics & Function**	D	D		D	A
Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution	D	D		D	A
Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron & Single Photon Level	D	D		D	A
Design of Materials & Chemical Processes: The Genomic Approach	D	D		D	
Sci-Mix		E			
PHYS Award Symposium			A		
Physical Electrochemistry of Electrocatalytic Processes			P	D	A
Ahmed Zewail Prize in Molecular Sciences			P		
Physical Chemistry Poster Session				E	
Molecular Mechanics* (COMP)	D	A		A	
Computational Design, Discovery & Optimization of Organic Semiconductor Materials* (COMP)	D	A			
Electronic Structure Methods for Highly Polarizable Systems* (COMP)	D	D			
Quantum Chemistry* (COMP)	P	P	P	D	
WCC Rising Stars Awards Symposium* (WCC)		D			
ACS Award for Computers in Chemical & Pharmaceutical Research: Honoring David A. Case* (COMP)		P	D		
Computational Chemistry in the Undergraduate Curriculum: What Is Working & How Do We Assess It?* (CHED)				D	

PROGRAM SUMMARY

Division of Polymer Chemistry

POLY

M. Jeffries-El, D. Boday, T. White, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Putting Renewable Polymers To Work	D	A	E		
Macromolecular & Nanoparticle Separation Science**	D	D	DE		
Next Generation Smart Materials**	D	D	E	D	D
General Topics: New Synthesis & Characterization of Polymers	D		AE	E	
Celebrating the Fifth Year Anniversary of Polymer Chemistry (RSC)	D				
Electrical, Thermal & Mass Transport in Polymer Nanocomposites & Alloys**		D	E		
Excellence in Graduate Polymer Research**		D	E		
Innovations in Macromolecular Network Chemistry**		P	E	P	D
Sci-Mix		E			
Carl S. Marvel Creative Polymer Chemistry Award in Honor of Todd Emrick			D		
Energy & Materials**			DE	D	D
Undergraduate Research in Polymer Science**			DE		
Polymer Composites & High Performance Materials			PE	D	D
Interacting with the Immune System Using Polymeric Systems			E	D	D
POLY/PMSE Plenary Lecture & Awards Reception**				E	
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Integrating Chemistry & Polymer Science Research into the Classroom* (CHED)		A			
Undergraduate Research Posters* (CHED)		P			
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum* (CHED)		E			
Joint PMSE/POLY Poster Session* (PMSE)			E		

Division of Polymeric Materials: Science & Engineering

PMSE

A. Tsou, Q. Lin, C. Stafford, M. Becker, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Design Principles of Functional Macromolecular Materials	D	D	A		
Stimulus-Responsive Assemblies & Materials	D	D	D		
Advances in X-ray & Neutron Scattering Techniques for Elucidating Polymer Morphology	D	D	D		
Graphene & Carbon Nanotubes: Synthesis, Devices & Applications	D	D			
Nanostructured Porous Polymers: Synthesis, Properties & Applications	D	D			
ACS Award in Applied Polymer Science: Honoring Geoffrey W. Coates	D				
General Papers/New Concepts in Polymeric Materials	P	D		D	A
Cooperative Research Award: Honoring Andy Tsou & Benjamin Hsiao		A			
Polymeric Biomaterials**		P	D	D	A
Sci-Mix		E			
Nanoscale Spectroscopic & Microscopic Characterization			D	D	
Polymer Modeling: Structure, Dynamics & Function			D	D	
ACS Award in Polymer Chemistry: Honoring Nikos Hadjichristidis			D	D	
Drug Delivery & Drug Device Combination Products			P	D	A
Joint PMSE/POLY Poster Session**			E		
Macromolecular & Nanoparticle Separation Science* (POLY)	D	D	DE		
Next Generation Smart Materials* (POLY)	D	D	E	D	D
Integrating Chemistry & Polymer Science Research into the Classroom* (CHED)		A			
WCC Rising Stars Awards Symposium* (WCC)		D			
Innovations in Macromolecular Network Chemistry* (POLY)		P	E	P	D

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

PROGRAM SUMMARY

Division of Polymeric Materials: Science & Engineering (continued)

PMSE

A. Tsou, Q. Lin, C. Stafford, M. Becker, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Undergraduate Research Posters* (CHED)		P			
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum* (CHED)		E			
Smart & Responsive Composites from Renewable Building Blocks* (CELL)			A	D	
Energy & Materials* (POLY)			DE	D	D
POLY/PMSE Plenary Lecture & Awards Reception* (POLY)				E	

Division of Professional Relations (continued)

PROF

R. D. Libby, Program Chair

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Terry L. Brewer* (SCHB)		A			
Excellence in Graduate Polymer Research* (POLY)			D	E	
WCC Rising Stars Awards Symposium* (WCC)			D		

Division of Professional Relations

PROF

R. D. Libby, Program Chair

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Native American Women Chemists of Color**	A				
Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations**	P				
ACS Award for Encouraging Women into Careers in the Chemical Sciences: Honoring E. Ann Nalley**		A	A		
Chemical Angel Network: Chemists Investing in Chemical Companies**		P			
Proposing & Administering a Successful REU Program			P		
Hands-On STEM Enrichment Programs for Persons with Disabilities				P	
Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Best Practices for Success with SBIR & STTR Grants* (SCHB)	P				
Starting a Successful Research Program at a Predominantly Undergraduate Institution* (YCC)	P				
Diversifying STEM: Uniting through our Differences for a Brighter Scientific Future* (CMA)		A			

Rubber Division

RUBB

T. R. DeLapa, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum* (CHED)		E			

Division of Small Chemical Businesses

SCHB

J. Sabol, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Best Practices for Success with SBIR & STTR Grants**	P				
Entrepreneurs' Poster Session**	P				
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Terry L. Brewer**		A			
Water Is the Next Oil: Small Businesses Percolating to the Top** <small>CNR</small>		P			
Sci-Mix		E			
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

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 (continued)

SCHB

J. Sabol, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations* (PROF)	P				
Chemical Angel Network: Chemists Investing in Chemical Companies* (PROF)		P			
Chemical Tales of Success: Helpful Tips for Younger Chemists* (YCC)			A		

Committee on Chemical Safety

CCS

E. Howson, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Legalized Marijuana & Health & Safety* (CHAS)		P			
Safety in Undergraduate Teaching* (CHAS)			P		
Ask Dr. Safety: EH&S Support of Nanotechnology R&D* (CHAS)			A		

Committee on Chemistry & Public Affairs

CCPA

S. Butts, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community* (PRES)			A		

Committee on Corporation Associates

CORP

D. Mason, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

Committee on Divisional Activities

DAC

M. J. Morello, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Frontiers in Glycoscience* (CELL)		D	D		

Committee on Environmental Improvement

CEI

C. Middlecamp, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Green Chemistry & the Environment* (ENVR)	D	A		E	
Uranium in Seawater* (I&EC)	D	D			
Assessing Toxicity of Environmental Contaminants* (ENVR)	D			E	
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community* (PRES)			A		
ACS-CEI Award for Incorporating Sustainability into Chemistry Education* (CHED)			A		
Citizens First: Communicating Climate Science to the Public* (CHED)			A		
Green Chemistry: Theory & Practice* (CHED)				D	
Water Sustainability in Oil & Gas Exploration: Treatment Issues* (ENVR)				DE	

Committee on Minority Affairs

CMA

J. Sarquis, Program Chair

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Diversifying STEM: Uniting through Our Differences for a Brighter Scientific Future**		A			
Native American Women Chemists of Color* (PROF)	A				
ACS Award for Encouraging Disadvantaged Students in Chemistry: Honoring Catherine H. Middlecamp* (CHED)		P			

PROGRAM SUMMARY

Committee on Science

COMSCI

D. Crans, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Transitioning between Academic Research into Practical Use: Solar Energy & Advanced Materials**		A			
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders* (PRES)	A				
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

International Activities Committee

I A C

H.N. Cheng, Program Chair

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences**	D				
The Interface of Chemical & Biological Sciences International Disarmament Efforts**			D		
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders* (PRES)	A				
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

Senior Chemists Committee

S C C

G. Heinze, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum* (CHED)		E			

Society Committee on Education

SOCED

D. Swartling, Program Chair

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Forensic Toxicology of Marijuana** <small>CNR</small>		A			
Biomass to Fuel & Products** <small>CNR</small>		A			
Sustainability in the 21st Century: Optimizing Complex Interdependent Systems** <small>CNR</small>		P			
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders* (PRES)	A				
Undergraduate Research Papers* (CHED)	D	D			
High School Program* (CHED)	D				
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Excellence in Graduate Polymer Research* (POLY)		D	E		
Undergraduate Research Posters* (CHED)		P			

Women Chemists Committee

W C C

K. Woznack, A. Debaillie, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
WCC Rising Stars Awards Symposium**		D			
Native American Women Chemists of Color* (PROF)	A				
Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Honoring Emily A. Weiss* (INOR)	D				
ACS Award for Creative Work in Fluorine Chemistry: Honoring Véronique Gouverneur* (FLUO)	D				
ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Honoring Kim R. Dunbar* (INOR)	E	P	D	A	

PROGRAM SUMMARY

Women Chemists Committee (continued)

W C C

K. Woznick, A. Debaille, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
ACS Award for Encouraging Women into Careers in the Chemical Sciences: Honoring E. Ann Nalley* (PROF)		A	A		
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Honoring Vickie M. Williamson* (CHED)		D			
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Honoring Jaqueline L. Kiplinger* (INOR)		P	D		
ACS Award for Encouraging Disadvantaged Students in Chemistry: Honoring Catherine H. Middlecamp* (CHED)		P			
E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Honoring Ruth R. Wexler* (MEDI)			A		
National Fresenius Award: Honoring Abigail G. Doyle* (ORGN)				A	
Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Honoring Hilka I. Kenttämaa* (ANYL)				P	

Younger Chemists Committee (continued)

Y C C

T. Matos, A. Gavrilenko, Program Chairs

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Terry L. Brewer* (SCHB)		A			
Excellence in Graduate Polymer Research* (POLY)		D	E		
Water Is the Next Oil: Small Businesses Percolating to the Top* (SCHB)		P			
Environmental Chemistry: Pedagogical Models & Practices* (ENVR)				E	A

Younger Chemists Committee

Y C C

T. Matos, A. Gavrilenko, Program Chairs

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Starting a Successful Research Program at a Predominantly Undergraduate Institution**	P				
Chemical Tales of Success: Helpful Tips for Younger Chemists**			A		
Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Young Investigators in Medicinal Chemistry* (MEDI)	P				
Best Practices for Success with SBIR & STTR Grants* (SCHB)	P				
Entrepreneurs' Postor Session* (SCHB)	P				

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

TECHNICAL PROGRAM

How to Read the Technical Program

1. Search for the Division—listed in alphabetical order

3. Locate the session name

4. Locate the time or poster #

CHAS

Division of Chemical Health and Safety

D.M. Decker, F. K. Wood-Black and
J. M. Pickel, Program Chairs

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Silverton Ballroom 1

Legalized Marijuana & Health & Safety

Cosponsored by CCS

N. R. Langerman, R. W. Phifer, Organizers, Presiding

1:30 Introductory Remarks.

1:40 CHAS 1. Taking care of Mary Jane's workers. J. Lieberman

2:10 CHAS 2. Safety considerations in the development of sensible workplace drug testing

Note:

Times represent the start of oral presentations and numbers represent poster numbers.

2. Locate the day

5. Locate the venue and room for each session



Amy (Vocals)



ACS Members are
ROCKSTARS of **CHEMISTRY**

ACS members who joined in the last 12 months are invited to attend our ROCKSTARS RECEPTION.

ACS looks forward to welcoming you to this very special event, Monday, March 23, from 3:00 p.m. to 4:00 p.m. in the Colorado Convention Center Room 601. New members will network with other Rockstars of Chemistry, such as award winners, published authors, and notable scientists. Light refreshments will be served. Guests will receive reserved seating for the Kavli Lecture Series.

Not a member yet?

Join today for your ticket to the Rockstars Reception. Go to www.acs.org/ROCKSTAR

Been a member for years?

Stop by the ACS Booth and take a commemorative ACS Rockstars photo at the open air photo booth!

Learn about your benefits at the *Membership Rocks* presentation in the ACS Theater on Monday at 10:30 a.m. and 11 a.m. or Tuesday at 11 a.m. and 11:30 a.m.

American Chemical Society

CHEMISTRY OF NATURAL RESOURCES

Denver, CO • March 22-26, 2015

WWW.ACS.ORG/DENVER2015

Where to Find Meeting Information

Official Meeting Website
www.acs.org/denver2015

Announcements & Changes
www.acs.org/meetingupdates

Digital Meeting Program
www.acs.org/denver2015



follow us @acsnatlmtg
tweet using #acsdenver



[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

Text your question to
754.227.2012 *(Standard text rates apply)*



ACS
Chemistry for Life®

PRES

Presidential Events

D. G. Schmidt, Program Chair

SUNDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 3A**The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders****Building a Global Technical Workforce**

Cosponsored by BMGT, COMSCI, IAC and SOCED

J. L. Benham, S. Hill, B. Miller, Organizers, Presiding

8:00 Introductory Remarks.

8:05 PRES 1. Global landscape: Chemistry-related transnational mobility and global talent innovation. J.L. Benham

8:30 PRES 2. Building a global technical workforce. T. Connelly

9:00 PRES 3. Science in diplomacy and global relations: "Good guys only win if they work together". D. Hupaylo

Section A

Colorado Convention Center
Mile High Ballroom 3A**The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders****Attracting and Preparing Chemists for the Global Chemical Enterprise**

Cosponsored by BMGT, COMSCI, IAC and SOCED

J. L. Benham, S. Hill, B. Miller, Organizers, Presiding

10:00 PRES 4. School of pharmaceutical science and technology of Tianjin University: A demo project as an international center of excellence in Chin. J.S. Siegel

10:30 PRES 5. From international/multinational ventures to transnational/global chemistry: Lowering activation barriers across national borders. L. Echegoyen

11:00 PRES 6. Chemistry in a global economy: Can our curriculum meet the challenge? J.S. Francisco

11:30 PRES 7. Connecting the dots: Interdisciplinary relationships case study in 21st century global workforce. A. Phillips Diaz

12:00 Concluding Remarks.

Basic Research in Colloids, Surfactants & Nanomaterials Metal Nanomaterials

Sponsored by COLL, Cosponsored by PRES

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Sponsored by COLL, Cosponsored by PRES

Particles at Fluid Interfaces

Sponsored by COLL, Cosponsored by PRES

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 3A**Nanotechnology: Delivering on the Promise Research & Development**

Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

D. G. Schmidt, Organizer

L. J. Doemeny, C. Geraci, Organizers, Presiding

1:30 Introductory Remarks.

1:35 PRES 8. Nanotechnology: Delivering the promise — R&D. C.A. Mirkin

2:05 PRES 9. NSF: Building foundational knowledge and infrastructure for nanotechnology. M. Roco

2:35 PRES 10. National Institutes of Health: The impact of nanotechnology in biology and medicine. L. Henderson

3:05 Intermission.

3:15 PRES 11. Nanoscience and technology for energy. H. Kung

3:45 PRES 12. Nanomaterials and nanomanufacturing with an emphasis on national security. L. Slotter

4:15 Keynote Address. L. Whitman

5:00 Discussion.

Basic Research in Colloids, Surfactants & Nanomaterials

Sponsored by COLL, Cosponsored by PRES

Department, University, and National Models for Faculty Development to Support Adoption of Evidence-Based Teaching

Sponsored by CHED, Cosponsored by INOR, ORGN and PRES

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Sponsored by COLL, Cosponsored by PRES

Particles at Fluid Interfaces

Sponsored by COLL, Cosponsored by PRES

SUNDAY EVENING

Fundamental Research in Colloids, Surfaces & Nanomaterials

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Sponsored by COLL, Cosponsored by PRES

Nanoscience

Sponsored by INOR, Cosponsored by PRES

MONDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 3A**Nanotechnology: Delivering on the Promise Opportunities and Challenges for Health, Safety and the Environment**

Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

D. G. Schmidt, Organizer

L. J. Doemeny, C. Geraci, Organizers, Presiding

8:30 Introductory Remarks.

8:35 PRES 13. Innovation trends, policies, and practices. T. Earles

9:05 PRES 14. The regulatory void. L. Bergeson

9:35 PRES 15. Adaptive governance.

V. Murashov

10:05 Intermission.

10:20 PRES 16. Sustainability and life cycle issues. J.T. Morris

10:50 PRES 17. What is responsible development of nanotechnology? A. Lin

11:20 Discussion.

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys Barrier and Separation Behavior

Sponsored by POLY, Cosponsored by PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion Sensing, Electronics, & Photophysics

Sponsored by COLL, Cosponsored by PRES

Particles at Fluid Interfaces

Sponsored by COLL, Cosponsored by PRES

Plasmonic Catalysis and Sensing

Sponsored by COLL, Cosponsored by PRES

Transitioning between Academic Research into Practical Use: Solar-Energy and Advanced Materials

Sponsored by COMSCI, Cosponsored by MPPG† and PRES

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 3A**Nanotechnology: Delivering on the Promise Bridging the Gap to a Thriving US Marketplace**

Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

D. G. Schmidt, Organizer

L. J. Doemeny, C. Geraci, Organizers, Presiding

1:30 Introductory Remarks.

1:35 PRES 18. Nanomaterials in the marketplace. M. Philbert

2:00 PRES 19. University tech transfer issues. M. Liehr

2:30 PRES 20. Nanotech market forecasting. B. Giles

3:00 Intermission.

3:15 PRES 21. Regulation: Facilitating advancement or serving as a barrier — a shared responsibility. T.L. Medley

3:45 PRES 22. Nanomanufacturing, nanomarkets, and applications. A. Malshe

4:15 Discussion.

Advances in Formulations Science & Technology

Sponsored by COLL, Cosponsored by PRES

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys Energy, Electrical and Thermal

Sponsored by POLY, Cosponsored by PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion Spectroelectrochemistry, Imaging, & Surface

Sponsored by COLL, Cosponsored by PRES

Plasmonic Catalysis and Sensing

Sponsored by COLL, Cosponsored by PRES

TUESDAY MORNING

Section A

Colorado Convention Center
Room 506**DOE Nanoscience Research Centers National Resources for the Nanoscience Community**

Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG

M. V. Buchanan, Organizer

G. Maracas, Organizer, Presiding

8:30 Introductory Remarks.

8:40 PRES 23. User opportunities at the Center for Nanophase Materials Sciences: From materials-by-design to neutron nanoscience. H.M. Christen

9:10 PRES 24. Molecular foundry: A knowledge-based user facility for nanoscale science. J. Neaton

9:40 PRES 25. Hybrid nanomaterials and tailoring nanoscale interactions at the Center for Nanoscale Materials. A. Roelofs

10:10 Intermission.

10:30 PRES 26. Nanomaterials integration: A pathway to technological innovation. N.D. Shinn, Q. Jia

11:00 PRES 27. Center for Functional Nanomaterials and its unique capabilities for research on nanomaterials by design and *in operando*. E. Mendez

11:30 Concluding Remarks.

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

Sponsored by CHAS, Cosponsored by AGFD, CCS and PRES

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion**Biosensing, Energy Conversion & Catalysts**

Sponsored by COLL, Cosponsored by PRES

Nanoscience and Nanotechnology of Natural Resources

Sponsored by MPPG, Cosponsored by PRES

Plasmonic Catalysis and Sensing

Sponsored by COLL, Cosponsored by PRES

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

TUESDAY AFTERNOON

Applied Nanotechnology for Food & Agriculture

Sponsored by AGFD, Cosponsored by PRES

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

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.

† Cooperative Cosponsorship

TUESDAY EVENING**Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys**

Sponsored by POLY, Cosponsored by PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY MORNING**Applied Nanotechnology for Food & Agriculture**

Sponsored by AGFD, Cosponsored by PRES

Basic Research in Colloids, Surfactants & Nanomaterials Amphiphilic Systems

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion**Biosensing, Catalysts, & Electrochemistry**

Sponsored by COLL, Cosponsored by PRES

Nanoscience

Sponsored by INOR, Cosponsored by PRES

Plasmonic Catalysis and Sensing

Sponsored by COLL, Cosponsored by PRES

WEDNESDAY AFTERNOON**Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion****Fabrication for Biosensing, Energy Conversion & Catalysts**

Sponsored by COLL, Cosponsored by PRES

Nanoscience**Metals**

Sponsored by INOR, Cosponsored by PRES

Plasmonic Catalysis and Sensing

Sponsored by COLL, Cosponsored by PRES

THURSDAY MORNING**Basic Research in Colloids, Surfactants & Nanomaterials**

Sponsored by COLL, Cosponsored by PRES

Nanoscience

Sponsored by INOR, Cosponsored by PRES

THURSDAY AFTERNOON**Basic Research in Colloids, Surfactants & Nanomaterials**

Sponsored by COLL, Cosponsored by PRES

Nanoscience Semiconductors

Sponsored by INOR, Cosponsored by PRES

MPPG**Multidisciplinary Program Planning Group**

R. Weber, Program Chair

SUNDAY MORNING**Assessing Toxicity of Environmental Contaminants**

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs

Sponsored by ENVR, Cosponsored by MPPG‡

Catalysis for Un-conventional Energy Sources**Fuel Cell, Solar Cell and Solar Fuel**

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage

Sponsored by INOR, Cosponsored by MPPG‡

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by CEI and MPPG‡

Nanomaterials for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by MPPG‡

Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)

Sponsored by ENFL, Cosponsored by MPPG‡

Understanding the Geochemical Interactions of Organic Compounds in the Subsurface

Sponsored by GEOC, Cosponsored by MPPG‡

Uranium in Seawater The Chemistry

Sponsored by I&EC, Cosponsored by CEI, MPPG‡, and NUCL

SUNDAY AFTERNOON**Section A**

Colorado Convention Center

Belco Theatre

Chemistry of Natural Resources Plenary

R. S. Weber, Organizer, Presiding

3:00 Introductory Remarks.

3:05 MPPG 1. Fundamentals of gas hydrates and their role in energy transportation and storage. C.A. Koh

3:45 MPPG 2. Four horsemen of the advanced biofuels apocalypse: Sustainability, technology, profitability, and politics. P.F. Bryan

4:25 MPPG 3. Water in the Anthropocene: too much, too little, too dirty. P. Kareiva

5:05 Discussion.

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs

Sponsored by ENVR, Cosponsored by MPPG‡

Catalysis for Un-conventional Energy Sources**Biofuel and CO₂ Utilization**

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage

Sponsored by INOR, Cosponsored by MPPG‡

Environmental Reactivity of Organic**Micropollutants and Their Transformation Products in Receiving Waters**

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by CEI and MPPG‡

Nanomaterials for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by MPPG‡

Nanotechnology: Delivering on the Promise Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)

Sponsored by ENFL, Cosponsored by MPPG‡

Understanding the Geochemical Interactions of Organic Compounds in the Subsurface

Sponsored by GEOC, Cosponsored by MPPG‡

Uranium in Seawater**The Sorbents**

Sponsored by I&EC, Cosponsored by CEI, MPPG‡, and NUCL

MONDAY MORNING**Biomass to Fuel and Products**

Sponsored by SOCED, Cosponsored by CELL, ENFL and MPPG‡

Catalysis for Un-conventional Energy Sources**Novel Catalysts**

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Chemical Technology in Antiquity

Sponsored by HIST, Cosponsored by MPPG‡

Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR and Novel Approaches

Sponsored by ENFL, Cosponsored by MPPG‡

Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter

Sponsored by ENVR, Cosponsored by MPPG‡

Geochemistry and Reactive Transport in Nano-Pore Geomaterials

Sponsored by GEOC, Cosponsored by MPPG‡

Hydraulic Fracturing Impacts on Water, Soil and Air Quality**Groundwater Impacts**

Sponsored by ENVR, Cosponsored by MPPG‡

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

Sponsored by ENVR, Cosponsored by ANYL and MPPG‡

Use of Mass Spectrometry and Other Methods to Characterize NOM in Diverse Environments

Sponsored by ENVR, Cosponsored by ANYL and MPPG‡

Nanomaterials for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by MPPG‡

Nanotechnology: Delivering on the Promise Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Transitioning between Academic Research into Practical Use: Solar-Energy and Advanced Materials

Sponsored by COMSCI, Cosponsored by MPPG‡ and PRES

Uranium in Seawater**Sorbents and Analysis**

Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

MONDAY AFTERNOON**Section A**

Colorado Convention Center

Belco Theatre

The Kavii Foundation Emerging Leader in Chemistry Lecture

R. S. Weber, Organizer, Presiding

4:00 Introductory Remarks.

4:05 MPPG 4. Radical frontiers in catalysis.

T. Betley

Section A

Colorado Convention Center

Belco Theatre

The Fred Kavii Innovations in Chemistry Lecture

R. S. Weber, Organizer, Presiding

5:30 Introductory Remarks.

5:35 MPPG 5. Us vs. them: Distinguishing humans from microbes with carbohydrate. L.L. Kiessling

Chemical Technology in Antiquity

Sponsored by HIST, Cosponsored by MPPG‡

Chemistry in the Marine Boundary Layer

Sponsored by ENVR, Cosponsored by MPPG‡

Hydraulic Fracturing Impacts on Water, Soil and Air Quality**Surface Water Impacts/Fluid Chemistry**

Sponsored by ENVR, Cosponsored by MPPG‡

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment**Extraction Techniques to Isolate NOM and Characterization of Pyrogenic Organic Matter (Biomass Burning)**

Sponsored by ENVR, Cosponsored by ANYL and MPPG‡

Nanomaterials for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by MPPG‡

Nanotechnology: Delivering on the Promise Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Solutions to Metals Contamination of Water

Sponsored by ENVR, Cosponsored by MPPG‡

Uranium in Seawater**Analysis and Toxicity/Cost**

Sponsored by I&EC, Cosponsored by CEI, MPPG‡, and NUCL

TUESDAY MORNING**Section A**

Colorado Convention Center

Mile High Ballroom 3A

Nanoscience and Nanotechnology of Natural Resources

Cosponsored by PRES

P. Alivisatos, P. S. Weiss, Organizers, Presiding

9:00 Introductory Remarks.

9:05 MPPG 6. Your anion is my plasmonic nanostructure: Discovering molecular plasmonics. N.J. Halas

9:35 MPPG 7. Silicon nanostructures for new energy applications. S. Lee

10:05 MPPG 8. Design of colloidal heterostructures for photocatalytic hydrogen generation. A. Rogach

10:35 MPPG 9. Dimensionality matters: Dimensionality effects on optoelectronic behavior of semiconductor nanocrystals. U. Banin

11:05 MPPG 10. Nanomaterials design for programmed multi- and staged release. P.T. Hammond

11:35 Concluding Remarks.

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Sponsored by ENVR, Cosponsored by AGRO, ANYL and MPPG‡

C1 Chemistry**Methane Activation**

Sponsored by ENFL, Cosponsored by MPPG‡

DOE Nanoscience Research Centers National Resources for the Nanoscience Community

Sponsored by PRES, Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG‡

Iron Oxides: Formation, Structure, Reactivity and Applications**Formation and Transformation**

Sponsored by GEOC, Cosponsored by MPPG‡

Hydraulic Fracturing Impacts on Water, Soil and Air Quality**Air & Water Quality**

Sponsored by ENVR, Cosponsored by MPPG‡

Nanotechnology: Delivering on the Promise**Research & Development**

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING**Section A**

Colorado Convention Center
Room 113

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Cosponsored by AGRO and MEDI

C. L. Cantrell, V. Jeliakov, Organizers, Presiding

8:30 Introductory Remarks.

8:35 AGFD 20. Production of essential oils for the personal care industry: Quality and regulatory issues. **B. Schmidt**

9:00 AGFD 21. Green extraction of natural products: From innovations to industrial applications. **F. Chemat**

9:25 AGFD 22. Dual utilization of medicinal and aromatic crops: For plant chemicals and biofuels. **V. Jeliakov, C.L. Cantrell, N. Stewart, B. Joyce, E. Jeliakov**

9:50 AGFD 23. Selected aspects of environmental protection in the processing of coal-monitoring and revitalization in relation to the isolation, identification and utilization of isolated organic compounds. **I. Salamon, J. Sandor, J. Mitra**

10:15 Intermission.

10:30 AGFD 24. Breeding of German chamomile, *Matricaria recutita* L., with the high content of *l*- α -bisabolol. **I. Salamon, S. Mudroncekova, J. Fejer**

10:55 AGFD 25. Biosynthesis of amphetamine-like alkaloids in *Catha edulis* and *Ephedra* spp., two distantly related taxa. **E. Lewinsohn, J. Hagel, R. Krizevski, E. Bar, R.A. Groves, A. Levy, K. Kilpatrick, Y. Zhang, N. Dudai, C.W. Sensen, S. Ben Shabat, S. Yaron, M. Frederic, P.J. Facchini**

11:20 AGFD 26. Saline water management strategy on growth and tuber yield of *Helianthus tuberosus* (L.) cv. Stampede. **J.F. Ferreira, N. Dias, X. Liu, D. Suarez**

Section B

Colorado Convention Center
Room 112

Agricultural & Food Chemistry General Papers**Health and Nutrition in Food Chemistry**

K. Deibler, Organizer, Presiding

8:00 AGFD 27. Innovative tactic toward rapid isolation of unique bioactive sphingoids from dietary natural resources. **S. B., K. Monde**

8:20 AGFD 28. Common juniper (*Juniperus communis* L.) and its qualitative and quantitative characteristics of essential oil in Albania. **I. Salamon, A. Ibralui, S. Mudroncekova, J. Fejer**

8:40 AGFD 29. Treatment with soluble phenolic antioxidants significantly improves antioxidant capacity of insoluble wheat bran. **E. Doğan, V. Gökmen**

9:00 Intermission.

9:15 AGFD 30. Study of the synergy between soluble and dietary fiber bound antioxidants. **E.E. Çelik, V. Gökmen, L. Skibsted**

9:35 AGFD 31. Carotenoid content and composition in winter squash, (*Cucurbita maxima* Duch.) and (*Cucurbita moschata* Duch.): Variability associated with different cultivars, harvest dates, and storage times. **J. Noseworthy**

9:55 AGFD 32. Effect of xanthan/enzymatically modified guar gum mixtures on the stability of oil-in-water emulsions. **P. Chityala, H. Khouryieh, K. Williams**

10:15 Intermission.

10:30 AGFD 33. Rice (*Oryza sativa* L.) resistant starch and novel processing methods to increase resistant starch concentration. **S.A. James, T. Pushparaj, D. Thavarajah, S. Premakumara, K. Abeysekara, S. Sotheeswaran**

10:50 AGFD 34. Fractionation and characterization of glabrous canary seed components for food and non-food applications. **E.M. Abdelal, P. Hucl, C. Patterson**

11:10 AGFD 35. Induced resistance in ash (*Fraxinus* spp.) against emerald ash borer: A proteomic investigation. **S. Chakraborty, S. Opiyo, A. Hill, D. Cipollini, D.A. Herms, P. Bonello**

Nanotechnology: Delivering on the Promise Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON**Section A**

Colorado Convention Center
Room 113

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Cosponsored by AGRO and MEDI

C. L. Cantrell, V. Jeliakov, Organizers, Presiding

1:00 Introductory Remarks.

1:05 AGFD 36. Chemical composition and antimicrobial activity of crude extract preparations from the medicinal plant *Vexibia alopecuroides* (L.) Jakovl. **T. Kustova, T. Karpenyuk, M. Jacob, C.L. Cantrell, S. Ross**

1:30 AGFD 37. β -Triketones from *Leptospermum scoparium* as natural herbicides Inhibiting *p*-hydroxyphenylpyruvate dioxygenase. **F. Dayan, D. Owens, D. Nanayakkara**

1:55 AGFD 38. Cilantro essential oil and its major constituents as a source of new drugs against Leishmaniasis. **M.A. Donega, S. Mello, R.M. Moraes, S.K. Jain, B.L. Tekwani, C.L. Cantrell**

2:20 AGFD 39. Essential oils in prevention and treatment of human opportunistic fungal diseases. **T. Markovic, V. Jeliakov**

2:45 Intermission.

3:00 AGFD 40. Effects of plant-derived bioactive compounds on rumen fermentation, nutrient utilization, immune response, and productivity of ruminant animals. **A.N. Hristov, J. Oh**

3:25 AGFD 41. Hairy roots and human health: Production and discovery of bioactive compounds. **F. Medina-Bolivar, T. Yang, L. Fang, K. Mockaitis, N. Joshee**

3:50 AGFD 42. Bioactive constituents isolated from essential oils from plants in *Asteraceae* and *Apiaceae* families. **K.M. Meepagala**

4:15 AGFD 43. Recent research and development of *Antrrodia cinnamomea*: An endemic medicinal mushroom of Taiwan. **S. K. J, S. Wang**

4:40 Concluding Remarks.**Section B**

Colorado Convention Center
Room 112

Agricultural & Food Chemistry General Papers

K. D. Deibler, Organizer, Presiding

1:00 AGFD 44. Bacteriophage-based scheme to enable rapid MALDI-TOF screening of samples for bacterial contaminants. **S.D. Alcaine, L. Tilton, Z. Wang, S.R. Nugen**

1:20 AGFD 45. Quantification of plant sterols and plant stanols in phytoosterol-enriched foods and dietary supplements. **C.T. Srigley, E. Haile**

1:40 AGFD 46. Phytochemical composition and in vitro antimicrobial activity of selected essential oils on foodborne pathogens. **R. Tardugno, F. Pellati, A. Serio, A. Paparella, S. Benvenuti**

2:00 Intermission.

2:15 AGFD 47. Determination of quantitative sodium mass transfer coefficient during osmotic processing of potatoes. **A. Kinchla, T. Hinkley**

2:35 AGFD 48. Feline bitter receptors TAS2R38 and TAS2R43 have response profiles distinct from the human homologues. **J. Rucker, M. Sandau, J. Goodman, A. Thomas, N. Rawson**

2:55 AGFD 49. Physics and chemistry of brewing better coffee. **C.H. Hendon, L. Colonna-Dashwood, M. Colonna-Dashwood**

3:15 Intermission.

3:30 AGFD 50. Estimation of procyanidin/prodelphinidin and *cis/trans* flavanol ratios of condensed tannin fractions by ^{13}C HSQC NMR spectroscopy: Correlation with thiolysis. **W. Zeller, A. Ramsay, H. Ropiak, C. Fryganas, I. Mueller-Harvey, R.H. Brown, C. Drake, J.H. Grabber**

3:50 AGFD 51. Impact by condensed tannins with different mean degrees of polymerization on protein precipitation. **W. Zeller, M.L. Sullivan, I. Mueller-Harvey, J.H. Grabber, A. Ramsay, C. Drake, R.H. Brown**

4:10 AGFD 52. Determination of amygdalin in apple seeds, fresh apples, and processed apple juices. **I. Bolarinwa**

4:30 AGFD 53. Withdrawn.**Nanotechnology: Delivering on the Promise Bridging the Gap to a Thriving US Marketplace**

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY EVENING**Section A**

Colorado Convention Center
Halls C/D

Sci-Mix

K. D. Deibler, Organizer

8:00 - 10:00

74, 77-78, 84, 92-97, 100, 103, 115, 118-120, 124-125. See subsequent listings.

TUESDAY MORNING**Section A**

Colorado Convention Center
Room 113

Agricultural & Food Chemistry General Papers**Agricultural and the Environment**

K. Deibler, Organizer

B. Park, Presiding

8:00 AGFD 53. Highly sensitive colorimetric sensors for fumigants. **G. Sun**

8:20 AGFD 54. Evaluation of biochar in three soil types for nutrient and water retention toward increased crop yield. **B.J. Winters**

8:40 AGFD 55. Positive role of lignin in enzymatic hydrolysis of lignocellulosic biomass. **Y. Huang, M. Tu**

9:00 Intermission.

9:15 AGFD 56. Green technologies for the generation of value added cotton. **S. Chang, B. Condon, J. Smith**

9:35 AGFD 57. Withdrawn.

9:55 AGFD 58. Phytotoxic and mosquito larvicidal constituents from *Ammi visnaga* seeds. **K.M. Meepagala, J.J. Beonel**

10:15 AGFD 59. Mustard meal extract as a natural herbicide for liverwort control. **I.E. Popova, J.S. Dubie, M.J. Morra**

10:35 Intermission.

10:50 AGFD 60. Phage amplification-based paper-fluidic device for the detection of generic *E. coli*. **S.D. Alcaine, S.R. Nugen**

11:10 AGFD 61. Is tomato worth an electron?

Bioelectrochemical treatment of waste residues from tomato processing Industry. **V. Gadhamshetty, A. Fogg**

11:30 AGFD 62. Herbicide metabolism database. **J. Yao, W. Xu, M. Lin, J. Hu, Q. Tang**

Section B

Colorado Convention Center
Room 112

Phenolic & Polyphenolic Chemistry in Food Processing**Reactions/Properties**

Cosponsored by AGRO, BIOT, COMP and MEDI

B. D. Guthrie, Organizer, Presiding

9:30 Introductory Remarks.

9:35 AGFD 63. Understanding physical-chemical, biological (antioxidant) and optical properties of natural polyphenols at an atomistic-scale. **P. Trouillas, M. Otyepka**

9:55 AGFD 64. Beyond ORAC: Dietary polyphenolics as metal-binding a98ntioxidants and food preservatives. **N.R. Perron, H.C. Wang, J.L. Brumaghim**

10:15 Intermission.

10:30 AGFD 66. Carbonyl-scavenging ability of phenolic compounds: A second barrier defense against the damage caused by lipid oxidation and oxidative stress. **R. Zamora, F.J. Hidalgo**

10:50 AGFD 65. Antiglycation activity of tannic acid in ovalbumin-glucose model system. **H. Akilloglu, V. Gökmen**

11:10 AGFD 67. Phenolic acids: Precursors for desirable aroma-active compounds and the undesirable toxicologically relevant styrene in wheat beer. **M. Granvogel, D. Langos, P.H. Schieberle**

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

Sponsored by CHAS, Cosponsored by AGFD, CCS and PRES

TUESDAY AFTERNOON**Section A**

Colorado Convention Center
Room 113

Applied Nanotechnology for Food & Agriculture

Cosponsored by PRES

M. Appell, B. Park, Organizers, Presiding

1:00 Introductory Remarks.

1:05 AGFD 68. Effect of nano size reduction on absorption and bioavailability of calcium from fortified milk powder in rats. **H. Mirhosseini, A. Erfanian, M. Abd Manap, b. rasti, S. Bin Mustafae**

1:35 AGFD 69. Green synthesis and electro-spray atmospheric pressure ionization mass spectral studies of hydrazinocurcumin: A potentially important derivative for intestinal absorption studies at the nanolevel. **B. Dayal, A. Mehta, D. Kulkarni, A. Pandey, S. Li, M.A. Lea**

2:05 AGFD 70. Withdrawn.

2:35 Intermission.

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at:

www.acs.org/denver2015

- 2:50 AGFD 71.** Nanocompositions for enhancing shelf life and quality of fruits, vegetables, and flowers. G. Paliyath, P. Padmanabhan, S. Mihindukulasurya, J. G.J., I. El Sharkawy, S. Jayasankar, L. Lim, A. Sullivan, S. K.S., G. R. K. Gill
- 3:20 AGFD 72.** Investigation of materials for the removal of arsenic from foodstuffs. T. Reed, A.W. Apblett
- 3:50 AGFD 73.** Bionanosensor adjusting the farming cultural practices in emergent nations. J. Reyes, N.D. Becerra-Mora, Y. Moreno, C.L. Macias, N.A. Marinho, A. Kohli, P. Kohli
- 4:20 Concluding Remarks.**

Section A

Colorado Convention Center
Room 113

Agricultural & Food Chemistry General Posters

K. Deibler, *Organizer, Presiding*

3:30 - 5:30

- AGFD 74.** Thermal stability of food allergens and nonallergenic proteins: A comparative study. Y. Wu, T. Fu
- AGFD 75.** Grain quality traits in a sorghum association mapping panel. S. Bean, T. Herald, J.D. Wilson, P. Gadgil, R.C. Kaufman, B.P. Ioerger
- AGFD 76.** Factors related to reduced *in-vitro* protein digestibility in a diverse sorghum population. S.L. Adriano, D.L. Blackwell, S. Bean, B.P. Ioerger, M. Tilley, T. Herald, P. Gadgil
- AGFD 77.** Smell of the entrance to the heaven: Volatiles from the coffee berry blossom end and their potential applications in pest managements of coffee berry borer *Hypothenemus hampei* (Coleoptera: Curculionidae). Y. Yu, E. Jang, M. siderhurst
- AGFD 78.** Influence of plant maturity on anthocyanin levels, phenolic composition, and antioxidant properties of purple basil (*Ocimum basilicum* L.). K.R. McCance, E.D. Niemeyer
- AGFD 79.** Determination of the antioxidant properties of flavanones and flavanone glucuronide metabolites. K.A. Costello, E.D. Niemeyer
- AGFD 80.** Withdrawn.
- AGFD 81.** Chiral and achiral profiling of a pesticide formulation using ultraperformance convergence chromatography (UPC²) with PDA and mass detection. M. Thwoigh, M. O'Leary, P.G. Alden
- AGFD 82.** Effectiveness of flocculants on inorganic and metallic species removal during aerobic digestion of wastewater from poultry processing plant. N. Lovanh, J.H. Loughrin, K. Cook, K. Sistani, P. Silva
- AGFD 83.** Novel structural modifications of plant oils. A. Biswas, H. Cheng
- AGFD 84.** QSAR and density functional approaches to evaluate trichothecene toxicity and detection. M. Appell, W.B. Bosma
- AGFD 85.** Cross species amplification of thirteen distinct microsatellite loci in *Z. aquatica*. B.J. Pinto
- AGFD 86.** Influence of biological fertilization on seed production of winter wheat. D. Trifan, M. Bularda
- AGFD 87.** Sorption of organic dyes by straw biochar and its effective factor. X. Ji, L. Lyu, C. Yang
- AGFD 88.** Detoxification with enzymes for tung meal. R. Liu
- AGFD 89.** Distribution and enantiomeric profiles of organochlorine pesticides in surface sediments from Bering Sea, Chukchi Sea, and Arctic Ocean. M. Jin, B. Xue, S. Zhou
- AGFD 90.** Enhanced anti-ultraviolet and thermal stability of a pesticide by modification of a volatile organic compound (VOC)-free vinyl-silsesquioxane in severe environments. D. Lin, X. Han, L. Hu
- AGFD 91.** Antilipidemic actions of the dietary fiber extract of soybean residues in Kunming mice. D. Lin, Z. Tu
- AGFD 92.** Advanced glycation endproducts may affect digestion and antigen processing of food allergens. C.P. Mattison, J. Dinter, M. Berberich, S. Chung, S. Reed, S. Le Gall, C.C. Grimm
- AGFD 93.** Behavior of whey protein concentrates under extreme storage conditions. M.H. Tunick
- AGFD 94.** Alternative hop processing. C. Knuston, B.E. Sturgeon
- AGFD 95.** Mechanism behind the antibacterial properties of hop acid investigated with model cell membranes. Y. Park, A. Sostarecz
- AGFD 96.** Determination of the presence of flavor- and aroma-affecting compounds in beer resulting from various yeast washing techniques. D. Kazal, W.H. Steel
- AGFD 97.** Improving lag time in second-generation washed beer yeast. W.H. Steel
- AGFD 98.** Changes of volatile compounds in Muscadine grape (*Vitis rotundifolia*) during ripening. B. Lee, F. Chen
- AGFD 99.** Vapor-infusion of wine flavor volatiles in specialty dark chocolate and analysis via GC-M. S. Richards, S. Bremer, K.L. Nuckles, C.R. Thurman, P.J. Iles, L.D. Giddings, M. Alvarez, N.R. Bastian
- AGFD 100.** Volatile-organic component sensitive colorimetric chemosensor: Application for determination of apple quality. Y. Kim, S. Jin, G. Kim, J. Park
- AGFD 101.** Withdrawn.
- AGFD 102.** Effect of fat concentration and fermentation on thermal properties of milk bases. Z. Bao, J. Xiong, J. Ye
- AGFD 103.** Production of lactic acid from cheese whey in controlled pH batch fermentation using *Lactobacillus plantarum* DSA 20174. A.A. Ayad, D. Gad El-Rab, S. Ibrahim
- AGFD 104.** Mineral and trace element analysis of berry liquors from Northern Europe. N.J. Ronkainen, N.S. Olson, S. Mustaly
- AGFD 105.** Roasting effects on phenolic content and free-radical scavenging activities of pulp pre-conditioned and fermented cocoa (*Theobroma cacao*) beans. E. Afoakwa, E. Ofosu-Ansah, J. Takrama, A.S. Budu
- AGFD 106.** Synthesis and characterization of cationic starches and their application in preparation of fertilizer nanoparticles through four-Inlet vortex mixer. Y. Shi, S. Zhang, X. Jia, K. Chen, X. Guo
- AGFD 107.** Multiplex real-time PCR detection and identification of food-borne pathogens *Salmonella enterica*, *Escherichia coli* and *Shigella flexneri*. K.C. Sweetin, K.M. Elkins
- AGFD 108.** Multiplex real-time PCR detection and differentiation of food-borne pathogen *Bacillus cereus* and related *Bacillus* species. J.D. Roussillon, K.M. Elkins
- AGFD 109.** Determination of heavy metals in tomatoes sauces. M. Reyna Lirano, R. Tremont
- AGFD 110.** Mold population on freshly-harvested rice and factors affecting prevalence. S. Thote, G. Atungulu, H. Zhong
- AGFD 111.** Fatty acid analysis of tilapia. E.M. Crosier, M.J. Yurkevicius, A.L. Rhyne, N.E. Breen
- AGFD 112.** Comparison of the fatty acid profiles of wild caught and farm raised salmon. M.J. Yurkevicius, E.M. Crosier, D.L. Taylor, N.E. Breen, A.L. Rhyne
- AGFD 113.** Antioxidant effect of porcine pancreatic phospholipase A2 and detection and pro-oxidative activity of ferryl-hemoglobin in washed cod muscle. N. Tatiyaborworntam, M.P. Richards
- AGFD 114.** Effect of porcine pancreatic phospholipase A2 on trout hemoglobin-promoted lipid oxidation and heme partitioning in washed cod muscle. N. Tatiyaborworntam, M.P. Richards
- AGFD 115.** Isolation and characterization of chitin from the mushroom *Pleurotus ostreatus* with possible application in biomedical and pharmaceutical application. B. Calderon
- AGFD 116.** Methylglyoxal scavenging activity of deacetylaseperulosidic acid. S. Deng, B. West, J. Jensen, C. Su
- AGFD 117.** Dietary sources of iridoids inhibit advanced glycation end product formation. B. West, A. Bogdanov, S. Deng, C. Su, C. Jensen, Z. Zaynudinov
- AGFD 118.** Exploration of curcumin, UV-Vis absorption, and degradation kinetics. H. Goemann, T. Roettgen, J.D. Alia
- AGFD 119.** Role of polyphenols of *Artemisia nova* and *Artemisia wyomingensis* in sage grouse dietary preferences. A.H. Nguyen, J.S. Forbey, G.G. Frye, J.W. Connolly, C.Y. Dadabay
- AGFD 120.** Antioxidant protection in human blood plasma of varying triglyceride content utilizing a ferric reduction assay. R. Chandra, C. Chidi, K. Huerta-Ruiz-Garza
- AGFD 121.** Withdrawn.
- AGFD 122.** Antioxidant activity assay based on rapid colorimetric measurement of gold nanoparticles. J. Chou, X. Li, Y. Yin, N. Indrisek, J. Merozo
- AGFD 123.** Chemical constituents and biological evaluation of leaves' essential oils of *Vitex agnus-castus* L. growing in the southern-west of Algeria. K. Sekkoum
- AGFD 124.** Block ionomer complexes formed by carboxymethyl-dextran-block-poly(ethylene glycol) copolymer and α -lactalbumin. J. Du, O.G. Jones
- AGFD 125.** Antioxidant activities of supercritical carbon dioxide and ethanol extracts of *Aronia melanocarpa* (black chokeberry) pomace. J. Wenzel, T. Dixon, E. Tucker, L. Wang, M. Ammerman, C. Samaniego
- AGFD 126.** Digestibility, viscosity, and microstructural properties of waxy and non-waxy rice starches resulting from microwave heat-moisture treatment. A. Anderson
- AGFD 127.** Beauvericin as virulence factor of entomopathogenic fungus *Beauveria bassiana* (BALS.) used on bark beetles attacking spruces. S. Mudronceková, I. Salamon, M. Barta
- AGFD 128.** Lyophilization technology for isolation of anthocyanins from fruits of the high bush blueberry (*Vaccinium corymbosum* L.). I. Salamon, R. Mariychuk, S. Mudronceková, D. Grulova
- AGFD 129.** Distribution of residues in various muscles of cattle following intramuscular administration of hormones. S. Sklenka, P.S. Chu, J. Ward, A. Chiesa, T. Johnson
- AGFD 130.** Comparison of kinetic profile of two total antioxidant capacity assays. C. Krzykwa, S.P. Canete
- AGFD 131.** Identification of toxic metal ions in water using a gold nanoparticle based colorimetric sensor array. G. Sener, I. Uzun, A. Denizil
- AGFD 132.** Effect of different proportions of ethanol on the crystalline structure of bacterial celluloses. J. Xiong, Z. Wang, J. Ye
- AGFD 133.** Teaching laboratory for food analysis: Titration and HPLC characterization of kombucha fermentation. N. Lawton, W. Hall, S. Tachibana
- AGFD 134.** Polyphenol antioxidants in savory snacks: Are any there? J. Goodman, J.A. Vinson
- AGFD 135.** Isoflavone metabolism leading by the human intestinal bacteria. M. Kim, J. Han
- AGFD 136.** Analysis of aroma compounds in whiskey by DLLME-GC/MS. J.E. Owens, L.B. Zimmerman, M.A. Gardner, L. Lowe, D.A. Orban, C.N. Goolsby
- AGFD 137.** Biosorption of various mushrooms. W. Ryan, C. Fowler, K. Yuan, D.J. Schauer
- AGFD 138.** Active site analysis of lepidopterans Farnesyl diphosphate synthase: Implications in omologous juvenile hormone biosynthesis. S.E. Sen, T. Horsfield, A. Jones
- AGFD 139.** Mercury analysis of tuna using a low-cost cold vapor spectroscopy apparatus. J. Hernandez
- AGFD 140.** Analysis of lipid transfer proteins in *Arabidopsis thaliana* by means of epitope tags to decipher the role of LTP4's lipid in plant senescence. J. Bautista
- AGFD 141.** Efforts toward the development of a titrimetric method for measuring biosorption capacity. S. Ardon, H. Duke, B. Stewart, T. Robertson, D.J. Schauer
- AGFD 142.** Withdrawn.
- AGFD 143.** Antioxidant and aldose reductase inhibitory activities of color-fleshed potatoes. D. Kalita, B. Shieh, H. Ali, D.V. LaBarbera, D.G. Holm, J.M. Pettrash, S.S. Jayanty

Section B

Colorado Convention Center
Room 112

Phenolic & Polyphenolic Chemistry in Food Processing

Sources

Cosponsored by AGRO, BIOT, COMP and MEDI

B. D. Guthrie, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 144. Ultrasound-assisted extraction of phenolic compounds from hazelnut shells. B. Yuan, M.A. Hanna

1:25 AGFD 145. Effects of pod storage and fermentation duration on total polyphenols, *o*-diphenols, and anthocyanin concentrations in cocoa (*Theobroma cacao*) beans. E. Afoakwa, J.E. Kongor, J. Takrama, A.S. Budu, H. Mensah-Brown

1:45 AGFD 146. Effect of solvent composition on grafting gallic acid onto chitosan via carbodiimides. P. Guo, J.D. Anderson, J.J. Bozell, S. Zvanovic

2:25 AGFD 148. Analysis of grape seed tannins by mass spectrometry (MALDI-TOF and ORBITRAP ESI-MS). E. Salas, N. Teixeira, S. Maia, J. Oliveira, N. Mateus, V. De Freitas

2:45 Concluding Remarks.

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 113

Applied Nanotechnology for Food & Agriculture

Cosponsored by PRES

M. Appell, B. Park, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 AGFD 149. Potentiometric PVC membrane sensors and their analytical applications in pharmaceuticals analysis: One example potentiometric PVC membrane sensors determination of moxifloxacin in pharmaceutical dose form. G.A. Mostafa

9:05 AGFD 150. Development of phage-conjugated magnetic nanopores for bacterial separation. S.R. Nugen, J. Chen

9:35 Intermission.

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.

- 9:50 AGFD 151.** Label-free detection of *Salmonella typhimurium* with ssDNA aptamers. **B. Park, B. Wang, Z. Lou, B. Xu, Y. Kwon**
- 10:20 AGFD 152.** Integration of nanostructured dielectrophoretic device and surface-enhanced Raman probe for highly sensitive rapid bacteria detection. **F. Madiyar, S. Bhana, L. Swisher, X. Huang, C.T. Culbertson, J. Li**
- 10:50** Discussion.

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 113

Agricultural & Food Chemistry General Papers

K. Deibler, *Organizer*
B. Park, *Presiding*

- 1:00 AGFD 153.** Accurate experimental design for the characterization and quantitation of *Antrodia cinnamomea* triterpenoids with RSM, qNMR, and HPLC-tandem MS: A tough case to crack. **T. Wu, Y. Du, M. El-Shazly, M. Lu, Y. Hsu, K. Lai, C. Chiu, F. Chang, Y. Wu**
- 1:20 AGFD 154.** Anti-inflammatory constituents of *Cordyceps militaris*. **C. Chiu, T. Wu, C. Lee, Y. Du, M. El-Shazly, Y. Chan, C. Tang, F. Chang, Y. Wu**
- 1:40 AGFD 155.** Isolation and structural characterization of five constituents from *Eucommia ulmoides* Oliv. by multistep process. **M. Zhu, J. Wen, Y. Dong, Y. Su, Q. Wei, R. Sun**
- 2:00** Intermission.
- 2:10 AGFD 156.** Improved the emulsion stability of phosvitin from hen egg yolk against different pH by the covalent attachment with dextran. **H. Chen**
- 2:30 AGFD 157.** Protein level determination in foods: A comparison of analytical methods. **M.C. Azih**
- 2:50** Intermission.
- 3:00 AGFD 158.** Influence of branched limit dextrin on wheat starch gels retrogradation. **J. Xu, X. Fan, X. Xu**
- 3:20 AGFD 159.** Modified fermentation method of producing virgin coconut oil. **N.D. Flores, J. Cuya**

Section B

Colorado Convention Center
Room 112

Water Our Most Critical Resource

Cosponsored by MPPG

J. Finley, *Organizer*
S. Ahuja, J. N. Seiber, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05 AGFD 160.** Water is indeed a crucial resource. **S. Ahuja**
- 1:35 AGFD 161.** Water and wine. **J.N. Seiber, V. Tianco, J. Real**
- 2:05 AGFD 162.** Foundations of water quality monitoring and assessment in the United States. **D.N. Myers**
- 2:35** Intermission.
- 2:45 AGFD 163.** Chemical characterization of brackish groundwater resources of the United States. **P. McMahon, J. Böhle, K. Dahm, J. Stanton, D. Parkhurst**
- 3:15 AGFD 164.** Water challenges in unconventional in situ energy resource extraction technologies. **T.J. Gallegos, C. Bern, J.E. Birdwell, S.S. Haines, M. Engle**
- 3:45 AGFD 165.** Energy and water nexus in urban environments. **T. Younos**
- 4:05** Intermission.
- 4:15 AGFD 166.** Effect of upflow velocity on nutrient recovery from swine wastewater by fluidized bed struvite crystallization. **R.M. Abarca, R.S. Pusta, R.B. Labad, J.A. Andit, C.M. Rejas, M.G. de Luna, M. Lu**

- 4:35 AGFD 167.** Contaminated irrigation water and the associated human health risks. **T. Tongesayi**

THURSDAY MORNING

Section B

Colorado Convention Center
Room 112

Water Our Most Critical Resource

Cosponsored by MPPG

S. Ahuja, *Organizer*
J. Finley, J. N. Seiber, *Organizers, Presiding*

- 8:00 AGFD 168.** Optimizing water resources: An Israeli approach. **H.L. Taft**
- 8:30 AGFD 169.** Impacts of EPA's Clean Power Plan on electricity generation and water use in Texas. **P. Faeth**
- 9:00** Intermission.
- 9:10 AGFD 170.** Desalination for expanding water supplies. **J.H. Lienhard**
- 9:40 AGFD 171.** Improving water use estimates for the United States. **N.L. Barber**
- 10:10 AGFD 172.** Water security in a warming world. **D. Michel**
- 10:40** Intermission.
- 10:50 AGFD 173.** Decreasing the severity of chemical pretreatment processes of switchgrass through storage. **D. Carrier, M. Wilkins, M. Buser, N. Frederick**
- 11:20 AGFD 174.** Coupling surface water remediation to sustainable energy: Toward off-grid production of algae for biofuels. **J.B. Miller**
- 11:50 AGFD 175.** Water for food production: Will we have enough? **J.W. Finley**
- 12:20 AGFD 176.** Sustaining groundwater resources for global food security. **T. Harter**

AGRO

Division of Agrochemicals

P. Rice, *Program Chair*

SUNDAY MORNING

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

SUNDAY AFTERNOON

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Nanotechnology: Delivering on the Promise Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Sponsored by AGFD, Cosponsored by AGRO and MEDI

Nanotechnology: Delivering on the Promise Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Sponsored by AGFD, Cosponsored by AGRO and MEDI

Nanotechnology: Delivering on the Promise Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

TUESDAY MORNING

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Sponsored by ENVR, Cosponsored by AGRO, ANYL and MPPG

Phenolic & Polyphenolic Chemistry in Food Processing

Reactions/Properties

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMIP and MEDI

TUESDAY AFTERNOON

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Sponsored by ENVR, Cosponsored by AGRO, ANYL and MPPG

Phenolic & Polyphenolic Chemistry in Food Processing Sources

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

WEDNESDAY MORNING

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment

Sponsored by ENVR, Cosponsored by AGRO

Surface Physicochemical Processes in Engineered and Natural Systems

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

WEDNESDAY AFTERNOON

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment

Sponsored by ENVR, Cosponsored by AGRO

Surface Physicochemical Processes in Engineered and Natural Systems

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

WEDNESDAY EVENING

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

THURSDAY MORNING

Surface Physicochemical Processes in Engineered and Natural Systems

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

ANYL

Division of Analytical Chemistry

D. C. Duckworth, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

DOE Nanoscience Research Centers National Resources for the Nanoscience Community (see PRES, Tue)

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment (see ENVR, Mon, Tue, Wed)

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment (see ENVR, Tue, Wed)

Macromolecular and Nanoparticle Separation Science (see POLY, Sun, Mon, Tue)

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Aspen Room A

Environmental Analytical Chemistry: A Tool for Introducing Research

M. Crowe, J. C. Ingram, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 1. Environmental analytical chemistry summer research for high school students. **J.C. Ingram**

1:30 ANYL 2. General Chemistry assignment analyzing environmental contamination for the DePue, IL, National Superfund site. **F.M. Geiger**

1:50 ANYL 3. Environmental analytical chemistry research: An undergraduate's perspective. **J. Credo, J.C. Ingram**

2:10 ANYL 4. Environmental analytical chemistry research with undergraduate students at Union College: Case studies and lessons learned. **L. MacManus-Spencer**

2:30 Intermission.

2:45 ANYL 5. Environmental analytical chemistry at James Madison University. **R.D. Foust, D.M. Downey, C.A. Hughey**

3:05 ANYL 6. Laboratory and field-based environmental analytical chemistry research experiences for undergraduates at Villanova University. **A.M. Grannas**

3:25 ANYL 7. Novel scan method for differential ion mobility spectrometry separations. **R. Harris, B. Santiago, S. Isenberg, G.L. Glish**

3:45 ANYL 8. Electrochemistry and "biofilms": Undergraduate research at the interface of chemistry and biology. **R.J. Lesuer, A. Maselli**

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Aspen Room A

Advances in Analytical Separations

J. L. MacLachlan, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL 9. Award Address (ACS Award in Chromatography) sponsored by Sigma-Aldrich/Supelco). Framework for the development of several new bioanalytical methods. **M.T. Hearn**

ANYL 147. Environmental variables influencing surfactant mobility and soiling on artists' acrylic dispersion paints. **A.F. Lagalante**, R.C. Wolbers, I. Ziraldo, K. Watts

ANYL 148. Electrospun polymer nanofibers with entrained explosives as potential field calibration standards for explosives. **S. Robertson**, A. Heflin, B. Bui, J. Lamb, C. Kneapler, D.E. Flegner, R. Hoff

ANYL 149. Comparison of MEKC-UV and GC-MS in the analysis of explosives in environmental samples. **A.M. Genzman**, J.M. Rine, K.A. Brensinger, C.M. Rollman, I.S. Lurie, M. Moini, C.L. Copper

ANYL 150. Separation of transition and heavy metal ions using gradient thin layer chromatography. **S. Stegall**, M. Collinson

ANYL 151. Development of standard reference materials (SRMs) for quantitative nuclear magnetic resonance (qNMR) spectroscopy. **J.A. Widegren**, T.J. Bruno, T.M. Lovestead, T.J. Fortin

ANYL 152. Interactions of drugs with model membrane systems: Focusing on the interactions near the water interface. **C. Beuning**, C. Rithner, D.C. Crans

ANYL 153. Characterization of aqueous choline chloride deep eutectic solvents. **S. Asare**

ANYL 154. Inorganic thermogravimetric analysis of hydrates of first-row transition metal salts revisited. **D.A. Habboush**, M.A. Arab, N.M. Alanazi

ANYL 155. Magnesium wire templated microfluidic construction. **S. Toussaint**, T. Torgersen, J. Wickes, C. Lamb, L.M. Miller, S.L. McKay, C.F. Monson

ANYL 156. Probing the sensitivity and applicability of differential magnetic catch and release for magnetic nanoparticle purification. **J. Morse**, R.E. Schaak, M.E. Williams

ANYL 157. Mathematical models for quantitative spectrophotometric spectral bandwidth measurements. **A. Reid**, M. Labrie, J. Messman

ANYL 158. Metrological evaluation of a potential certification bias for potassium dichromate solution measurement standards. **M. Labrie**, A. Reid, J. Messman

ANYL 159. Particle size paradox. **J.G. Saad**, P.A. Webb

ANYL 160. Characterization of earth pigments and study of their influence on the drying properties of linseed oil. **E. Portero**, L. de Viguierie, P. Walter

ANYL 161. Effect of linked gold nanoparticles on the oxidation of silver nanoparticles. **K. Elmer**, R. Masitas, F.P. Zamborini

ANYL 162. Tailored to suit: Fabricating specialized DETECHIP arrays. **R.M. Burks**, J. Atwater, A.E. Holmes

ANYL 163. Determination of pyrazole and pyrrole pesticides in environmental water samples by Magnetic Metal-Organic Framework (MOF) as a novel adsorbent coupled with high performance liquid chromatography. **J. Ma**, Z. Yao, Y. Xia

ANYL 164. Integrated geochemical fingerprinting of uranium deposits for sustainable exploration and development. **L.L. Van Loon**, N.R. Banerjee, M. Fayek, D. Quirt

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.

WEDNESDAY MORNING

Section A

Embassy Suites Denver—Downtown Convention Center
Aspen Room A

Advances in Electrochemistry

S. H. Pratt, *Organizer*
D. Polcari, C. A. Rusinek, *Presiding*

8:00 Introductory Remarks.

8:05 ANYL 165. High-efficiency generation-collection microelectrochemical platform for interrogating electroactive thin films. **M.J. Anderson**, R.M. Crooks

8:25 ANYL 166. New insights into magnesium alloy corrosion using scanning electrochemical microscopy. **P. Dauphin Ducharme**, U.M. Tefashe, R.M. Asmussen, M. Danaie, W.J. Binns, P. Jakupi, G. Botton, D.W. Shoesmith, J. Mauzeroll

8:45 ANYL 167. Anodic stripping voltammetry at platinum-mercury nanoelectrodes: Trapping of Mn²⁺ by crown ethers. **L. Danis**, S.M. Gateman, M.E. Snowden, I.C. Halalay, J.Y. Howe, J. Mauzeroll

9:05 ANYL 168. Fabrication of carbon, gold, platinum, silver, and mercury ultramicroelectrodes with controlled geometry. **D. Polcari**, L. Danis, A. Kwan, S. Gateman, J. Mauzeroll

9:25 ANYL 169. New electrochemical sensors for wearable applications: Sniffing environmental inhalation hazards with ultralow power devices. **M.T. Carter**, J. Stetter, M. Findlay, V. Patel

9:45 Intermission.

10:05 ANYL 170. 1000-fold sensitivity increase on solid-contact ion-selective electrodes by controlling the ionophore/polymer interface. **S. Granados Focil**, L. Mendecki, K.A. Stockmal, A. Radu

10:25 ANYL 171. Erbium (III) tetraphenylporphyrin-based ion selective electrodes. **A.J. Kane**, E.D. Steinle

10:45 ANYL 172. Electrochemical studies into the possible formation of germanene. **M. Ledina**, Y. Kim, J. Jung, J.L. Stickney

11:05 ANYL 173. Cloud point extraction for electroanalysis: Anodic stripping voltammetry of cadmium. **C.A. Rusinek**, A.F. Bange, I. Papautsky, W.R. Heineman

11:25 Concluding Remarks.

Section B

Embassy Suites Denver—Downtown Convention Center
Aspen Room B

Analytical Chemistry of Natural Resources

Environmental Analysis: Analytical Methods for Natural Resource Assessment and Protection

Cosponsored by MPPPG†

W. T. Cooper, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL 174. Raman study of the adsorption behavior of silver nanoparticles at mineral- and natural organic matter-water interfaces. **K.A. O'Neil**, J. Fraley, S.W. Brittle, J. Purvis, S.R. Kanel, S.R. Higgins, I.E. Pavel Sizemore

8:25 ANYL 175. SP-ICP-MS for nanoparticle detection and size distribution determinations: Current state of the art and future perspectives. **C. Stephan**

8:45 ANYL 176. Efficient association of chiral HPLC, polarimetric detection and chemometrics: Discrimination of lavender and lavandin essential oils using chiroptical fingerprint. **S. Lafhal Sakiou**, I. Bombarda, N. Dupuy, M. Jean, J. Kister, C. Roussel, P. Vanloot, N. Vanthuyne

9:05 ANYL 177. Comparative assessment of analytical methods for the determination of total sugar content of energy drinks consumed in Nigeria. **J. U. Okere**

9:45 Intermission.

10:05 ANYL 179. Toward chemiluminescence detection of cytotoxics in surface waters. **T. Reeves**, R. Popelka-Filcoff, C. Lenehan

10:25 ANYL 180. Preparation, characterization, and application of activated tassel for the remediation of eutrophic phosphorus in contaminated water. **A.M. Shofolahan**, J. Okonkwo, N. AgyeiA

10:45 ANYL 181. Withdrawn.

11:05 ANYL 182. Analysis of trace elements in fuel gas for the prediction of masking events. **T. Bruno**, J. Burger

11:25 ANYL 183. Comprehensive analytical approach for characterizing the impacts of climate change on carbon sequestration in Arctic peatlands. **S.B. Hodgkins**, R. Wilson, J. Chanton, W.T. Cooper

WEDNESDAY AFTERNOON

Section A

Embassy Suites Denver—Downtown Convention Center
Aspen Room A

Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Symposium in Honor of Hilikka I. Kenttämää
Cosponsored by WCC

L. Yang, *Organizer, Presiding*

V. M. Bierbaum, *Presiding*

1:00 Introductory Remarks.

1:05 ANYL 184. Mass spectrometry as a synthetic method. **R.G. Cooks**

1:40 ANYL 185. Peptide and protein aggregation: The latest news. **M.T. Bowers**

2:15 ANYL 186. SID-IM-SID: A new tool for substructure characterization of protein complexes. **V.H. Wysocki**

2:50 Intermission.

3:05 ANYL 187. Remote but not disinterested: Measuring influence of charge on radical energetics in dicationic radical ions. **S. Blanksby**, D. Marshall

3:40 ANYL 188. Award Address (Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry sponsored by Waters Corp.). Recent studies on dicationic mono- and polyradical cations. **H. I. Kenttämää**

4:15 Concluding Remarks.

Section B

Embassy Suites Denver—Downtown Convention Center
Aspen Room B

Analytical Chemistry of Natural Resources Instrumentation and Methods

Cosponsored by MPPPG†

M. Fayek, A. Karamalidis, A. Koenig, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 189. Withdrawn.

1:25 ANYL 190. Multicollector ICP-MS for isotope ratio analysis of uranium. **G.L. Hart**, S.H. Pratt

1:45 ANYL 191. Variations in hydrogen isotopes of individual plant waxes from four plant species during the growing season. **A. Oakes**, M.T. Hren

2:05 ANYL 192. Dual isotopic ($\delta^{13}\text{C}$, $\delta^3\text{H}$) evidence for long-range transport of mining-related PAHs in the Athabasca oil sands region. **J.J. Jautzy**, J.M. Ahad, C. Gobeil, A. Smirnov, B.D. Barst, M.M. Savard

2:25 ANYL 193. Isotopic variability of nitrogen oxides (NO_x) from biomass burning. **D.L. Flibiger**, M. Hastings

2:45 Intermission.

3:00 ANYL 194. Design and implementation of quantitative carbon detector (QCD) for calibration-free gas chromatography. **C. Krumm**, S. Maduskar, A.R. Teixeira, A. Paulsen, T. Mountziaris, W. Fan, P.J. Dauenhauer

3:20 ANYL 195. Vapor sampling by PLOT-cryoadsorption: Examples in forensic sample analysis. **T. Bruno**

3:40 ANYL 196. HPTLC and clustering analysis for the classification of colored wheat varieties by anthocyanin patterns. **S. Böhmderfer**, G. Genta-Jouve, H. Grausgruber, T. Rosenauer

4:00 ANYL 197. Multichannel high frame-rate beam-scanning microscopy based on Lissajous scanning trajectories and model based image reconstruction. **S. Sullivan**, J. Newman, R. Muir, S. Sreeharu, C.A. Bouman, G.J. Simpson

4:20 ANYL 198. Polymer screen-printing for paper-based device fabrication. **Y. Sameeoni**, P. NaNongkai, S. Nouanthatong, C. Henry

THURSDAY MORNING

Section A

Embassy Suites Denver—Downtown Convention Center
Aspen Room A

Nakanishi Prize: Symposium in Honor of Fred W. McLafferty

N. L. Kelleher, *Organizer*

P. Compton, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL 199. Native electron capture dissociation: A droplet dissociation process used to elucidate iron-binding motifs in biological macromolecules. **O. Skinner**, M. McAnally, R.P. Van Dyne, P.D. Compton, N.L. Kelleher

8:50 ANYL 200. New approaches to multiplex newborn screening of lysosomal storage disorders by tandem mass spectrometry. **F. Turecek**, M.H. Gelb, C.R. Scott

9:35 ANYL 201. Developing native top-down mass spectrometry as a tool for protein structural biology. **J.A. Loo**

10:20 Intermission.

10:35 ANYL 202. Top-down mass spectrometry of modified ribonucleic acids. **K. Breuker**

11:20 ANYL 203. Award Address (Nakanishi Prize sponsored by the Nakanishi Prize Endowment). Analytical chemistry of gaseous ubiquitin ions. **F.W. McLafferty**, S. Castro, O. Skinner, K. Breuker

THURSDAY AFTERNOON

Section A

Embassy Suites Denver—Downtown Convention Center
Aspen Room A

Advances in Analytical Spectroscopy

X. Yu, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL 204. Finding the needle in the haystack: Characterization of trace crystallinity in a commercial formulation of paclitaxel protein-bound particles by Raman spectroscopy and synchrotron X-ray diffraction enabled by second harmonic generation microscopy. **P.D. Schmitt**, N.S. Trasi, F. Deng, S. Zhang, L.S. Taylor, G.J. Simpson

1:25 ANYL 205. Four-wave mixing imaging of nanorod aggregates. **K.A. Antonio**, Z.D. Schultz

1:45 ANYL 206. Spectroscopic analyses of chemical adaptation processes within microalgal biomass in response to changing environments. **F. Vogt**

2:05 ANYL 207. Correlative imaging of cancer cell and drug interactions in the liquid microenvironment. **X. Hua**, C. Szymanski, Z. Wang, B. Liu, Z. Zhu, J. Evans, G. Orr, S. Liu, X. Yu

2:25 ANYL 208. Biomarker VOC concentration and desorption coupled with a TIR-Raman system. **R. Dodson**, A.R. Mercer-Smith, K. Park, P. Koonath, H. Lu, V. Sapirstein, A. Niemz, C. Taylor

2:45 Intermission.

† Cooperative Cosponsorship

3:00 ANYL 209. Optimizing uptake and identification of volatile organic compounds for clinical diagnoses. **A.R. Mercer-Smith**, R. Dodson, K. Park, P. Koonath, H. Lu, V. Sapirstein, A. Niernz, C. Taylor

3:20 ANYL 210. Spectroscopic analysis of weakly turbid systems: A generally useful simple algorithm. **P. Dent**, R. McDonough, K. Rawlins, S. Ortiz, J. Goodisman, J. Chaiken

3:40 ANYL 211. Rapid, broadband, precision spectroscopy of carbon dioxide near 5000 cm⁻¹ using optical frequency combs. **A. Klose**, G. Truong, L. Sinclair, I. Coddington, N. Newbury, S. Diddams

4:00 ANYL 212. Brightness-equalized quantum dots. **S. Lim**, M.U. Zahid, D. Entenberg, A.S. Harney, J. Condeelis, A. Smith

4:20 ANYL 213. Trace chemical sensing by photoionization through Rydberg states followed by detection of the laser induced plasma via microwave radiation. **F. Rudakov**, P. Weber

BIOT

Division of Biochemical Technology

M. Lazzara and A. Kantardjiev, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Phenolic & Polyphenolic Chemistry in Food Processing (see *AGFD, Tue*)

Undergraduate Research Posters (see *CHED, Mon*)

Rising Stars Awards Symposium (see *WCC, Mon*)

SOCIAL EVENTS:

Membership Desk, 8:00 AM: Sun, Mon, Tue, Wed, Thu

Reception, 6:30 PM: Sun

Poster Session, 6:00 PM: Tue

Program Chair's Lunch 6:00 PM: Tue

Company Seminars 12:30 PM: Sun, Mon, Wed

Networking/ Mentoring Session 6:00 PM: Wed

BUSINESS MEETINGS:

BIOT Executive Committee Meeting, 7:00 PM: Mon

Future Programming Meeting, 12:30 PM: Tue

SUNDAY MORNING

Section A

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes

Advances in Systems Biology

M. R. Antoniewicz, **B. Mulukutla**, *Organizers, Presiding*

8:30 BIOT 1. New insight of the CHO cell transgene production level using next-generation genomic tools. **H. Fu**, N. Vishwanathan, M. Xiong, A. Bandyopadhyay, Y. Yang, W. Hu

8:50 BIOT 2. Automated RNA-Seq analysis pipeline to identify and visualize differentially expressed genes and pathways in CHO cells. **C. Chen**, H. Le, C. Goudar

9:10 BIOT 3. Transcriptome, methylome, and genome analysis in clonal variability. **L. Zhao**, N. Vishwanathan, H. Fu, A. Bandyopadhyay, W. Hu

9:30 BIOT 4. Updating the Chinese hamster reference genome and applications to CHO HCP studies. **K.H. Lee**

10:10 BIOT 5. Development of a comprehensive *Escherichia coli* kinetic metabolic model consistent with multiple genetic and environmental perturbations. **A. Khodayari**, C. Maranas

10:30 BIOT 6. Reconstructing anaerobic microbiomes from the "bottom-up": New techniques to decipher interwoven metabolism. **J.A. Sexton**, K. Solomon, J. Henske, M.K. Theodorou, D.L. Valentine, M.A. O'Malley

10:50 BIOT 7. Genome scale metabolic network reconstruction of *Synechocystis* sp. PCC6803 taking into account molecular mechanisms under photoautotrophic conditions. **C. Joshi**, F.E. Estep, M. Tracey, C.A. Peebles, A. Prasad

11:10 BIOT 8. Development of regulated metabolic models for anaerobic organisms. **S. Dash**, C.D. Maranas

Section A

Grand Hyatt Denver
Mt. Evans

David Perlman Memorial Lectureship and Van Lanen and Peterson Award Presentations

M. Lazzara, *Organizer, Presiding*

11:30 BIOT 9. Overcoming obstacles to expression and characterization of difficult proteins. **A.S. Robinson**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Advances in Chromatographic Separations

A. Hewig, **J. Hubbuch**, **A. R. Lajmi**, **S. Yamamoto**, *Organizers, Presiding*

8:30 BIOT 10. Scalability of mechanistic models for ion exchange chromatography. **T. Huuk**, T. Hahn, J. Griesbach, H. Stefan, J. Hubbuch

8:50 BIOT 11. Competitive binding of antibody monomer-dimer mixtures on CEX resins: Equilibrium and kinetics. **J. Reck**, T. Pabst, A. Hunter, X. Wang, G. Carta

9:10 BIOT 12. Development of robust orthogonal methods for impurity clearance using high throughput screening. **S. Chollangi**

9:30 BIOT 13. Optimization of monomer separation processes by electrostatic-interaction chromatography. **S. Yamamoto**, N. Yoshimoto, Y. Isakari, A. Podgornik

9:50 Intermission.

10:10 BIOT 14. Chromatographic retention prediction using quantitative structure property relations. **M.E. Klijn**, A. Hanke, M. Ottens

10:30 BIOT 15. Insights into the nature of multimodal chromatographic selectivity using *in silico* designed Fab fragment variants. **H. Karkov**, H. Ahmadian, B. Olsen Krogh, A. Boggsnes, S.M. Cramer

10:50 BIOT 16. Modelling of pH and dual gradient ion exchange and multi modal chromatography for the purification of mAbs. **S. Kluters**, Y. Lee, C. Frech

11:10 BIOT 17. Systematic exploration of homologous ligand library leads to improved design principles and tools for the prediction of protein selectivity in mixed-mode chromatographic systems. **J. Woo**, H. Chen, M.A. Snyder, S.M. Cramer

Section C

Grand Hyatt Denver
Grays Peak A

Biomolecular & Biophysical Processes

Protein Characterization Technologies

J. Kaar, **A. R. Lajmi**, *Organizers, Presiding*

8:30 BIOT 18. Rapid screening of monoclonal antibody stability in serum using affinity-capture self-interaction nanoparticle spectroscopy. **S. Geng**, X. Li, M. Chiu, D. Saro, P.M. Tessier

8:50 BIOT 19. Time evolution of protein gel bead microstructure. **D. Greene**, A.M. Lenhoff, N.J. Wagner, S.I. Sandler

9:10 BIOT 20. Fitness landscapes as comprehensive measures of adaptive tradeoffs in the engineering of protein function. **B. Steinberg**, M.A. Ostermeier

9:30 BIOT 21. Asparagine-repeat peptides: Synthesis, characterization, and comparison to glutamine repeats. **X. Lu**, R.M. Murphy

9:50 Intermission.

10:10 BIOT 22. Quantifying the surface hydrophobicity of human gamma-D crystallin and its cataract-associated P23T mutant using molecular dynamics simulations. **E. Wu**, S. Garde

10:30 BIOT 23. Biophysical characterization of reflectin isoforms from squid and cuttlefish. **L. Phan**, W.G. Walkup IV, D. Ordinario, A.A. Gorodetsky

10:50 BIOT 24. Azo-group based novel Naked eye DNA sensors for alcoholic media. **A. Altar**, U. Hashmat, A. Badshah, **B. Lal**, S. Ullah

11:10 BIOT 25. Comparison of real-time and post-mortem techniques for detection of protein fouling. **A. Greenberg**, E. Kujundzic, A. Lajmi, X. Wu

Section D

Grand Hyatt Denver
Grays Peak B

Emerging Technologies

Molecular Delivery

W. Porter, **G. Thurber**, *Organizers, Presiding*

8:30 BIOT 26. Near infrared-degradable crosslinkers for on-demand delivery of hydrophilic molecules. **C. de Gracia Lux**, S. Lee, M. Chan, A. Almutairi

8:50 BIOT 27. Novel light-triggered therapeutics for selective cell phenotypes. **S.M. Goodman**, C.M. Courtney, J. McDaniel, A. Chatterjee, P. Nagpal

9:10 BIOT 28. Kinome-level screening identifies kinase targets for enhancing transient transgene expression. **M. Christensen**, J. Elmer, S. Eaton, L. Gonzalez-Malerva, J. LaBaer, K. Rege

9:30 BIOT 29. Local sustained co-delivery of 25-hydroxyvitamin D3 and parathyroid hormone-related peptide for overcoming antimicrobial resistance. **J. Xie**, J. Jiang

9:50 Intermission.

10:10 BIOT 30. Phosphoramidation-based bioorthogonal reactions for synthesis of nucleic acid conjugates potentially useful in target delivery of DNA/RNA therapeutics. **Y. Su**, T. Wang

10:30 BIOT 31. Histone-targeted gene delivery scaffolds for bone regeneration. **E.V. Munsell**, M.O. Sullivan

10:50 BIOT 32. CMP-based method for achieving tunable, cell-mediated gene delivery. **M. Urello**, K.L. Kiick, M. Sullivan

11:10 BIOT 33. Biomimetic pH-responsive polymers for intracellular therapeutic delivery and theranostic applications. **R. Chen**

Section E

Grand Hyatt Denver
Mt. Elbert B

Colorado Biotechnology

Biomedical Research

N. Boyle, **C. A. Eckert**, *Organizers*
S. Khetani, **M. Krebs**, *Presiding*

8:30 BIOT 34. Modified aptamers and their uses in biomedical research and development. **N. Janjic**

9:10 BIOT 35. Biodegradable, micropatterned wound dressings for enhanced epithelialization. **C.M. Magin**, M.C. Drinker, E.E. Mann, S.T. Reddy, G.S. Schultz, A.B. Brennan

9:50 Intermission.

10:10 BIOT 36. Induced ketosis in mild to moderate Alzheimer's disease. **S. Henderson**

10:50 BIOT 37. Intervening in complex disease biology with microRNA-targeting therapeutics. **W. Marshall**

SUNDAY AFTERNOON

Section A

Grand Hyatt Denver
Grays Peak A

Upstream Processes

Engineering Natural Product Biosynthesis

V. Roy, **M. Thomas**, *Organizers, Presiding*

2:00 BIOT 38. Structure and substrate specificity of AtxE2, a lasso peptide isopeptidase. **J.D. Koos**, **M. Maksimov**, **A. Link**

2:20 BIOT 39. Peptide that neutralizes rattlesnake venom in mice can be expressed in *E. coli*. **E.E. Sanchez**, **M. Suntravat**, **Z. Ahmad**, **A. Cifelli**, **A.S. Rathore**, **C.F. Komives**

2:40 BIOT 40. Synthetic biochemical production of medicinal protoberberine alkaloids in yeast. **S. Galanie**, **C.D. Smolke**

3:00 BIOT 41. Reinventing central carbon metabolism in *Saccharomyces cerevisiae* for high-volume biofuel production. **A. Tsong**, **Y. Tsegaye**, **A. Meadows**, **L. Pickens**, **A. Tai**, **E. Antipov**, **Q. Mitrovich**, **K.A. Curran**

3:20 Intermission.

3:40 BIOT 42. Combinatorial design and assembly for engineering multi-gene systems. **M. Smanski**

4:00 BIOT 43. Diverse opportunities for engineered biosynthesis of complex natural products. **B.A. Pfeifer**

4:20 BIOT 44. Protein interactions in type II fatty acid and polyketide biosynthesis. **M.D. Burkart**

4:40 BIOT 45. Carbon-neutral chemicals from sunlight and CO₂. **S. Liu**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Advances in Chromatographic Separations

A. Hewig, **J. Hubbuch**, **A. R. Lajmi**, **S. Yamamoto**, *Organizers, Presiding*

2:00 BIOT 46. Using powerful HT chromatography screenings to develop purification steps modulating charge-related isoform patterns. **F. Rudolph**, **G. Anja**, **M. Pauers**, **D. Michael**, **J. Studts**, **M. Hampel**

2:20 BIOT 47. Right tool for the job? A critical look at the needs of a diverse product pipeline. **L.W. Pampel**, **J. Aucamp**, **B. Guelat**

2:40 BIOT 48. Robo-characterization: Can HTS miniature columns predict a manufacturing future? **J. Pollard**, **H. Bao**, **M. Petroff**, **S. Kandula**, **N. Tugcu**, **J. Welsh**, **T. Linden**

3:00 BIOT 49. Comparison of PAT based approaches for making real-time pooling decisions for process chromatography – use of feed forward control. **A.S. Rathore**

3:20 Intermission.

3:40 BIOT 50. Optimal elution gradient preparative chromatography. **A. Holmqvist**, **F. Magnusson**, **A. Sellberg**, **B. Nilsson**, **A. Staby**

4:00 BIOT 51. Molecular study on the MabSelect SuRe ligand after treatment under alkaline conditions. **T. Bjorkman**, **F. Berqvist**, **M. Wetterhall**

4:20 BIOT 52. Understanding the effect of salt ions on protein adsorption in novel responsive hydrophobic interaction membrane chromatography. **Z. Liu**, **S.R. Wickramasinghe**, **X. Qian**

4:40 BIOT 53. New generation sorbents for the purification of biomolecules. **J. Champagne**, **M. Schofield**, **A. Uzel**, **G. Balluet**, **R. Gantier**, **M. Touelle**

Section C

Grand Hyatt Denver
Mt Elbert A

Biomolecular & Biophysical Processes**High Concentration Therapeutics: Development, Production & Delivery**

T. Randolph, N. Warne, *Organizers, Presiding*

2:00 **BIOT 54.** Biopharmaceutical informatics: Understanding behavior of highly concentrated antibody solutions at molecular level via coarse-grained modeling and simulations. **D. Tomar**, P. Buck, S. Kumar, S.K. Singh

2:20 **BIOT 55.** Relating protein – protein and protein – solute interactions to protein aggregation rates for low to high protein concentration solutions. **R. Ghosh**, A. Saluja, C.J. Roberts

2:40 **BIOT 56.** Biochemical characterization of the low viscosity reversible protein nanocluster platform. **J. Laber**, B.J. Dear, A. Borwankar, J. Maynard, T. Truskett, K.P. Johnston

3:00 **BIOT 57.** Computational modeling of bulk scale freezing to predict freeze duration and cryoconcentration of biologics in a liquid nitrogen blast freezer. **K. Greco**, R. Falk, J. Cape, T.R. Gervais

3:20 Intermission.

3:40 **BIOT 58.** Role of spatial heterogeneity in protein adsorption on polymeric membrane materials at the single-molecule level. **B. Langdon**, R. Mirhossani, J. Mabry, I. Sriram, A.R. Lajmi, D.K. Schwartz

4:00 **BIOT 59.** Probing protein denaturation at the solid-liquid interface with single-molecule fluorescence microscopy. **J. Weltz**, D.K. Schwartz, J. Kaar

4:20 **BIOT 60.** High concentration abstract TBD. **H. Samra**

4:40 Panel Discussion.

Section D

Grand Hyatt Denver
Grays Peak B

Emerging Technologies**Disease & Biomedical Applications**

K. Lampe, J. Zartman, *Organizers, Presiding*

2:00 **BIOT 61.** Peptoids modulate A β aggregation and alter morphology of fibril species. **J.P. Turner**, M. Moss, S.L. Servoss

2:20 **BIOT 62.** Using backscattering interferometry to characterize interactions of the cystic fibrosis transmembrane conductance regulator with small molecule modulators. **A. Lockwood**, D. Heidary, C.I. Richards, M. Baksh, M. Finn

2:40 **BIOT 63.** Mobile phone based microscopy for imaging and sizing of single DNA molecules. **Q. Wei**, W. Luo, S. Chiang, T. Kappel, C. Mejia, D. Tseng, R. Chan, E. Yan, H. Qi, F. Shabbir, H. Ozkan, S. Feng, A. Ozcan

3:00 Intermission.

3:20 **BIOT 64.** Multifunctional hydrogel assays for 3D culture of melanoma cells reveal increased matrix metalloproteinase activity and migration in response to BRAF/MEK inhibitors. **E.Y. Tokuda**, J. Leight, K.S. Anseth

3:40 **BIOT 65.** Cross species meta-analysis of transcriptome data to unveil the road block of stem cell differentiation to hepatocytes. **R. Raju**, D. Chau, H. Pei, W. Hu

4:00 **BIOT 66.** Design principles of a robust genetic switch using antisense transcription in naturally occurring systems. **A. Escalas Bordoy**, U.S. Varanasi, A. Chatterjee

4:20 **BIOT 67.** Engineered Prussian blue nanoparticles as multimodal molecular imaging agents. **R. Fernandes**

Section E

Grand Hyatt Denver
Mt. Elbert B

Colorado Biotechnology**The Science of Colorado's Craft Beer, Wine & Spirits Industries**

N. Boyle, *Organizer*
C. A. Eckert, *Organizer, Presiding*
R. Sclafani, *Presiding*

2:00 Introductory Remarks.

2:20 **BIOT 68.** Reticulated regulatory network governing glucose fermentation by yeasts. **M. Johnston**

2:40 **BIOT 69.** Utilization of next generation sequencing to develop a real-time qPCR assay for cross-contamination of house brewing yeasts. **D. Driscoll**

3:00 **BIOT 70.** Rapid measurement of beer flavor stability: Application of UPLC-MS metabolomics to develop non-volatile markers of beer stability. **D.L. Sedin**, A. Heuberger, C. Broeckling, J. Prenni

3:20 Intermission.

3:40 **BIOT 71.** Operation of a craft brewery within a major brewery: An overview of Blue Moon Brewing Company. **K. Villa**

4:00 Panel Discussion.

MONDAY MORNING**Section A**

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes**Mammalian Cell Culture Process Development**

N. Jacob, S. T. Sharfstein, *Organizers, Presiding*

8:30 **BIOT 72.** Understanding cell line bubble sensitivity and preparing for future challenges. **R. Ferguson**, W. Hu, H. Peng, K. Wiltberger, T.K. Ryll

8:50 **BIOT 73.** Genome-wide analysis of transgene expression in Chinese hamster ovary cells. **K. Lee**, H. Fu, W. Hu

9:10 **BIOT 74.** Shear contributions to cell culture performance and product recovery in ATF and TFF perfusion systems. **S. Wang**, H. Lin, S. Godfrey, R.W. Leighty, J. Ravikrishnan, A. Osborne, J.L. Coffman, J. Vogel

9:30 **BIOT 75.** Evaluating the impact of copper on CHO cell metabolism and antibody Fc glycan galactosylation using enzymatic assays. **J. Huang**, H. Zhang, M. Trentalange, B. Shah, Z. Zhang, C. Goudar

9:50 Intermission.

10:10 **BIOT 76.** Developing a perfusion process for a novel protein. **S.G. Vajjala**, B. Holman, J.H. Lee, A.E. Schmeizer

10:30 **BIOT 77.** Understanding the transcriptome responses of Chinese hamster ovary (CHO) cells using RNA-seq. **Y. Gowtham**, C. Saski, S.W. Harcum

10:50 **BIOT 78.** Concentrated fed-batch cell culture increases manufacturing capacity without additional volumetric capacity. **W. Yang**, D. Minkler, R.R. Khirsagar, T.K. Ryll, Y. Huang

11:10 **BIOT 79.** Challenges associated when moving from a peptone-containing early stage cell culture process to a chemically-defined late stage cell culture process. **L. Brown**

Section A

Grand Hyatt Denver
Mt. Evans

Marvin J. Johnson Award in Microbial and Biochemical Technology

M. Lazzara, *Organizer, Presiding*

11:30 **BIOT 80.** Mammalian cell factories: Taking small steps forward to keep from drowning in big data. **M.J. Betenbaugh**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes**Non-Chromatographic Separations & Process Integration**

R. Aires-Barros, J. Cyganowski, *Organizers, Presiding*

8:30 **BIOT 81.** High pressure refolding as an alternative technology in protein manufacturing. **L. Gombos**

8:50 **BIOT 82.** Exploring options for continuous diafiltration. **M. Westoby**, A. Brinkmann

9:10 **BIOT 83.** Integrated flocculation and depth filtration high-throughput process development for CHO supernatants. **G. Espuny Garcia del Real**, J.L. Davies, D.G. Bracewell

9:30 **BIOT 84.** Smaller is better: Depth filtration at the 0.2 cm² scale. **A. Noyes**, J. Basha, S. Cook, B. Huffman, D.P. LaCasse, R.S. Wright, R. Fahrner, R. Godavarti, N. Titchener-Hooker, J. Mullin, D. Millard, J. Frostad, K. Sunasara, T. Mukhopadhyay

9:50 Intermission.

10:10 **BIOT 85.** Evaluation of precipitation driven processes for monoclonal antibody downstream processing. **U. Bhaskar**, K. Wei, P. Jorjorian, S. Shrivastava

10:30 **BIOT 86.** Parvovirus filter robustness investigation: The characterization of higher order aggregates and membrane fouling. **B.V. Bhut**, M. Jin, J. Savard, D. Brody, N. De Mas, I. Pla, Z. Li

10:50 **BIOT 87.** Understanding and modeling retention of mammalian cells in a fluidized bed centrifuge. **W.J. Kelly**, J. Scully, J. Rubin, V. Kamaraju, P. Wnukowski, R. Bhatia

11:10 **BIOT 88.** Modelling high concentration tangential flow filtration unit operations. **Y. Lam**, M. Westoby, A. Brinkmann

Section C

Grand Hyatt Denver
Mt. Sopris A

Biomolecular & Biophysical Processes**Engineering Protein Function & Stability**

E. Boder, D. Colby, A. Link, *Organizers, Presiding*

8:30 **BIOT 89.** NMR-guided rational engineering of an ionic liquid tolerant lipase. **E. Nordwald**, G. Armstrong, J. Kaar

8:50 **BIOT 90.** Sense codon reassignment in E. coli: Toward 22 amino acid genetic codes (and beyond). **J.D. Fisk**

9:10 **BIOT 91.** Highly soluble and active human paraoxase variants for quorum quenching. **C. Li**, X. Ge

9:30 **BIOT 92.** Rational design of protein switches based on the ensemble model of allostery. **J.H. Choi**, A.H. Laurent, V.J. Hilsner, M. Ostermeier

9:50 Intermission.

10:10 **BIOT 93.** Laser extraction from micropore arrays enables high-throughput enzyme engineering. **A. Kannan**, B. Chen, F. Sundan, S. Alford, S. Lim, I. Dimov, D. Herschlag, T. Baer, J. Cochran

10:30 **BIOT 94.** Directed evolution of self-cleaving intein purification tags using yeast surface display. **S.D. Stimple**, M.J. Coolbaugh, M. Shakalli Tang, D.W. Wood

10:50 **BIOT 95.** Library-scale evaluation of a computational design and thermostable cel-lulase. **L. Johnson**, L. Gintner, S. Park, C. Snow

11:10 **BIOT 96.** Ultrahigh throughput method for the identification of orthogonal aminoacyl tRNA synthetase/tRNA pairs. **A. Hohl**, X. Liu, J. Eppinger

Section D

Grand Hyatt Denver
Grays Peak

Emerging Technologies**Stem Cells & Regenerative Medicine**

Y. Kim, C. Kirschner, *Organizers, Presiding*

8:30 **BIOT 97.** Emerging technologies for biomaterials at the biological interface. **K. Anseth**

9:10 **BIOT 98.** Photopatterning of site-specifically modified proteins within hydrogel biomaterials. **J.A. Shadish**, C.K. Arakawa, C.A. DeForest

9:30 **BIOT 99.** Hydrogels for controlling stem cell fate through intracellular redox state. **K. Lampe**, L. Russell

9:50 Intermission.

10:10 **BIOT 100.** *Ex vivo* platelet production from hematopoietic stem cells: Understanding the environment and signaling pathways directing proplatelet formation. **T. DeLuca**, L. Hellrich, P. Weingarden, A. Schlinker, L. Shea, W.M. Miller

10:30 **BIOT 101.** Scalable hepatic differentiation of human pluripotent stem cells. **H. Pei**, R. Raju, D. Chau, W. Hu

10:50 **BIOT 102.** Chemical biology technologies to identify small-molecule regulators of cancer stem cells. **J. Lee**

11:10 **BIOT 103.** Thiol-ene Photoclick chemistry as an approach for user directed covalent tethering of bioactive proteins to synthetic hydrogel scaffolds. **I. Marozas**, D. Alge, K.S. Anseth

Section E

Grand Hyatt Denver
Mt. Sopris B

Biosimilars & Follow-on Biologics**Process Development & Manufacturing Considerations for Biosimilars**

F. He, S. Vunnum, *Organizers, Presiding*

8:30 Introductory Remarks.

8:50 **BIOT 104.** Development and commercialization of biosimilar Products: challenges and opportunities. **A.S. Rathore**

9:30 **BIOT 105.** High-throughput multi-parametric clone screening approach for the generation of biosimilar production cell lines. **K. Le**, H. Le, H. Victor, S. Fodor, C. Rollins, T. Munro

9:50 Intermission.

10:10 **BIOT 106.** Overcoming challenges in biosimilar process development: Innovative purification tools to fine-tune biosimilarity. **O.A. Jaquez**, R.S. Gronke

10:30 **BIOT 107.** Purification of a fusion protein containing high HMWs and LMWs. **B. Wang**, D. Wu, J. Shou, S. Liao, J. Fan

10:50 **BIOT 108.** Development of biosimilar drug product in prefilled syringe presentations: Considerations and challenges. **M. Jayaraman**, K. Sampathkumar

11:10 Panel Discussion.

MONDAY AFTERNOON**Section A**

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes**Mammalian Cell Culture Process Development**

V. Janakiraman, I. H. Yuk, *Organizers, Presiding*

2:00 **BIOT 109.** Achieving glycosylation comparability and similarity through cell culture medium optimization. **L. Zhang**, I. Liu, M. Ambhaikar, V. Dandekar, C. Jung, C. Goudar

2:20 **BIOT 110.** Epigenetic studies of anti-body-producing CHO cells for therapeutic applications. **S. Nicoletti**, H. Dahodwala, Z. Kereszteszy, S.T. Sharfstein

- 2:40** **BIOT 111.** Matching dissolved carbon dioxide profiles to achieve comparable cell culture performance across scales. **J.J. Wu, A. Meier, S. Bhardwaj, L. Zheng, K. Tschudi, S.J. Meier**
- 3:00** **BIOT 112.** Control of antibody glycosylation: Application of statistical analysis of manufacturing data coupled with DOE in scale down models to significantly reduce variation in antibody glycosylation. **R.G. Beri, V. Canning, B. Hadley, A. Maxwell, J. Kauten, J. Heimbach, R. Gerber**
- 3:20** Intermission.
- 3:40** **BIOT 113.** Inhibition of intracellular histone deacetylase (HDAC) enzymes for enhancement of transient transgene expression. **J. Elmer, M. Christensen, S. Barua, J. Lehman, K. Haynes, K. Rege**
- 4:00** **BIOT 114.** Application of metabolomic analysis to systematically design fed-batch media for process improvement. **Y. Li, N. Aranibar, B.M. Warrack, J. Yee, M.C. Bony, Z. Li**
- 4:20** **BIOT 115.** Production of highly gamma carboxylated recombinant human factor II with consistent sialylation level in a fed-batch process. **J.H. Lee, J. Reier, K. Heffner, C. Barton, D. Spencer, A. Schmetzer**
- 4:40** **BIOT 116.** Impact of pH control strategies on CO₂ accumulation in bioreactors at different scales. **S. Xu, H. Chen**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Non-Chromatographic Separations & Process Integration

R. Aires-Barros, J. Cyganowski, Organizers, Presiding

- 2:00** **BIOT 117.** Aqueous two-phase systems from natural products to large biomolecules. **R.M. Aires-Barros, A. Azevedo, D. Silva, R. Soares, V. Chu, J. Conde**
- 2:20** **BIOT 118.** Practical experiences in the development of a lab-scale process for the production and recovery of fucoxanthin from *Isochrysis galbana*. **A. Gómez-Loredo, J. González-Valdez, J. Benavides, M.A. Rito-Palomares**
- 2:40** **BIOT 119.** Strategy for primary recovery of a mAb employing harvest treatment and depth filtration. **Z. Tan, R. Martel, N. Singh, M. Jin, A.T. Lewandowski, Z. Li**
- 3:00** **BIOT 120.** Optimizing clarification of feed streams when nanoparticles are the product. **M. Collins, A. Onraedt, R. Leibnitz**
- 3:20** Intermission.
- 3:40** **BIOT 121.** Constrained by the membrane: A case study of harvest process streams fouling single pass tangential flow filters. **K. Petty, E. Gelfroh, N. Soice, A. Hewig**
- 4:00** **BIOT 122.** Novel system design and cleaning strategies for single pass tangential flow filtration systems. **J. Parrella, S. Lau, K. Chan, J. Steen, H. Lutz**
- 4:20** **BIOT 123.** Effect of operating parameters on parvovirus retention by membranes during flow interruption. **D.M. Bohonak, A. Leahy, P. Greenhalgh**
- 4:40** **BIOT 124.** Avoiding the pitfalls of viral clearance experimental design: utilizing representative spiking conditions. **D. Strauss, A. Schwartz, N. Hirotoni**

Section C

Grand Hyatt Denver
Grays Peak

Biomolecular & Biophysical Processes

Engineering Protein Function & Stability

E. Boder, D. Colby, A. Link, Organizers, Presiding

- 2:00** **BIOT 125.** Human therapeutic enzyme specifically sabotages tumor metabolism by an engineered cystine/cysteine degrading activity. **S. Cramer, A. Saha, S. Tiziani, J. Digiovanni, E. Stone, G. Georgiou**

- 2:20** **BIOT 126.** Toward rational design of viscosity reducing mutants of monoclonal antibody therapeutics. **S. Kumar, D. Tomar, P.E. Nichols, L. Li, S.K. Singh**
- 2:40** **BIOT 127.** Biophysical properties of antibody drugs: Predicting and engineering developability. **K. Wittrup**
- 3:20** Intermission.
- 3:40** **BIOT 128.** Structure-based design of CDR mutations that increase the solubility of multi-domain antibody fragments. **L. Zhang, S. Kumar, K. Sunasara, M. Allen, P.M. Tessier**
- 4:00** **BIOT 129.** Genetically encoded unstrained olefins for live cell labelling with tetrazine dyes. **Y. Lee, W. Liu**
- 4:20** **BIOT 130.** Rational identification of scaffolds for combinatorial discovery of ligands. **M. Kruziki, P. Holec, D. Woldring, H. Zhou, B. Hackel**
- 4:40** **BIOT 131.** Withdrawn.

Section D

Grand Hyatt Denver
Mt. Sopris A

Emerging Technologies

New Tools and Approaches

- Y. Kim, J. Zartman, Organizers, Presiding**
- 2:00** **BIOT 132.** Sequence-specific synthetic RNA silencing overcomes antibiotic resistance. **C. Courtney, A. Chatterjee**
- 2:18** **BIOT 133.** Endogenous CRISPR-Cas systems as convenient platforms for genetic screens and pathway engineering. **M. Luo, C. Beisel**
- 2:36** **BIOT 134.** Zeolitic imidazolate framework nanoparticles for imaging and biomedical applications. **C.G. Jones, V. Stavila, C. Ashley, M. Allendorf**
- 2:54** **BIOT 135.** Cell penetrating peptides for stem cell applications. **G. Jin, F. Ghasemi Tahrir, W. Ma, W.H. Suh**
- 3:12** Intermission.
- 3:30** **BIOT 136.** Dynamic stiffening of poly(ethylene glycol)-based hydrogels to direct valvular interstitial cell phenotype in a 3D environment. **K. Mabry, K.S. Anseth**
- 3:48** **BIOT 137.** Layered hydrogels to study development of iPSC-derived neural progenitor cells in 3D. **Z. Zhang, J. Karpiak, A. Muotri, A. Almutairi**
- 4:06** **BIOT 138.** "Sandwich-type" nanofiber skin grafts for skin regeneration. **J. Jiang, J. Xie**
- 4:24** **BIOT 139.** Development of a cellularly degradable PEG hydrogel to promote articular cartilage extracellular matrix deposition. **B.V. Sridhar, J.L. Brock, J.S. Silver, M.A. Randolph, J. Leight, K.S. Anseth**
- 4:42** **BIOT 140.** Photonic crystal platform for biomolecular sensing. **K. MacConaghy, J. Kaar, M.P. Stoykovich**

Section E

Grand Hyatt Denver
Mt. Elbert B

Colorado Biotechnology

Biofuels

- C. A. Eckert, Organizer**
N. Boyle, Organizer, Presiding
K. A. Brown, Presiding
- 2:00** **BIOT 141.** Research in biofuels and bio-products in Colorado. **R.M. Baldwin**
- 2:40** **BIOT 142.** Biobased chemical and fuel development at OPXBIO. **D. Hogsett**
- 3:20** Intermission.
- 3:40** **BIOT 143.** Novel sensors for continuous monitoring of fermentations for biofuels and bioproducts. **K.F. Reardon**
- 4:20** **BIOT 144.** Development and commercialization of fermentative isobutanol production. **A. Hawkins**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

M. Lazzara, A. Kantardjieff Organizers

8:00 - 10:00

223-224, 234-235, 252, 257, 266, 269, 271-272, 274, 301, 320-321, 323, 332, 374, 377. See subsequent listings.

TUESDAY MORNING

Section A

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes

Control of Protein Quality Attributes

B. Hackel, P. M. Hossler, Organizers, Presiding

- 8:30** **BIOT 145.** Process development to lower tryptophan oxidation of a biopharmaceutical produced in chemically defined medium. **L.B. Hazeltine, K.M. Knueven, Y. Zhang, A. Ouyang, Z. Lian, D.J. Olson**

8:50 **BIOT 146.** Controlling the glycosylation profile in MAbs by amino acid supplementation. **D. Radhakrishnan, A.S. Robinson, B. Ogunnaike**

9:10 **BIOT 147.** Framework for real-time peptide-mapping (RT-PM) in bioreactor cultures of recombinant protein producing CHO cells. **T. Tharmalingam, C. Wu, R. Hong, S. Benchaar, C. Goudar**

9:30 **BIOT 148.** Controlling fucose content of glycoproteins expressed in different CHO cell lines. **A. Zhang, V.L. Tsang, L. Markely, G. Kennedy, S. Prajapati, Y. Huang**

9:50 Intermission.

10:10 **BIOT 149.** Unraveling the effect of energy metabolism on N-glycosylation of recombinant protein produced in mammalian cells. **T. Le, A. Yongky, S. Grimm, W. Hu**

10:30 **BIOT 150.** Ways to improve process performance and product quality in high performing fed-batch and perfusion CHO cultures. **T. Falkman, E. Fältt, O. Larsson, A. Vitina, C. Kaisermayer, A. Castan**

10:50 **BIOT 151.** Engineering secretion machinery for high-throughput protein production. **A. Azam, K.J. Metcalf, D.T. Ercek**

Section A

Grand Hyatt Denver
Mt. Evans

BIOT Young Investigator Award

M. Lazzara, Organizer, Presiding

11:30 **BIOT 152.** Toward antibodies by design. **P.M. Tessier**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Vaccines, Non-Antibody & Non-Protein Biological Products

A. Noyes, T. M. Przybycien, Organizers, Presiding

8:30 **BIOT 153.** Virus flocculation and recovery with osmolytes. **M. Gencoglu, C. Heldt**

8:50 **BIOT 154.** Purification of viruses and virus-like particles by ion-exchange and hydrophobic interaction monoliths. **A. Jungbauer, P. Steppert**

9:10 **BIOT 155.** Downstream processing of a large live virus: Challenges in developing a sterile purification process. **A. Kristopeit, M. Wenger, M. Woodling, J. Konietzko, T. Nguyen, S. Wang, K. Phillips, A. Swartz**

9:30 **BIOT 156.** Aminoglycoside antibiotic derived anion-exchange microbeads and monoliths for plasmid DNA binding and in-situ DNA capture. **T. Grandhi, A. Mallik, N. Lin, B. Miryala, T. Potta, Y. Tian, K. Rege**

9:50 Intermission.

10:10 **BIOT 157.** Accelerated process development for the purification and conjugation of a novel protein carrier for a polysaccharide conjugate vaccine candidate. **M.A. Winters, T.J. Svab, S. Wang, J.G. Joyce**

10:30 **BIOT 158.** Integrated bioprocess development based on microscale cultivations and feed stock characterization by chromatography modeling. **P. Baumann, T. Hahn, J. Hubbuch**

10:50 **BIOT 159.** Design and optimization of peptide affinity resins for downstream processing. **S. Timmick, D. Chandra, D. Shastry, C. Goodwine, S. Ruppel, P. Karande, S.M. Cramer**

11:10 **BIOT 160.** Protecting target glycoenzyme from proteolysis during purification. **X. He, M.A. Snyder**

Section C

Grand Hyatt Denver
Mt. Sopris A

Biomolecular & Biophysical Processes

Biomolecular Sensing & Actuation in Membranes

A. Brown, J. Rucker, Organizers, Presiding

8:30 **BIOT 161.** Manipulation of vesicle formation and characteristics using photo-initiated chemistry. **D. Konetski, T. Gong, W. Xi, A.D. Baranek, C. Bowman**

8:50 **BIOT 162.** Developing a chemically specific stimulus-response nanopore. **A. Geiger, L. Keranen Burden, D. Burden**

9:10 **BIOT 163.** Exosome capture technology based on peptide-lipid interactions. **J.P. Saludes**

9:30 Intermission.

9:50 **BIOT 164.** Aggregation of alpha-synuclein in functional model membrane systems. **S. Convalgia, D. Scaini, L. Casalis**

10:10 **BIOT 165.** Understanding the significance of fibroblast activation protein (FAP) homo- and heterodimerization in relation to proteolytic activity. **B. Berger, B. Wonganu**

10:30 **BIOT 166.** Nanodiscs for purification and functional studies of family B G protein-coupled receptors (GPCRs). **Y. Liu, Y. Cai, K. Cuihane, R. Sunahara, E.C. Yan**

10:50 **BIOT 167.** Discovery and characterization of antibodies against membrane proteins using virus-like particles. **J. Rucker**

Section D

Grand Hyatt Denver
Grays Peak

Emerging Technologies

Cellular & Molecular Engineering

A. Chatterjee, D. Colby, Organizers, Presiding

8:30 **BIOT 168.** Transition between multipotent stem cells and embryonic stem cells by chemical factors. **D. Cho, B. Kuang, H. Pei, C.M. Verfaillie, W. Hu**

8:50 **BIOT 169.** High-throughput single-cell imaging reveals that CD4⁺ CAR⁺ T-cell can participate in multikilling through simultaneous conjugation with multiple tumor cells. **I. Liadi, H. Singh, G. Romain, N. Rey-Villamizar, A. Merouane, P. Kebriaei, H. Huls, P. Qiu, B. Roysam, L. Cooper, N. Varadarajan**

9:10 **BIOT 170.** DNA strand displacement induced prodrug activation for cancer treatment. **R.P. Chen, W. Chen**

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at:

www.acs.org/denver2015

- BIOT 236.** Developing optimal MWCNT-modified electrodes for studying the electrochemistry of key redox cofactors and their complexes with aptamers. **I. Emahi, M.P. Mitchell, P.R. Gruenke, D.A. Baum**
- BIOT 237.** Expanding electrochemical DNA biosensors to detect ricin. **L. Fetter, A.J. Bonham**
- BIOT 238.** Diagnostic application of molecular recognition element. **K.L. Hong, K. Imlay, L. Battistella, R.M. Williams, K.M. Hickey, C.D. Bostick, P.M. Gannett, L.J. Sooter**
- BIOT 239.** Peptide internalization triggered by temperature. **M. Oh, C. Hu, M. Arostegui, K. Slowinska**
- BIOT 240.** Recombinant Pif80 protein for nacre-mimicking calcium carbonate biomineralization. **S. Bahn, Y. Choi, H.J. Cha**
- BIOT 241.** Developing microscale themophoresis techniques for analysis of proteins. **J. Devriendt**
- BIOT 242.** Rapid identification of *Listeria monocytogenes* using bacteriophage A511 amplification and enhanced lateral flow immunochromatography. **N. Stambach, S. Carr, C. Cox, K.J. Voorhees**
- BIOT 243.** "Sequence-specific" and "pathogen-specific" antimicrobials using phage-delivered CRISPR-Cas9 gene targeting. **P.B. Oupual, K.E. Erickson, A. Chatterjee**
- BIOT 244.** Comparison of serotonin-expressing mammalian and yeast responses to selected ligands. **K.M. Blocker, A.S. Robinson**
- BIOT 245.** Detection of toxin producing *Vibrio cholerae* and *Escherichia coli* using double biomolecular marker microarray. **H. Shin, C. Kim, B. Hwang, J. Seo, H. Cha**
- BIOT 246.** Directed evolution of haptocorrin into an oral zinc supplement. **Y. Nie**
- BIOT 247.** Investigation of the evolutionary relationship between Rio2 kinases and the canonical eukaryotic protein kinases using X-ray crystallography. **S. Bahmanjah, N.O. Laronde**
- BIOT 248.** Mechanistic study of unusual enzyme activation caused by addition of inert betaine-type metabolite and the analogs. **Y. Nakagawa, K. Koumoto**
- BIOT 249.** Direct observation of single-molecule adsorption/desorption kinetics on ion-exchange adsorbents. **S. Dhmane, M. Poongavanam, W. Chen, U. Patil, L. Kiskey, J. Chen, A.P. Mansur, B. Shuang, S. Dominguez Medina, E. Kulla, M. Kang, K. Kourantzi, C.F. Landes, R.C. Willson**
- BIOT 250.** Bacterial adhesion to complex surfaces: Pair-additive model and pattern-matching. **S. Yoon, L. Edens, J.A. Brozik, D. Keller**
- BIOT 251.** Enzyme-based approaches to kill *Bacillus* spores and other resistant pathogens. **R.V. Mundra, K. Mehta, X. Wu, E. Paskaleva, R.S. Kane, J.S. Dordick**
- BIOT 252.** Identification of the amidase activity and in vitro characterization of the cortex lytic enzyme CwlJ1 of *Bacillus anthracis* spores. **X. Wu, N. Grover, E.E. Paskaleva, R.V. Mundra, M.A. Page, J.S. Dordick, R.S. Kane**
- BIOT 253.** Neuronal differentiation of human stem cells via electrostimulation. **F. Ghasemi Tahrir, G. Jin, W. Ma, W.H. Suh**
- BIOT 254.** Effects of cross-sequence interaction between β -amyloid and human islet amyloid polypeptide on the structure and aggregation of amyloids. **R. Hu, M. Zhang, H. Chen, J. Zheng**
- BIOT 255.** Analysis of monoclonal antibodies using capillary zone electrophoresis: Application to formulation screening. **A. Brousseau, P. Casaz, S. Ozturk**
- BIOT 256.** Feasibility of targeting cells without unique molecular targets. **K. Slowinska, M. Oh, C. Hu, M. Arostegui**
- BIOT 257.** Deimmunization of lectins using computational prediction and membrane-anchored display of correctly folded proteins. **X. Zheng, Y. Choi, C. Bailey-Kellogg, K.E. Griswold, M.P. DeLisa**
- BIOT 258.** Bending lasso peptide structure. **C. Allen, A. Link**
- BIOT 259.** Selective $C(sp^2)$ -H bond functionalization with engineered P450 catalysts. **R. Fasan**
- BIOT 260.** Probing the binding interactions of peptide-polymer coated gold nanoparticle encapsulated drugs with tumor cells by SPR. **A. Brown, Y. Miranda, G. Knoll, I.A. Banerjee**
- BIOT 261.** Improved stability of a model, difficult to formulate IgG3 by DoE-based evaluation of buffer formulations. **B. Chavez, C. Agarabi, E. Read, M. Khan, K.A. Brorson**
- BIOT 262.** Measurement of charge: An important molecular property for predicting high concentration behavior. **B. Balthazor, S. Goswami, Y. He, R. Walters, S. Kumar, D. Boardman, D. Luisi**
- BIOT 263.** Evaluation of different commercially available Protein A resins on the DBC to Nanobodies. **W. Van De Velde, W. Martens, B. Van Der Jeugt, R. Lievrouw, A. Naresh**
- BIOT 264.** Evaluation of various wash and elution buffers across a panel of four monoclonal antibodies for host cell protein reduction during Amsphere Protein A chromatography. **A. Naresh, R. Lievrouw, M. Siwak**
- BIOT 265.** Systematic approach for evaluation of the different DOE designs for biotech applications. **V. Kumar, A.S. Rathore**
- BIOT 266.** Binding mechanisms of viral clearance utilizing multimodal anion exchange chromatography. **M. Brown, K.A. Brorson, S. Lute, B. Chavez, D.J. Roush, T. Linden**
- BIOT 267.** Charge-tunable polyampholytes for the enhanced flocculation of cellular biomass. **K.L. Morrissey, Y. Inaba, M.J. Keirn, A.J. Denham, G.J. Henry, M.P. Stoykovich**
- BIOT 268.** Characterization of CaPure-HA, a new hydroxyapatite resin for the purification of monoclonal antibodies (mAbs) and other biomolecules. **W. Evans, K. Motter, A. Chakrabarti**
- BIOT 269.** Purification of a bispecific antibody using hydrophobic interaction chromatography. **N. Gupta, P.J. Alfonso, D. Bezila, R. Bertrand, M. Capaldi, M. Chiu, P. Haytko, T. Seagreaves**
- BIOT 270.** Development and characterization of a protein A capture step for improved impurity clearance. **N.E. Levy, J.R. Molek, K.E. Goklen**
- BIOT 271.** Engineering of novel staphylococcal Protein A ligands to enable milder elution pH and high dynamic binding capacity. **R. Palmgren, J. Vasic, B. Noren, A. Fors**
- BIOT 272.** Affinity purification of Fab feedstreams. **M. Holstein, N. Bian, M. Jung, M. Bruce, J. Orlando**
- BIOT 273.** HCP clearance strategies for protein A chromatography. **M. Holstein, K.A. Cotroni, N. Bian**
- BIOT 274.** Investigation of variability in the throughput of a platform viral filter. **B. Olson, R. Tedstone, S. Rajendran**
- BIOT 275.** Automated scale-down model for characterization of an affinity chromatography step. **A. Mohanty, R. Tedstone, S. Rajendran**
- BIOT 276.** Ensuring long term robustness of a CIEC chromatographic step for separation of charge variants with optimized yield. **K. Haeringer, E. Rosenberg, S. Heppbildikler, K. Lacki, E. Brekkan, M. Ahnfeldt**
- BIOT 277.** Model-based biopurification process development. **S. Pirrung, A. Hanke, L. van der Wielen, P. Verhaert, E. van de Sandt, M. Eppink, M. Ottens**
- BIOT 278.** Model-based comparison of protein aggregation in integrated and batch-wise downstream processing. **A. Sellberg, F. Ojala, B. Nilsson**
- BIOT 279.** Subtractive panning in phage display for identification of chromatographic affinity peptide ligands. **C. Goodwine, D. Shastry, S.M. Cramer, P. Karande**
- BIOT 280.** Use of multimodal chromatography and protein-protein interaction studies to create separation between antibodies and associated host cell proteins. **S. Ranjan, W.K. Chung, M. Zhu, D. Robbins, S.M. Cramer**
- BIOT 281.** Comparison of binding capacity of TOYOPEARL AF-F Protein A HC-650F affinity resin at varying bed heights. **K. Motter, A. Chakrabarti**
- BIOT 282.** Improvements in downstream processing: minimization in chromatographic steps for early milestones. **D. Shah, H. Li, T. Linden, M. lammarino**
- BIOT 283.** Feasibility study of Raman probe for online measurement of protein concentration during UFDF. **J. Wylie, Y. Xie, H. Cui**
- BIOT 284.** Virus detection using restricted-access adsorbents. **S. Dhmane, M. Adhikari, U. Patil, A. Hagström, K. Kourantzi, U. Strych, R.C. Willson**
- BIOT 285.** Purification of a non-enveloped virus using an aqueous two-phase system. **K. Vijayaragan, A. Zahid, J. Young, C. Heldt**
- BIOT 286.** Chromabolt® prepacked and pre-validated columns: A three-resin validation approach. **S. Rahane, M. Turiano, S. Josephson, N. Bian**
- BIOT 287.** Adsorption characteristics of newly developed protein A and ion exchange media for affinity chromatography. **M. Kiyono**
- BIOT 288.** Method comparison for determining steric mass action isotherm parameters for a multicomponent chromatography model. **K. Tolley, T. Larsen, S. Hunt, R.J. Todd, W. Heymann**
- BIOT 289.** Metal-catalyzed fragmentation of a mAb: A case study. **M. Grooms, E. Wilson, T.B. Vickroy, R.G. Collier, M. Monck, J. Dally, R. Luo, K.E. Goklen**
- BIOT 290.** Development of a novel affinity chromatography medium for platform purification of lambda Fabs. **L. Laurin, P. Hermans, N. Eiler**
- BIOT 291.** Avoiding antibody aggregation in downstream processing: Establishing hold time. **V. Yadav, A.S. Rathore**
- BIOT 292.** Circular dichroism spectroscopy as a tool for rapid screening of monoclonal antibody stability. **V. Yadav, A.S. Rathore**
- BIOT 293.** Neutron reflectivity for characterization of chromatographic interfaces in bioprocessing. **A. Mazzer, L. Clifton, C.J. Roberts, D.G. Bracewell**
- BIOT 294.** Process analytical technologies using a multipath length UV/vis spectroscopy flow cell. **R. Orozco, J. Miller, S. Godfrey, W. Chang, J. Vogel, J.L. Coffman**
- BIOT 295.** Connecting molecular adsorption processes to liquid chromatography. **J. Mabry, M. Skaug, D.K. Schwartz**
- BIOT 296.** High throughput tools and methods for faster protein purification process development. **M. Touelle, J. Champagne, G. Balluet, R. Gantier**
- BIOT 297.** Rapid characterization of HCP removal on adsorptive membranes using protein surrogate markers. **M. Siwak**
- BIOT 298.** Design of a novel agarose-based resin platform. **H.J. Johansson**
- BIOT 299.** High-throughput screening and analytics as tools for efficient purification process design. **J. Spitz, J. Studts**
- BIOT 300.** Toward high-throughput protein refolding and purification: Model-based process development. **P. Saremirad, Y. Zhang, A. Ray**
- BIOT 301.** Investigation and mitigation of high molecular weight species formation on cation exchange chromatography for a monoclonal antibody. **A. White**
- BIOT 302.** Facility fit prediction and debottlenecking of antibody purification facilities. **Y. Yang, S. Farid, N. Thornhill**
- BIOT 303.** Optimization of tangential flow filtration: Control and characterization of aggregates and particles. **E. Schutsky, D. Yu, A.T. Lewandowski, Z. Li**
- BIOT 304.** Automated scale-down model of a commercial chromatography process. **A. Mohanty, R. Tedstone, S. Rajendran**
- BIOT 305.** Effective synthesis of cadaverine from L-lysine using recombinant decarboxylase under CO₂ purging condition. **S. Jeong, E. Choi, S. Byun, D. Cho, Y. Kim**
- BIOT 306.** Influenza vaccine titre determination using Biolayer Interferometry (BLI). **D. Wheatley**
- BIOT 307.** On-column low pH viral inactivation of a pH sensitive protein. **J. Armand, J.P. Pieracci, M. Bakhshayeshi, D. Houde**
- BIOT 308.** Pulse gradient experiments for fast chromatography model development. **K. Westerberg, K. Tolley, S. Hunt, O. Kaltenbrunner**
- BIOT 309.** Process fit modeling to aid in contract manufacturer selection. **S. Howwald, M. Gallup, A. Goerke**
- BIOT 310.** Biopharmaceutical process monitoring using statistical stability metrics. **T. Mistretta**
- BIOT 311.** Reverse phase high performance liquid chromatography (RP-HPLC) as an in-process analytics core competency for upstream and downstream process development. **K. McLaughlin, D. Shah, E. Wu, S.D. Schussler, B. Kilgore, H. Li, T. Linden**
- BIOT 312.** Production planning, scheduling, and debottlenecking practices in the biopharmaceutical industries. **D. Carmichael, C.A. Siletti, D. Petrides**
- BIOT 313.** Biomaterial production process intensification, analysis, and optimization with process simulation tools. **D. Carmichael, C.A. Siletti, D. Petrides**
- BIOT 314.** Engineering synthetic fungal cellulose-degrading complexes. **S.P. Gilmore, C.H. Haitjema, M.A. O'Malley**
- BIOT 315.** Process analytical technology solutions for robust measurement and control of upstream bioprocesses. **E.R. Gibson, K. Lanz, E. Koerperick, D. Cooley, J. Olesberg, C. Evans, G. Small, M. Arnold**
- BIOT 316.** Translating unnatural amino acids with phenotypically-diverse, computationally-engineered EF-Tu variants. **V. Cox, E. Gaucher**
- BIOT 317.** Effect of plant and microbe associated compounds on bacterial cellulose production. **J.L. Strap, A.J. Varley**
- BIOT 318.** Understanding the effect of glycosylation on the stability and biochemical characteristics of cutinases. **A. Shirke, A. Su, D. Basore, M. Ullo, C. Bystroff, R.A. Gross**
- BIOT 319.** In vitro transcription/translation in emulsion produced by a simple flow-focusing device. **M. Murzabaev, T. Mizoguchi, T. Kojima, I. Kobayashi, H. Nakano**
- BIOT 320.** Rapid and high throughput fluorescent protein engineering performed in micro-pore arrays. **S.C. Alford, B. Chen, T. Baer, J. Cochran**
- BIOT 321.** Toward engineering bacterial transcriptional regulators through continuous directed evolution. **T. Cook, A. Yaguchi, M.A. Blenner**
- BIOT 322.** Engineering transcriptional and post-transcriptional repression for synthetic cellular circuits. **T.J. Mansell, A.D. Corts, A. Choudhury, R.T. Gill**
- BIOT 323.** Direct production of propene from the thermolysis of poly(β -hydroxybutyrate). **A. Mittal, H.M. Pilath, D.K. Johnson**

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.

- BIOT 324.** Chaperone overexpression to enhance domain antibody secretion in *E. coli*. **J. Brady, D.B. Ritz, Y. Zhu**
- BIOT 325.** Engineered bacterium with periplasmic carbonic anhydrase as a biocatalyst for CO₂ sequestration. **B. Jo, J. Seo, H. Cha**
- BIOT 326.** Molecular toolkit development for a model cyanobacterium. **H.R. Aucoin, W.E. Sinclair, C. Witherell, N.R. Boyle**
- BIOT 327.** Grafted cellulose with ferulic acid from the residual liquid of corn processing. **E. Torres, R. Manriquez Gonzalez, J. Meza-Contreras, J. Andrade-Hernandez, A. Méndez-Albores**
- BIOT 328.** Process parameter screening utilizing a Plackett-Burman design for a model monoclonal antibody and exploring the linkage between cell culture and downstream processing. **C. Agarabi, E. Read, S. Lute, M. Boyne, J. Schiel, B. Chavez, K.A. Brorson**
- BIOT 329.** Media components for reducing waste accumulation in mammalian cell culture. **C. Cafalletto, W. Yang, A. Ray, V. Shen, R.R. Kshirsagar, T.K. Ryll, Y. Huang**
- BIOT 330.** Microbial production of a hydrocarbon fuel intermediate polyhydroxybutyrate (PHB) from a process relevant lignocellulosic derived sugar stream. **W. Wang, A. Mittal, A. Mohagheghi, D.K. Johnson**
- BIOT 331.** Dosing considerations and impacts on the clarification of mammalian cell culture feed streams using polydiallyldimethylammonium chloride flocculant in conjunction with Clarisolve depth filters. **M. Peck**
- BIOT 332.** High-throughput screening metabolic assay to improve media design for mammalian fed-batch culture. **Y. Li, J. Yee, M.C. Borys, Z. Li**
- BIOT 333.** Methods for quantitative analysis in plant synthetic biology. **K. Schaumburg, W. Xu, C. Zalewski, T. Kassaw, M. Antunes, J. Medford, A. Prasad**
- BIOT 334.** Characterization and modeling of metabolic changes in cyanobacteria during photosynthesis. **F.E. Estep, A. Zimont, G. Peers, A. Prasad, C.A. Peebles**
- BIOT 335.** Analyzing the degradation capacity within *Pseudomonas* sp. strain ADP biofilm. **V. Henry, J.L. Jessop, T.L. Peeples**
- BIOT 336.** Uniaxially aligned, porous collagen-GAG scaffolds for in vitro modeling of human trabecular meshwork. **S. Bernier, M. Pantcheva, M. Krebs**
- BIOT 337.** Using backscattering interferometry to observe label-free observations of molecular interactions of membrane-associated species. **M. Baksh, A. Lockwood, C.I. Richards, M. Finn, D. Heidary**
- BIOT 338.** Ultrathin coatings on polymer substrates for chemically defined culture of human mesenchymal stem cells. **S. Schmitt, A. Xie, W.L. Murphy, P. Gopalan**
- BIOT 340.** Characterization of the alginate lyases from *Vibrio splendidus* 12B01. **A. Badur, G. Yalamanchali, C.V. Rao**
- BIOT 341.** Bioinspired silica nanoparticle with auto-encapsulated carbonic anhydrase as a robust biocatalyst for biomimetic CO₂ sequestration. **B. Jo, J. Seo, K. Baek, Y. Choi, S. Pack, S. Oh, H.J. Cha**
- BIOT 342.** Characterizing technical and biological variance in CHO cell time-series metabolomics data. **H. Le, C. Goudar**
- BIOT 343.** Differential gene expression variability underlies adaptive resistance in heterogeneous populations. **K.E. Erickson, A. Chatterjee**
- BIOT 344.** Effects of key cell culture process parameters on the quality attributes of a therapeutic protein produced by an NSO cell line. **T. Bui, M. Berge**
- BIOT 345.** Efficient approach to perfusion medium development using design of experiments (DoE). **A. Castan, E. Földt, T. Persson, H. Bergling**
- BIOT 346.** Process development to increase productivity with minimal impact to product quality. **L. Cella, Y. Yang, M. Dowling, P. Russo, G.A. Tulloch**
- BIOT 347.** Constraints-based modeling to elucidate the impacts of environmental dynamics on nitrogen gases production by the soil nitrifying bacteria *Nitrosomonas europaea* and *Nitrobacter winogradskyi*. **F. Chaplen, C. Ta, C. Higgins, P. Bottomley, L. Sayavedra-Soto**
- BIOT 348.** *Nitrobacter winogradskyi* responses to Fe limitation. **C. Ta, R. Ferrell, L. Sayavedra-Soto, F. Chaplen**
- BIOT 349.** Transcriptional activation of yeast by split intein-mediated reconstitution of synthetic peptide signals. **K. Siu, W. Chen**
- BIOT 350.** Modulation of gene expression via directed electrical signaling: Electrically sensitive promoters. **Y. Okasheh, R.M. McBee, N.M. Marshall, A.D. Ellington**
- BIOT 351.** Utilization of the separate out of *E. coli* for the development of a protein expression and purification platform. **E. Brune, M.S. Frucht**
- BIOT 352.** Large scale algal oil production for biofuel use: Techno-economic analysis and evaluation. **D. Carmichael, C.A. Siletti, D. Petrides**
- BIOT 353.** Specifically tuned light activated nano-therapeutics for selective cell phenotypes. **C. Courtney, S.M. Goodman, P. Nagpal, A. Chatterjee**
- BIOT 354.** Combinatorial synthesis and cheminformatics modeling of aminoglycoside lipopolymers for transgene expression. **B. Miryala, Z. Zhen, T. Potta, C.M. Breneman, K. Rege**
- BIOT 355.** Aqueous ionic liquid (IL) enzyme mixtures for single-step dissolution and hydrolysis of cellulosic materials. **T. Schutt, C.M. Maupin**
- BIOT 356.** Single cell capture and biochemical analysis using self-folding biocompatible devices. **Q. Jin, M. Li, I. Barman, D.H. Gracias**
- BIOT 357.** Silver nanoparticle-generating mussel adhesive fusion protein as a novel bioinspired surface-independent antibacterial coating material. **H. Hwang, Y. JO, J. Seo, B. Choi, B. Kim, H. Shin, H.J. Cha**
- BIOT 358.** Cellulose hydrolysis in acidified molten salt hydrate reaction media: Insights from kinetic and spectroscopic studies. **W. Deng, G. Tsilomelekis, J. Kennedy, V. Nikolakis**
- BIOT 359.** Response surface methodology for efficient production of biomass and lipids by *Rhodotorula glutinis* grown in pulp and paper wastewater. **M. AmirSadeghi, W.T. French, R. Hernandez, S. Shields-Menard, B. Sukhbaatar**
- BIOT 360.** Fabrication of a nanoconjugate for synergistic antibiotic and photothermal treatment of resistant bacteria. **S.V. Jenkins, D. Meeker, K.E. Beenken, M.S. Smeltzer, J. Chen**
- BIOT 361.** Comprehensive utilization of waste hemicelluloses during ethanol production to increase lactic acid yield: from pretreatment to fermentation. **L. Zhang, T. You, L. Zhang, F. Xu**
- BIOT 362.** Understanding population fluctuations in marine environment. **J. Gardner, N. Boyle, B. Hodge**
- BIOT 363.** Isotope tracer and mass spectrometry reveal engineered xylose metabolism in cyanobacteria. **W. Xiong, J. Yu**
- BIOT 364.** Integration of the alpha-amylase gene into single and high-copy number loci within the *Saccharomyces diastaticus* genome to elicit a high degradation efficiency on a unique starch source. **M.P. Pinto, W. Hagren, S.B. Braun-Sand**
- BIOT 365.** What makes phosphatidylserine a novel regulator of ceramide-1-phosphate transfer proteins? **X. Zhai, D.K. Simanshu, H. Pike, J. Mundy, J.G. Molotkovsky, D.J. Patel, L. Malinina, R.E. Brown**
- BIOT 366.** High throughput process development: Utilization of high-throughput bioreactors and high-throughput analytics for rapid and robust cell culture process development. **S. Rameez, S. Gopalakrishnan, J.S. Notey, S.S. Mostafa, A.A. Shukla**
- BIOT 367.** Evaluation of bicarbonate free medium for improved mammalian cell growth and monitoring in controlled bioreactors. **D. Odenwelder, S.W. Harcum**
- BIOT 368.** Development of a NSO monoclonal antibody producing scale-down model for support of a technical transfer. **E. Hodgman**
- BIOT 369.** Improving scale-up of medium filtration for cell culture processes through understanding of iron effect during large-scale preparation. **J. Tressel, A. Khetan, H. Lin**
- BIOT 370.** Identifying cell signaling regulators of epithelial-mesenchymal transition in carcinoma. **J.M. Buonato, S.S. Yee, E.L. Carpenter, M. Lazzara**
- BIOT 371.** Strategies and considerations for the development of perfusion process for continuous processing based on existing fed-batch platform. **H. Lin, S. Wang, R. Leighty, S. Godfrey, S. Yildirim, A. Osborne, R. Orozco, G. Setiabudi, J. Coby, J.H. Vogel, J.L. Coffman**
- BIOT 372.** Clarification platform evaluation and optimization. **K. Humbard, B. Wang, M. Wagner, K. Chefer, K. Dhanasekharan**
- BIOT 373.** Assessment of down-hole membrane-diffused hydrogen for stimulating uranium reduction and immobilization. **L. Haynes**
- BIOT 374.** Remote activation of TRPV1 for therapeutic effect. **J. Sauer, S. Stanley, R.S. Kane, J. Friedman, J.S. Dordick**
- BIOT 375.** Toward a unified process development strategy for batch and continuous chromatography. **A. Forss, H. Blom, K. Lacki**
- BIOT 376.** Chromatography in periodic counter current chromatography. **H. Blom, H. Skoglar, A. Åkerblom, L. Mathiasson, K. Lacki, A. Forss**
- BIOT 377.** Use of multivariate techniques to develop a predictive model for viral vaccine potency based on raw material components. **A. Purdy, C. Cameron, N. Afanador, H. Fahmy, J. O'Neill**

WEDNESDAY MORNING

Section A

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes

Advances in Biocatalysis

M. A. Blenner, I. R. Wheeldon, *Organizers, Presiding*

8:30 BIOT 378. Metabolic channeling and spatial effects of bifunctional enzymes. **W. Xu, A. Prasad**

8:50 BIOT 379. Controlling local substrate concentrations and enzyme kinetics through rationally designed intermolecular interactions. **Y. Gao, J. Zhu, J. Lin, I. Wheeldon**

9:10 BIOT 380. Microscale tools for rapid evaluation of the two-phase whole-cell bio-oxidation of highly volatile substrates. **J.F. Kolmar, F. Baganz, P. Engel**

9:30 BIOT 381. Engineering recombinant *Escherichia coli* for improved triacetic acid lactone production by screening transposon insertion libraries. **Y. Li, P. Cirino**

9:50 Intermission.

10:10 BIOT 382. Methods to increase substrate conversion in the fungus, *Beauveria bassiana*. **F. Nicolau Manterola, T.L. Peeples**

10:30 BIOT 383. De novo biosynthesis of 1,2-propanediol from renewable feedstock through lactic acid. **W. Niu, J. Guo**

10:50 BIOT 384. Engineering of *Saccharomyces cerevisiae* for the production of long and short chain fatty acids. **C. Leber, B. Polson, R. Fernandez-Moya, N.A. Da Silva**

11:10 BIOT 385. Biosynthesis of key gaso-line-range alkanes using engineered *E. coli*. **A.M. Kunjapur, M. Sheppard, K.L. Jones Prather**

Section A

Grand Hyatt Denver
Mt. Evans

Biotechnology & Bioengineering Awards Presentation and Gaden Award

M. Lazzara, *Organizer, Presiding*

11:30 BIOT 386. Sex and the better biocatalyst. **F.H. Arnold**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Advances and Case Studies in the Use of Disposables, Continuous Processing & Flexible Manufacturing

S. M. Cramer, J. Salm, *Organizers, Presiding*

8:30 BIOT 387. Continuous precipitation-based capture step for recombinant antibodies. **N. Hammerschmidt, S. Hobiger, A. Jungbauer**

8:50 BIOT 388. Control and optimization of a twin-column counter-current chromatography process for affinity capture of biopharmaceuticals. **T. Muller-Spath, N. Ulmer, L. Aumann, M. Bavand**

9:10 BIOT 389. Design and characterization of an incubation chamber for continuous viral inactivation. **R. Orozco, N. Guillen, S. Godfrey, J. Vogel, J.L. Coffman**

9:30 BIOT 390. Development of a continuous MAb purification process. **A. Forss, H. Blom, T. Bjorkman, A. Ljunglöf, B. Westerlund**

9:50 Intermission.

10:10 BIOT 391. Continuous downstream processing for monoclonal antibodies: Are we there yet? **J.Y. Zhang, L. Conley, D. Cecchini, V. Natarajan, S. Ghose**

10:30 BIOT 392. Process economics of continuous mAb processing with single-pass tangential flow filtration. **E. Ayturk, R. Gantier**

10:50 BIOT 393. PAT tool for chromatography supporting batch and continuous processing. **N. Brestrich, A. Sanden, T. Briskot, J. Hubbuch**

11:10 BIOT 394. Feasibility of pH measurement by spectroscopy during continuous low pH virus inactivation in monoclonal antibody production. **J. Goby, J.L. Coffman, E. Zimmermann, M. Strawn, M. Noguchi, J.A. Beller, M. Cortese, J.F. Breit, J. Vogel**

Section C

Grand Hyatt Denver
Grays Peak

Biomolecular & Biophysical Processes

Bionanotechnology

P. Millili, K. Schultz, *Organizers, Presiding*

8:30 BIOT 395. Biofabrication and engineering of ZnS:Mn nanocrystals. **B. Swift, W. Zhou, F. Baneyx**

8:50 BIOT 396. Photoresponsive on/off dormancy in polyplexes for patterned control of cell behavior. **C.T. Greco, T.H. Epps, III, M.O. Sullivan**

9:10 BIOT 397. Functionalization of hydrogels with matrix metalloproteinase-sensitive fluorogenic biosensors to measure cancer cell response to drug treatment. **J.L. Leight, E.Y. Tokuda, K.S. Anseth**

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

9:30 BIOT 398. Synthesis and characterization of a micelle-templated, sub-100 nm PLGA nanoparticle for targeted drug delivery. B.L. Miller, G. Nabar, M.C. Calhoun, J. Xu, M.N. Gurcan, V.K. Puduvali, J.O. Winter

9:50 Intermission.

10:10 BIOT 399. Quantum molecular-se- quencing (QM-Seq): Single molecule DNA and RNA sequencing. J. Casamada-Ribot, A. Chatterjee, P. Nagpal

10:30 BIOT 400. Therapeutic nucleic acid complex micelles. L. Leon Gibbons, E. Chung, Y. Fang, M.V. Tirrell

10:50 BIOT 401. Hemocompatibility of colloi- dally stable glycopolymer-DNA complexes for gene therapy. H.R. Phillips

11:10 BIOT 402. Tunable composite nano- carriers for magnetic resonance imaging, multimodal imaging, and theranostic applications. R.K. Prudhomme

Section D

Grand Hyatt Denver
Mt. Sopris A

Biofuels & Sustainable Energy

Biological Fuel & Energy Production Using Photons & Electrons

C. A. Peebles, A. Singh, *Organizers, Presiding*

8:30 BIOT 403. Prospective bioethylene production process from photosynthetical- ly-fixed CO₂ in recombinant cyanobacteria. J. Markham, J. Yu, L. Tao

8:50 BIOT 404. Understanding and optimizing free fatty acid production in *Synechocystis* sp. PCC 6803. Y. Cheah, C.A. Peebles

9:10 BIOT 405. Metabolic flux analysis of the micro-algae *Chlorella vulgaris* at different CO₂ concentrations under autotrophic, heterotrophic, and mixotrophic growth. M.R. Antoniewicz

9:30 BIOT 406. Role of PII in the nitro- gen-stress response of *Chlamydomonas reinhardtii*. J. Sweeley

9:50 Intermission.

10:10 BIOT 407. Impact of salinity on the kine- tics of CO₂ fixation by *Spirulina platensis* cultivated in semicontinuous photobioreac- tors. J. Ramirez-Perez, H. Janes

10:30 BIOT 408. Understanding the perfor- mance of sugar-yeast-ethanol biohybrid fuel cells. J. Jahnke, D. Mackie, M. Benyamin, S. Liu, R. Ganguli, J. Sumner

10:50 BIOT 409. Engineering the chemolitho- autotroph *Acidithiobacillus ferrooxidans* for chemical and fuel production. S. Banta, X. Li, T. Kernan, S. Majumdar, A. West

11:10 BIOT 410. High performance nanocom- posites produced with cross-linked glucose oxidase aggregates and graphitized meso- porous carbon. T. Garcia-Perez, J. Kim, S. Ha

Section E

Grand Hyatt Denver
Mt. Elbert B

Quality-by-Design for Biopharmaceuticals

Case Studies in QbD Implementation

B. Junker, A. S. Rathore, *Organizers, Presiding*

8:30 BIOT 411. Is QbD more difficult for less defined biopharmaceuticals? A comparison of 3 case studies. M. Streefland, S. Mercier, R. Wijffels

9:10 BIOT 412. Multivariate data analysis methods for qualifying scale-down models. A. Meier, S. Meier

9:30 BIOT 413. QbD as basis for effective development of biopharmaceuticals. J. Panek, J. Gampfer

9:50 Intermission.

10:10 BIOT 414. Implementation of QbD for development of a downstream process for a therapeutic biosimilar. A.S. Rathore

10:30 BIOT 415. Virus filtration QbD knowledge base. H. Lutz

10:50 BIOT 416. Effective strategy for a comprehensive QbD characterization of Viresolve® filter: A collaboration between medImmune and EMD millipore. G. Ferreira, J. Prentice, S. Rajarajan, M. Zhu, M.L. Dickson, H. Lutz, D. Robbins

11:10 BIOT 417. Design space assessment focused on value and probability of success. M. Trexler Schmidt, M. Mun, S. Khoo, N.L. McKnight, A. Mehta, S.J. Meier, R. St. John, B.D. Kelley

WEDNESDAY AFTERNOON

Section A

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes

Microbial Process Development

M. Lipscomb, D. B. Ritz, *Organizers, Presiding*

2:00 BIOT 418. Standardized two-stage bioprocess development using synthetic metabolic valves and dynamic metabolic control. M.D. Lynch, A. Trahan, Z. Ye

2:20 BIOT 422. Optimization of valuable inter- mediates synthesis by 11 alpha-hydroxyl- ation of steroid DHEA by solvent-enhanced biocatalyst. R. Gonzalez

2:40 BIOT 419. Optimization of microbes for industrial bioprocesses using high through- put genome engineering. Z. Serber

3:00 BIOT 424. Increasing soluble expression of an intact Fab (fragmented antibody) in *E. coli* by smart plasmid design and chaperone co-expression. V. Roy, K. Bhare, P. Navarathna, S. Machhi, M. Berge, L. Qu

3:20 Intermission.

3:40 BIOT 420. Engineering a modular network of nonnatural pathways for aromatic chemicals and muonic acid. B. Thompson, S. Pugh, R. McKenna, D.R. Nielsen

4:00 BIOT 421. Development of an enzyme- free process for converting lignocellulosic biomass to fuels and chemicals. B. Pfeleger, J.A. Dumesic, C. Maravelias

4:20 BIOT 339. Regulation of photosynthetic carbon partitioning in a cyanobacterium. M.A. Cano, W. Xiong, D.J. Carrieri, T. Paddock, P. Maness, M.L. Ghirardi, J. Yu

4:40 BIOT 423. New method for peptide production: Modular secretion from *Bacillus megaterium*. N. Marchand, C.H. Collins

Section A

Grand Hyatt Denver
Mt. Evans

Biotechnology & Bioengineering Daniel I. C. Wang Award

M. Lazzara, *Organizer, Presiding*

5:00 BIOT 425. Toward a holistic understanding of cellular metabolism. M.R. Antoniewicz

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Advances and Case Studies in the Use of Disposables, Continuous Processing & Flexible Manufacturing

S. M. Cramer, J. Salm, *Organizers, Presiding*

2:00 BIOT 426. Single-use nonchromato- graphic purification method for antibodies. P. Jorjorian

2:20 BIOT 427. Development and GMP production of novel antibody immuno-PET conjugates using single use/disposable technologies. T. Peram, D. Olson, J. Keba

2:40 BIOT 428. Antibody sieving analysis of multiple microfiltration membranes during a single perfusion cell culture. N. Pinto, W. Napoli, C. Kistler, M. Brower

3:00 BIOT 429. PALL single-use strategy to increase flexibility in manufacturing. J. Griffin

3:20 Intermission.

3:40 BIOT 430. Implementation and characteri- zation of solvent detergent viral inactivation in single use bags. M.A. Cunningham, V. Raman, N. Sood, J. Shea, L. Mullin, E. Youssef, P. Almeida, E.M. Goodrich

4:00 BIOT 431. Considerations when building a single use technology ADC manufacturing. D. Lok, E. Mahajan

4:20 Panel Discussion.

Section C

Grand Hyatt Denver
Mt. Sopris A

Biomolecular & Biophysical Processes

General Topics

C. J. Roberts, H. Samra, *Organizers, Presiding*

2:00 BIOT 432. Understanding the mechanism of in surfo crystallization of membrane pro- teins. A. Samadzoda, A. Vaish, A.S. Robinson, A.M. Lenhoff

2:20 BIOT 433. Specific-ion effects on the aggregation mechanisms and protein-protein interactions for antistreptavidin immunoglobulin Gamma-1. G.V. Barnett, V. Razinkov, B.A. Kerwin, T. Laue, A. Woodka, P. Butler, T. Perevozchikova, C.J. Roberts

2:40 BIOT 434. High-throughput passive microrheology of therapeutic protein solu- tions. L. Josephson, W.J. Galush, E.M. Furst

3:00 BIOT 435. Can aggregation prone states of an antibody fragment be predicted through biophysical analysis? D. Hilton

3:20 Intermission.

3:40 BIOT 436. Cell-material interactions in synthetic hydrogel scaffolds. K. Schultz, F. Escobar, K. Kyburz, D. McKinnon, K.S. Anseth

4:00 BIOT 437. Impact of asymmetric flow field-flow fractionation on antistrepta- vidin IgG1 protein aggregation. C. Bria, K.R. Williams

4:20 BIOT 438. Parameters influencing cavitation within therapeutic vials subjected to drop shock. C. Lengsfeld, D. Sederstrom, M. Puryear, R. Rodrigues

4:40 BIOT 439. Silicone oil microdroplets can act as an adjuvant in protein formulations containing foreign antigen or self antigen. C.F. Chisholm, J. Carpenter, T. Randolph

Section D

Grand Hyatt Denver
Grays Peak

Biofuels & Sustainable Energy

Synthetic Biology Approaches to Engineer Production of Fuels & Energy Molecules

J. Carothers, A. Froehlich, *Organizers, Presiding*

2:00 BIOT 440. Utilization of modular cell and pathway design for combinatorial synthesis of designer bioesters. D.S. Layton, C.T. Trinh

2:20 BIOT 441. 2-Keto acids based biosynthe- sis pathways for renewable fuels and chemi- cals. Y. Tashiro, S.H. Desai, G.M. Rodriguez, S. Atsumi

2:40 BIOT 442. Advanced pathways for micro- bial production of branched C₃ alcohols in *E. coli*. T. Lee, A. Kang, K. George

3:00 BIOT 443. Strain engineering, high-throughput screening, and systems biology analysis for the successful production of renewable chemicals and fuels. M. Leavell

3:20 Intermission.

3:40 BIOT 444. Genome-scale strategies for designing, building, and testing biological systems. R.T. Gill

4:20 BIOT 445. Synthetic biology-enabled strategies for improving ethylene production from engineered *E. coli*. S. Lynch, C.A. Eckert, J. Yu, P. Maness, R.T. Gill

4:40 BIOT 446. Building important molecules from methanol. I.W. Bogorad, C. Chen, M. Theisen, T. Wu, J.C. Liao

Section E

Grand Hyatt Denver
Elbert B

Quality-by-Design for Biopharmaceuticals

Approaches to Process Characterization & Design Space Definition

S. Ahuja, S. Tobler, *Organizers, Presiding*

2:00 BIOT 447. Characterization of a CHO- based monoclonal antibody production process using a quality by design approach. J.C. Goodrick

2:20 BIOT 448. Modeling the preparation of a concentrated nutrient feed solution for a large scale cell culture process. B. Russell, S. Ahuja, G. Miro-Quesada, L. Qu

2:40 BIOT 449. Addressing solution compo- sition variability for process buffers and product intermediates in PC studies and control strategy definition. S.A. Tobler

3:00 BIOT 450. Process characterization: A quality by design approach to scale-down studies across multiple HTPD formats. A. Berrill, J.S. Feliciano, A. Mattias, K. Nilsson Välimaa, Z. Fung, E. Brekkan, B. Evans, J. Salm, R. Godavarti, K. Lacki

3:20 Intermission.

3:40 BIOT 451. Development and charac- terization challenges of an ion exchange chromatography step. J.F. Hsui, A. Mehta, L. Gao, B. Thayer, R. St. John

4:00 BIOT 452. Employment of QbD principles to control charge variants with anion exchange chromatography. B.F. Marques, T. Wiley, S. Weisser, P.R. Smith, K.E. Goklen

4:20 BIOT 453. QbD approach to aggregate control in affinity chromatography. L. Leone, A.T. Lewandowski, Z. Li

4:40 BIOT 454. Quantitative process parameter classification approach for biopharmaceuti- cal development in QbD paradigm. S. Singh, G. Miro-Quesada, L. Qu, R.V. Venkat

THURSDAY MORNING

Section A

Grand Hyatt Denver
Mt. Evans

Upstream Processes

General Topics

N. Agarwal, C. F. Komives, *Organizers, Presiding*

8:30 BIOT 455. Evaluation of extended passing during inoculum expansion of a CHO cell line: a case-study of improving manufacturing flexibility. P. Apostolidis, L. Zhou, P. Thompson, H. Graham

8:50 BIOT 456. Can we predict production instability? Detection of karyotypic changes related to phenotypic changes in CHO cells. J. Baik, K.H. Lee

9:10 BIOT 457. Achieving comparable product quality profiles through cell culture process and media optimization. N.M. Jacob, V. Marczewski, R. Li, S.B. Flanna, E. Kraus, K. Camberg

9:30 BIOT 458. Real-time, continuous moni- toring of cellular nutrients and metabolites for optimization of upstream bioprocesses. M.A. Arnold, E.R. Gibson, K. Lanz, E. Koerperick, D. Cooley, J. Olesberg, C. Evans, G.W. Small

9:50 Intermission.

10:10 BIOT 459. UNICAN: Dual capability in single use bioreactors. E. Mahajan, E. Chan, T. Hudson

10:30 BIOT 460. Efficient, high-titer monoclonal antibody production in a fed-batch process using single-use stirred-tank and rocking bioreactor systems. T. Falkman, E. Fäldt, O. Larsson

10:50 BIOT 461. Sparger design for improved bubble-liquid hydrodynamics in bioreactors. Y. Liu, R. Ferguson, W. Hu, K. Wittberger, S. Hourn, F. Li

11:10 BIOT 462. Improved monitoring in upstream clean-in-place (CIP) operations. V. Saucedo, Z. Li, D. Schimizzi, M. Su, A. Phillips, T.W. Hudson, B. Gan

Section B

Grand Hyatt Denver
Mt. Sopris B

Downstream Processes**Antibodies, Drug Conjugates & Related Molecules**

G. Carta, S. Kandula, *Organizers, Presiding*

8:30 BIOT 463. Development of a manufacturable process to control IgG4 half antibody. **K. Brower**, R. Koduri, M. Yu, K. Karaveg, V. Dhawan, P. Finn, C. Hwang, V. Warikoo, K.B. Konstantinov

8:50 BIOT 464. Approaches to platforming antibody drug conjugate development. **J. Liddell**

9:10 BIOT 465. Downstream process solution to mAb occupancy in glycoengineered pichia. **S. Rios**

9:30 BIOT 466. Development of a downstream purification process for an early phase bispecific antibody: A case study. **A. Ladiwala**, J. Lee, M. Bhaumik, M. Lee, S. Woon, M. Fedesco, C.A. Teske, M. Butler, P. Lester

9:50 Intermission.

10:10 BIOT 467. Antibody drug conjugates: A new platform of protein therapeutic molecules with duocarmycins as cytotoxic agents. **M. Eppink**, G. De Roo, P. Beusker, R. Coumans, R. Versteegen, B. Kampp, H. Spijker

10:30 BIOT 468. Protein A affinity chromatography for efficient purification of recombinant antibody fragments. **A. Stein**, A. Heinen-Kreuzig, A. Kiesewetter, M. Jung, M. Holstein, M. Bruce, J. Orlando, N. Bian

10:50 BIOT 469. Capacity assessment: DBC is not the whole story – implications for resin lifetime and sequential multicolumn chromatography. **E. Trilisky**, J. Ladwig, S. Trimble, J.S. Moscarillo

11:10 BIOT 470. Thorough investigation of the effect of novel sanitization agents on affinity chromatography media. **E. Monie**, A. Grönberg, A. Ljunglöf, M. Wetterhall, T. Bjorkman

Section C

Grand Hyatt Denver
Grays Peak A

Biomolecular & Biophysical Processes**General Topics**

C. J. Roberts, H. Samra, *Organizers, Presiding*

8:30 BIOT 471. Mechanism of cholesterol binding by an RTX leukotoxin. **E. Koufos**, A.C. Brown

8:50 BIOT 472. Photocrosslinking with p-azidophenylalanine used to identify the location of Cic binding on ERK. **A. Futran**, S.Y. Shvartsman, A. Link

9:10 BIOT 473. Rare example of a protein where an isolated domain is more stable than the full-length. **S. Bandi**, S. Singh, K. Mallela

9:30 BIOT 474. Mechanistic details of pH dependent non-photochemical quenching mediated by CP29. **C.A. Lopez**, B. Gennady, R.T. Sayre, S. Gnanakaran

9:50 Intermission.

10:10 BIOT 475. Engineering cellulose-degrading complexes from anaerobic gut fungi. **C. Haitjema**, S. Gilmore, K. Solomon, M.A. O'Malley

10:30 BIOT 476. Promoting binding of protein-targeting substrates by regulating interdomain dynamics within a signal recognition particle: Implications for biotechnology. **F. Gao**, A. Kight, S. Jayanthi, P. Patel, R.L. Goforth, S.K. Thallapuranam, R. Henry, R. Henderson, C.D. Heyes

10:50 BIOT 477. Effect of DNA base orientation on charge transfer reaction. **A. Khan**

11:10 BIOT 478. Conformational study of Δ^5 -tetrahydrocannabinol (Δ^5 -THC) linear and nonlinear circular dichroism. **J. Donnelly**, F.E. Hernández

Section D

Grand Hyatt Denver
Grays Peak B

Biofuels & Sustainable Energy**Development and Deconstruction of Sustainable and Low-cost Feedstocks for Biofuels and Bioproducts**

H. Scheller, G. Sriram, *Organizers, Presiding*

8:30 BIOT 479. Dynamics of CO₂ consumption, and biomass and lipid production during photobioreactor cultivation of the diatom *Cyclotella* under constant incident and constant mean light modes. **A. Ozkan**, G. Rorer

8:50 BIOT 480. Use of synthetic biology to improve bioenergy crops. **A. Eudes**, Y. Liang, D. Loque

9:10 BIOT 481. Base-catalyzed depolymerization of residual solid biomass from a biochemical conversion process. **R. Katurahira**, A. Mittal, K.A. McKinney, G.T. Beckham

9:30 BIOT 482. Innovative pretreatment strategies to generate high-quality sugars from a broad spectrum of biomass resources. **Y.N. Guragain**, K.P. Bastola, R. Barrios, A.R. Kingsly, P.V. Vadlani

9:50 Intermission.

10:10 BIOT 483. Amberlyst 35DRY enhanced 1-butyl-3-methylimidazolium chloride pretreatment of *Arundo donax* Linn. **T. You**, L. Zhang, F. Xu

10:30 BIOT 484. Charge engineering of cellulases improves ionic liquid tolerance and reduces lignin inhibition. **E. Nordwald**

10:50 BIOT 485. Increased lipid production via genetically engineered oleaginous yeast *Rhodospiridium toruloides*. **S. Zhang**, C.V. Rao

11:10 BIOT 486. Over-expression and characterization of four alginate lyases from *Vibrio splendidus* 12B01. **A.H. Badur**, G. Yalamanchali, C.V. Rao

Section E

Grand Hyatt Denver
Mt. Sopris A

Downstream Processes**Mini Topics: Biobased Industry Challenges and a Focus on Impurities**

J. J. Stickel, S. A. Tobler, L. A. van der Wielen, R. C. Willson, *Organizers, Presiding*

8:30 BIOT 487. Continuous enzymatic hydrolysis: Membrane fractionation. **B. Adhikari**, D. Sievers, J.J. Stickel, J. Pellegrino

8:50 BIOT 488. On fractionation of organic fuel precursors from electrolytes with RO and NF membranes. **M. Rickman**, R.H. Davis, J. Pellegrino

9:10 BIOT 489. Flocculant-aided solid-liquid separation of algal and lignocellulosic biomass slurries. **N.C. Crawford**, M. Minot, J.J. Lischeske, D. Sievers, N. Nagle, J.J. Stickel

9:30 BIOT 490. Comparing In situ removal strategies for improving styrene biosynthesis. **R. McKenna**, B. Thompson, L. Moya, M. McDaniel, D.R. Nielsen

9:50 Intermission.

10:10 BIOT 491. Impact of elution pH on product and process related impurities in Protein A chromatography. **D. Yu**, E. Schutsky, L. Leone, Z. Tan, A. Lewandoski, M.C. Borys, Z. Li

10:30 BIOT 492. Two-stage chromatographic separation of aggregates for monoclonal antibody therapeutics. **V. Kumar**, A.S. Rathore

10:50 BIOT 493. Heterogeneous high molecular weight species in purification platform. **Y. Li**

11:10 BIOT 494. Development of platform host cell protein enrichment strategies for use in impurity spike challenge studies. **R.G. Soderquist**, R. Hart

THURSDAY AFTERNOON**Section A**

Grand Hyatt Denver
Mt. Evans

Upstream Processes**Engineering Non-model Hosts for Biological Production**

S. Atsumi, Y. Huo, A. Sato, *Organizers, Presiding*

2:00 BIOT 495. Production of bispecific antibodies in “Knobs-into-Holes” using a cell-free expression system. **Y. Xu**

2:20 BIOT 496. Robustness and productivity: Lessons from metabolic engineering and RNA-Seq studies in *Zymomonas mobilis*. **S. Yang**, M. Zhang, Y. Chou, T. Vander Wall, W. Michener, P. Pienkos

2:40 BIOT 497. Anaerobic advanced biofuel production in *Zymomonas mobilis*. **M. Zhang**, Y. Chou, M. Franden, S. Yang

3:00 BIOT 498. Engineering *Clostridium thermo- cellum* for hydrogen production. **K.J. Chou**, L. Magnusson, P. Maness

3:20 Intermission.

3:40 BIOT 499. Photosynthetic limonene and bisabolene production in wild type and a glycogen-deficient mutant of *Synechococcus* sp. PCC 7002. **F.K. Davies**, S.A. Jackson, J.J. Eaton-Rye, M. Posewitz

4:00 BIOT 500. Synthetic biology approach to improving cyanobacterial chemical production. **N. Nozzi**, S. Atsumi

4:20 BIOT 501. Transferring nitrogen fixing capabilities to an oxygenic photosynthetic organism. **A. Balassy**, M. Bhattacharyya, A. Hoynes-O'Connor, C. Immetun, M. Liberton, D. Liu, T. Mueller, Y. Xiao, J. Yu, T. Moon, F. Zhang, C. Maranas, H. Pakrasi

4:40 BIOT 502. Engineering ORCA3 and SGD in *Catharanthus roseus* hairy roots increase alkaloid production. **J. Sun**

Section B

Grand Hyatt Denver
Mt. Sopris B

Downstream Processes**Antibodies, Drug Conjugates & Related Molecules**

G. Carta, S. Kandula, *Organizers, Presiding*

2:00 BIOT 503. Toward improving selectivity in Protein A chromatography with PEGylated ligands: High throughput characterization of PEGylation strategies. **J.B. Weinberg**, T.M. Przybycien

2:20 BIOT 504. Alternative multimodal process for the capture of monoclonal antibodies based on phenylboronic acid chromatography. **A.M. Azevedo**, S. Rosa, R. Santos, R.M. Aires-Barros

2:40 BIOT 505. Antibody aggregation in the mobile phase. **F. Ojala**, A. Seilberg, T. Budde Hansen, E. Broberg Hansen, A. Staby, B. Nilsson

3:00 BIOT 506. Rapid ranking of high-concentration monoclonal antibody formulations using manufacturability indices. **Y. Yang**, A. Velayudhan, S. Farid, N. Thornhill

3:20 Intermission.

3:40 BIOT 507. Withdrawn.

4:00 BIOT 508. High capacity salt tolerant weak cation exchange media for mAb purification: Improved process performance through efficient pH transition and control. **D.M. Kanani**, N. Sidhu, N. Paghda, J. Stout

4:20 BIOT 509. Eliminate downstream facility constraints for high titer cell culture processes. **M. Zhu**, J. Savery, J. Bender, G. Miroquesada, D. Robbins

4:40 BIOT 510. Understanding HCP binding to depth filters: Can we qualify depth filters for purification? **N. Soice**, E. Zinn, K. Petty, R. Alvarado, J. Espinoza, A. Hewig

Section C

Grand Hyatt Denver
Grays Peak A

Biomolecular & Biophysical Processes**High-Throughput Biomolecular Engineering and Characterization**

I. V. Korendovych, I. R. Wheeldon, *Organizers, Presiding*

2:00 BIOT 511. Engineering a lasso peptide display system for directed evolution applications. **C. Zong**, A. Link

2:20 BIOT 512. Characterization and directed evolution of aminoacyl tRNA synthetases. **J. Tullman**, L. Wu, S. Li, J.P. Marino

2:40 BIOT 513. Physiological assay designed to quantify the efficacy and potency of antimicrobials. **M.A. Ketchum**, J.D. Rimer, P.G. Vekilov

3:00 BIOT 514. Application of automated micro-UF/DF system for high-throughput formulation development. **C. Ren**, K. Westland, R. Rajan, S. Lambert, R. Burge

3:20 Intermission.

3:40 BIOT 515. Design and selection of peptides with specific recognition properties for protein purification and analysis. **D. Chandra**, S. Timmick, C. Goodwine, D. Shastri, S.M. Cramer, P. Karande

4:00 BIOT 516. Computational design and directed evolution of allosterically regulated enzymes. **I.V. Korendovych**

4:20 BIOT 517. Design and discovery of short peptides for biocatalysis and self-assembly. **R. Uljin**

4:40 Panel Discussion.

Section D

Grand Hyatt Denver
Grays Peak B

Biofuels & Sustainable Energy**Biomass Pretreatment & Hydrolysis**

K. Brandon Sutton, M. A. O'Malley, *Organizers, Presiding*

2:00 BIOT 518. RAPT (reversible acid pretreatment) for cellulosic ethanol production. **P.R. Weider**, R. Blackburn

2:20 BIOT 519. Identification of topochemical features associated with cell wall recalcitrance to dilute acid pretreatment in *Miscanthus x giganteus*. **Z. Ji**, X. Zhang, Z. Ling, B. Wu, F. Xu

2:40 BIOT 520. Alkaline pretreatment of corn stover: Optimal pretreatment conditions and development of new analytical methods for quantification of chemical compounds within lignin rich liquors. **E.M. Karp**, P. Ciesielski, B. Donohoe, S. Deutch, M.J. Biddy, G.T. Beckham

3:00 BIOT 521. Comparative analysis of extremely thermophilic *Caldicellulosiruptor* species provides insights into cellular strategies for plant biomass deconstruction. **J. Zurawski**, H. Simpson, J.A. Izquierdo, J.M. Conway, L.L. Lee, S.E. Blumer-Schuetz, R.M. Kelly

3:20 Intermission.

3:40 BIOT 522. Combination of enzyme paradigms and biomass pretreatment reveal novel saccharification mechanisms. **M. Resch**, B. Donohoe, C.H. Haitjema, A. Mittal, P. Ciesielski, G. Beckham, M. Himmel, M.A. O'Malley, S. Decker

4:00 BIOT 523. Differential binding of biomass hydrolyzing enzymes to lignin: Conversion yields suggest a paradigm shift. **J. Yarbrough**, A. Mittal, L.E. Taylor, S.E. Hobday, E. Mansfield, D. Sammond, S. Decker, M.E. Himmel, T.B. Vinzant

4:20 BIOT 524. SPORL for robust bioconversion of Douglas-fir forest residue: Pilot scale-up design, lignin co-product, and high solids fermentation without detoxification. **J. Zhu**

4:40 BIOT 525. SSF-IL: Enabling simultaneous saccharification and fermentation in ionic liquid for high-yield conversion of cellulose into alpha-ketoglutaric acid. **S. Ryu**, N. Labbe, C.T. Trinh

Section E

Grand Hyatt Denver

Mt. Sopris A

Downstream Processes

Leveraging Fundamentals for Accelerated Downstream Process Development

A. C. Dumetz, M. Ottens, E. von Lieres,

Organizers, Presiding

2:00 BIOT 526. Robust characterization of the chromatographic behaviour of complex biological feedstocks. **A.T. Hanke**, P.D. Verhaert, L.A. van der Wielen, E.J. van de Sandt, M.H. Eppink, M. Ottens

2:20 BIOT 527. Efficient and reliable model calibration in column chromatography with Optimal Experimental Design (OED). **T. Hahn**, G. Wang, T. Huuk, J. Hubbuch

2:40 BIOT 528. Computational investigation into mAb adsorption behavior under high loading conditions for cation exchange chromatography. **S. Hunt**, K. Tolley, T. Larsen, B. Smith, E. von Lieres, R.J. Todd

3:00 BIOT 529. Model-based optimization and control of process scale ion exchange chromatography for therapeutic proteins. **V. Kumar**, E. von Lieres, A.S. Rathore

3:20 Intermission.

3:40 BIOT 530. Rationale purification development: Leveraging molecular biophysics to target purification modalities. **D.J. Roush**, F. Insaïdo, J. Welsh, T. Linden

4:00 BIOT 531. Binding of proteins to multimodal chromatographic surfaces: A molecular modeling perspective. **S. Banerjee**, S. Parimal, S. Garde, S.M. Cramer

4:20 BIOT 532. Mass transfer resistance as evidence of resin fouling: Accelerated experimental techniques. **P. Smith**, A. Pike, B.F. Marques, A.R. Ubiara, K.E. Goklen

4:40 BIOT 533. Multi-addition batch uptake: A novel high-throughput approach for measuring intra-particle mass transfer. **S.J. Traylor**, X. Xu, Y. Li, M. Jin, Z. Li

9:30 BIOL 4. Small-molecule modulation of apoptosis via direct targeting of pro-apoptotic BAX. **D. Reyna**, T. Garner, F. Kopp, Y. Wu, N. Biris, U. Steidl, R. Kitsis, **E. Gavathiotis**

9:50 BIOL 5. Chemoproteomic profiling of lysine acetyltransferases highlights an expanded landscape of catalytic acetylation. **J.L. Meier**, D. Montgomery, A. Sorum

10:10 Intermission.

10:30 BIOL 6. Tabtoxinine- β -lactam inhibits glutamine synthetase by an ammonia capture mechanism. **T.A. Wenczewicz**, U. Wanninayake, G.J. Patrick

10:50 BIOL 7. Evolution of Src homology 2 domain. **T. Ju**, W. Niu, **J. Guo**

11:10 BIOL 8. Quadruplet codon decoding. **N. Wang**, W. Niu, E.D. Hankore, **J. Guo**

11:30 BIOL 9. Substoichiometric hydroxynonylation of a single protein recapitulates whole-cell-stimulated antioxidant response. **Y. Aye**, S. Parvez

SUNDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Complex Enzymatic Transformations

V. Bandarian, Organizer, Presiding

2:30 BIOL 10. Gut reactions: Understanding radical enzymes from the human microbiota. **E.P. Balskus**

3:15 BIOL 11. Mechanism of the C5 stereo-inversion reaction catalyzed by the Fe(II)- and 2-oxoglutarate-dependent enzyme, CarC, in the biosynthesis of carbanemem antibiotics. **W. Chang**, Y. Guo, C. Wang, S.E. Butch, A.C. Rosenzweig, A.K. Boal, C. Krebs, J.M. Bollinger

4:00 BIOL 12. Experimental strategies for functional annotation and metabolism discovery: Targeted screening of solute binding proteins and unbiased panning of metabolomes. **S. Almo**

4:45 BIOL 13. Mechanistic studies of tRNA hypermodification. **V. Bandarian**

SUNDAY EVENING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Michael A. Marletta

C. M. Crews, Organizer, Presiding

7:00 BIOL 14. Award Address (Alfred Bader Award in Bioinorganic or Bioorganic Chemistry sponsored by the Alfred R. Bader Fund). At the interface between chemistry and biology: Two examples. **M.A. Marletta**

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Current Topics in Biological Chemistry

V. Bandarian, C. M. Crews, Organizers

8:15 - 9:45

BIOL 15. Quantifying vGlut2 terminals in the rat medial geniculate body. **Z.J. Diaz-Reguero**

BIOL 16. Identification of unique cell surface receptors on breast cancer stem cells by using combinatorial chemical library. **C. Long**, J. Lee

BIOL 17. Biophysical parameters that determine RNA-metal complex formation. **R. Whitaker**

BIOL 18. Characterization of the pyruvyltransferase WcfO from the CPSA biosynthetic pathway. **S. Sharma**, J.M. Troutman

BIOL 19. Advancing tetrazine ligations to develop fluorogenic probes for cellular imaging. **N.K. Devaraj**

BIOL 20. Design and biological screening of steroidal analogs as selective estrogen receptor modulators. **F.T. Halaweish**, A. Ahsayari, L. Kopel, M. Ahmed

BIOL 21. Thermostabilization of 3-dehydroshikimate dehydratase: A pivotal enzyme in commodity chemical biosynthesis. **L. Harrington**, R. Jha, T. Kern, C. Strauss, G. Canales, K. Hotta, A.T. Koppisch, **D.T. Fox**

BIOL 22. Helicase recruitment to sub-cellular granules during viral infection. **M. Corby**, A. Mahim, G. Biener, V. Raicu, D.N. Frick

BIOL 23. Exploiting molten salts for concerted pathogen neutralization and transdermal drug delivery. **T. Kern**, K.S. Lovejoy, M. Zakrewsky, M. Janicke, A. Newsham, M. Jones, S. Mitragotri, A.T. Koppisch, R.E. Del Sesto, **D.T. Fox**

BIOL 24. Characterization and manipulation of acylase enzymatic activity of calreticulin using redesigned ligands. **A. Akinyemi**, L. Larkin, W. Marsh, L. Maynard

BIOL 25. Structural biochemistry of a fungal LOV domain photoreceptor reveals an evolutionarily conserved pathway integrating blue-light and oxidative stress. **B.D. Zoltowski**, J. Lokhandwala

BIOL 26. Identification of novel inhibitors of 6-phosphogluconate dehydrogenase (6PGDH) in *Trypanosoma brucei* through virtual drug screening. **V. Gomez**, K. Kolavasi

BIOL 27. Detection of heavy metal ions using green fluorescent protein biosensors by quenching FRET from endogenous aromatic amino acids. **A. Beranek**, B. Hicks

BIOL 28. Alternative ELISA using a RNA aptamer against calf intestinal alkaline phosphatase. **V.D. Huynh**, E. Wei, G.M. Stovall

BIOL 29. Insights into the biochemical characterization of [FeFe]-hydrogenase Maturase HydF. **A. Byer**, J.B. Broderick

BIOL 30. Benefits of being contained: The protection of nucleic acids inside prebiotic cell models. **M. Joseph**, D. Gifeisman, **S.E. Maurer**

BIOL 31. Peptidomimetics as dual function antimicrobial and anti-inflammatory agents. **C. Smith**, J. Cai, H.H. Yin

BIOL 32. Withdrawn.

BIOL 33. Selective G-quadruplex DNA photocleavage agents: *N*-methyl-mesoporphyrin IX. **D. McBrayer**, M.L. Schoonover, S.M. Kerwin

BIOL 34. mRNA expression of amino acid transporters in *Eimeria tenella* infected broilers. **K. Miska**, J. Santiago-Feliciano

BIOL 35. H-loop and E-loop of human glutathione synthetase. **M.E. Anderson**, T.R. Cundari, B.L. Ingle

BIOL 36. Chemical tools to study E3 ubiquitin ligases. **A. Statsyuk**, S. Park, D.T. Krist, S.G. Kathman, Z. Xu

BIOL 37. Structural and functional studies of TSP0. **C.T. Nordyke**, N. Susanti, J. Sharpe, K. Varga

BIOL 38. Engineering virus-like particles toward directing protective immunologic responses. **D. Patterson**, A. Pynda-Apple, A. Hamsen, T. Douglas

BIOL 39. Biosynthetic studies on the antitumor antibiotic pactamycin. **C.J. Brumsted**, T. Mahmud, M.E. Abugreen

BIOL 40. Withdrawn.

BIOL 41. Studies toward the total synthesis of chrolactomycin and the development of novel small molecule telomerase inhibitors. **E.J. Lee**, K. Scheidt

BIOL 42. Thermal stability and functional implications of short RNA strands containing 7,8-dihydro-8-hydroxyadenosine. **M.J. Resendiz**

BIOL 43. Cellular response to sertraline, paroxetine, and fluoxetine of IMR-32 neuroblastoma cells in vitro. **M. Feuerstein**, M.L. Pajski

BIOL 44. Development of new BF₂ azadipyrromethene near-infrared fluorochromes. **D. Wu**

BIOL 45. Interaction of the antimicrobial peptide aurein 1.2 with lipid raft model membranes. **A. Alhewaitay**, A. Sunda-Meya, N. Pamburu

BIOL 46. Selectivity, cooperativity, and competition in the binding of heterocyclic diamidines to DNA. **S.A. Winkle**, A. Hassan, d. rodriguez, C. Vega, C. Winkle

BIOL 47. Sequence and topological specificity in the binding of tetra(*N*-methylpyridyl) porphines to DNAs. **S.A. Winkle**, A. Llodra, J. Barretta, M. Ballester, R. Castillo, D. Edgar

BIOL 48. Investigating the structural dynamics transitions of human adipocyte fatty acid binding protein by NMR spectroscopy. **K. Ha**, Y. Xia, Y. Tran, **A. Ojoawo**, G. Veglia, D. Bernlohr

BIOL 49. Use of site-directed mutagenesis and cyanide binding studies to understand the oxygen sensing mechanism of the SmFixL protein, a member of the heme-PAS and histidine kinase families. **M.F. Reynolds**

BIOL 50. What makes Lyme disease tick? Impact on DNA-protein interactions by mutations to regulator BosR. **S.E. Evans**, L. Evans

BIOL 51. Structure and inhibition of acyl protein thioesterases. **K.J. Labby**, B.R. Martin

BIOL 52. Characterization of the colanic acid biosynthesis pathway with a novel isoprenoid analog. **P. Scott**

BIOL 53. Mutant firefly luciferases catalyze light emission with complementary synthetically modified luciferins. **M.A. Paley**, W.B. Porterfield, D.C. McCutcheon, R.C. Steinhart, C.M. Rathbun, J.A. Prescher

BIOL 54. Structural and functional characterization of the antifreeze protein ApAFP752. **K.W. Elliott**, S. Follett, P. Jevtic, D. Levy, K. Varga

BIOL 55. Probing phagocytosis of Janus particles. **L. Sanchez**, Y. Yu

BIOL 56. Synthesis and evaluation of substituted coumarin derivatives as inhibitors of monoamine oxidase B. **I. Kieffer**, E. Oduaran

BIOL 57. Oxidation of α -crystallin Len protein resulting from xanthurenic acid radical. **C.N. Follou**, C. Knuston, J.E. Roberts, B.E. Sturgeon

BIOL 58. Lipoic acid organic nanoparticles (ONPs) for bacterial inhibition: Synthesis, characterization, and antibacterial studies of doped and undoped ONPs with Ag/Au NPs. **T. Pandiyan**, A. Pérez Jiménez, C. Huerta Aguilar, A. Romero Silva, J. Vázquez Ramos, J. Narayanan

BIOL 59. Biochemical analyses of ATP binding and hydrolysis in DEAD-box proteins. **H. Englert**, I. Garcia

BIOL 60. Blinking of quantum dot probes in measurements of molecular rotation on cell surfaces. **D. Zhang**, P. Winter, D. Roess, B. Barisas

BIOL 61. Molecular dynamics studies of the role of protein flexibility in immunological molecular recognition. **C. Ayres**, D. Scott, B. Baker, S. Corcelli

BIOL 62. Antimicrobial peptide and anisotropy. **S. Jocelin**, E.R. Middleton

BIOL 63. Effect of cell treatment conditions on glutathione levels and cell viability. **A.M. Khobeir**, J. Shultz, J. Cali, J. Kelts

BIOL 64. 2D Spectral-spatial rapid scan electron paramagnetic resonance imaging of spin trapped adducts at 250 MHz. **D.G. Mitchell**, J.R. Biller, S. Eaton, G.R. Eaton, G.M. Rosen, J.P. Kao

BIOL 65. Structural and kinetic characterization of *E. coli* oxidoreductase YqhD. **J.M. Ellis**, R. Verma, J. Bann, K.R. Mitchell-Koch

BIOL 66. Study and characterization of the sugar-modifying enzymes of the capsule biosynthesis pathway of *Vibrio vulnificus*. **J.M. Hazel**, K.M. Erickson, M.A. Chahoud, J.M. Troutman

BIOL 67. Characterization of the C-terminal domain of CGI-112, a protein involved in the ER-associated degradation pathway. **K.R. Gallagher**, N. Bachman, S. Bolde, A. Rothfuss

BIOL

Division of Biological Chemistry

C. M. Crews and V. Bandarian, Program Chairs

OTHER SYMPOSIA OF INTEREST:

Interfacial and Biomolecular Recognition

(see COLL, Sun, Tue, Wed, Thu)

Undergraduate Research Posters (see

CHED, Sun, Mon)

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis (see CHED, Tue)

SUNDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Young Investigators in Biological Chemistry

C. M. Crews, Organizer, Presiding

8:30 BIOL 1. Award Address (Nobel Laureate Signature Award for Graduate Education in Chemistry Sponsored by Avantor Performance Materials). Expansion of the genetic alphabet in vitro and in vivo. **D. Malyshev**, K. Dhami, T. Laverigne, T. Chen, N. Dai, J. Foster, I. Correa, F.E. Romesberg

8:50 BIOL 2. Chemical probes to explore histidine kinase signaling. **K. Wilke**, R. Godsey, E.E. Carlson

9:10 BIOL 3. Novel base-modified nucleotides terminating DNA synthesis and their applications in chemistry of life processes. **V.A. Litosh**

- BIOL 68.** Riboregulators as tunable gene switches for post-transcriptional control of gene expression. **M. Krishnamurthy**, S.P. Hennelly, K.Y. Sanbonmatsu, C.J. Unkefer
- BIOL 69.** Ribosome-associated complex antagonizes prion formation in yeast. **A. van Ooy**, D. Cameron, A. Amor, D. Selechnik, S. Delaney, D. Castanzo
- BIOL 70.** Magnetic field effects on charge transport through DNA. **T.J. Zwang**, S. Hurlimann, M.G. Hill, J.K. Barton
- BIOL 71.** Identifying the direct effects of Mn^{2+} , Fe^{2+} and small molecule drugs on the iron responsive element in the human FTH1 IRE/IRP complex. **E.T. Mendenhall**, B. Wang, M.L. Norton, W.L. Patterson, M. Rahman, B.S. Day
- BIOL 72.** Kinetic investigation of the active site base of recombinant F_{10} -dependent glucose-6-phosphate dehydrogenase from *Mycobacterium tuberculosis*. **M. Ouygi**, E. Joseph, K.L. Johnson-Winters
- BIOL 73.** Design, synthesis, and protein crystallography of novel potent inhibitors of macrophage migration inhibitory factor. **J. Cisneros Trigo**, P. Dziedzic, M.J. Robertson, W.L. Jorgensen
- BIOL 74.** Chemical modifications of catalytically important residues of enzyme lysyl oxidase. **E.J. SteMarie**, C. Gomes, C.D. Palmer, M. Zinter
- BIOL 75.** Excess iron and copper induced alterations in microRNA expression as a new role for metals in neurodegeneration. **N.L. Iyer**, C. Hung, S.K. Szwed, K. Khanuja, **M.J. Sever**
- BIOL 76.** Cytoskeletal protein analysis from *Tetrahymena thermophila* utilizing solution NMR studies and confocal microscopy. **R. Steiner**, J. Honts, A. Kilpatrick
- BIOL 77.** Progress toward the synthesis and evaluation of luciferin derivatives for bioluminescence imaging. **I. Fields**, K.S. Huang, C. Miller
- BIOL 78.** Profiling the role of galectin-9 in modulating the HA/CD44 interaction. **S.V. Durbin**, R.G. Barkley, L.N. Jude, A.M. Campbell, N.L. Snyder
- BIOL 79.** Menaquinone biosynthesis: An antibacterial target? **J. Matarlo**, C. Evans, D.S. Tan, P.J. Tonge
- BIOL 80.** Recycling histidine tagged thermophilic enzymes with magnetic beads. **D. Finocchietti**, J. Howland, **P. Woodruff**
- BIOL 81.** KinEXA-based immunosensor for measuring the salivary level of CA15-3: An efficient technology for diagnosis and management of breast cancer. **I. Darwish**, T. Wani
- BIOL 82.** Nanoluciferase fragments as sensitive probes for protein solubility in living cells. **J. Zhao**, Q. Vu, T. Truong, T. Nelson, C. Stains
- BIOL 83.** 2-Iminohydantoin, a mutagenic lesion, is a major oxidation product of 2'-deoxyguanosine with hydroxyl radical. **O. Alshykhyly**, A.M. Fleming, C.J. Burrows
- BIOL 84.** Fluorogenic chemical inducers of protein oligomerization. **B. Xu**, X. Zhou, C. Stains
- BIOL 85.** Isolation and purification of *Entamoeba histolytica* alcohol dehydrogenase 2 (EhADH2) enzymatic activities and inhibition by pyrazoline derivatives. **J.A. Leitao**, H. Kumar, L. Rossi, D. Oduaran, A. Espinosa
- BIOL 86.** Withdrawn.
- BIOL 87.** Controlling the phosphoproteome: Ligand activated split-kinases. **M. M.E. Ghaffari**, K. Camacho-Soto, J. Castillo-Montoya, I. Ghosh
- BIOL 88.** Disruption of insect isoprenoid biosynthesis with pyridinium biphosphonates. **S.E. Sen**, A. Jones, T. Horsfield
- BIOL 89.** Unique features of isoprenoid forming enzymes in moths: implications for the biosynthesis of homologous juvenile hormones. **S.E. Sen**, M. Grasso, J. Macor, L.M. Wood, R. Jacob, A. Jones, T. Horsfield, A. Tomasello, J. Hitchcock, M. Cusson
- BIOL 90.** C-reactive protein conformational states alter biological reactivity. **C.L. Moon**, A.A. Alnaas, I. Roche, M.K. Knowles
- BIOL 91.** Novel azo-stilbenes as photoresponsive chemical tools. **C.N. Streu**, M. Paterson, **Y. Yen**, K. Jensen, J. Jespersen, A.J. Engdahl, T. Scheckelhoff, T.S. Crum, A.D. Mesecar
- BIOL 92.** Increasing thermo- and pH stability in carbonic anhydrase II for bioremediation purposes: A novel approach to industrial CO₂ sequestration. **V. Rasi**, B.P. Mahon, A.M. Hendon, C.D. Boone, R. McKenna
- BIOL 93.** Cloning, expression, and characterization of bacterial enzymes with predicted structural similarity to mammalian cyclooxygenases. **B.S. Selinsky**, M. Butchy, S. Neumann, C. Nichols
- BIOL 94.** Predicting membrane binding interface of peripheral proteins and beyond. **L. Zhang**, M. Rajendram, A. Yethiraj, D.B. Weibel, Q. Cui
- BIOL 95.** Unraveling the slow onset inhibition of InhA, the enoyl ACP reductase from mycobacterium tuberculosis: Mechanism and inhibitor design. **W. Yu**, H. Li, S. Eltschkner, L.A. Spagnuolo, A. Peryman, A. Chang, C. Kisker, P.J. Tonge
- BIOL 96.** SialoPen: A new class of protease resistant membrane permeable peptides for intracellular biomolecule delivery. **E.M. Contreras**, A. Monreal, J.P. Saludes
- BIOL 97.** Re(II) polypyridyl complexes in chemotherapy. **P. Ahuja**, F.M. MacDonnell
- BIOL 98.** Connecting the global protein folding free energy and the heme affinity using the formal reduction potential of heme. **B.R. Gibney**
- BIOL 99.** Hemostats that target hidden injuries. **M. Gkikas**, T. Mesar, R.K. Avery, G. Velmachos, B.D. Olsen
- BIOL 100.** PLP proteomics: Probing and identifying of PLP-dependent proteins in bacteria. **Y. Liu**, B. Shome, D. Fedoseyenko, T.P. Begley
- BIOL 101.** Hapalindole-linked welwitindolone and ambiguous gene clusters from Stigonematalean cyanobacteria are delivering interesting chemistry via an unprecedented stereoselective halogenation of an sp³-carbon by a freestanding enzyme encoded within *wel*. **M.L. Hillwig**, X. Liu
- BIOL 102.** Compensatory kinetic effects of viscogen and crowding agent PEG8000 on the reaction of human uracil DNA glycosylase (HUNG). **A. Rodriguez**, S.L. Cravens, J.T. Stivers
- BIOL 103.** Withdrawn.
- BIOL 104.** Combination therapeutic nanoparticles for chemoresistant prostate cancer. **R. Pathak**, S. Dhar
- BIOL 105.** Kinetic characterization and optimization of mechanism-based inhibitors of BioA. **C. Eiden**, C.C. Aldrich, J.D. Lipscomb
- BIOL 106.** Differences in protein unfolding mechanisms revealed characterized in aqueous ionic liquid solutions. **M.C. Miller**, O.C. Fiebig, S.L. Hanna, M. Enriquez, G.A. Caputo, **T.D. Vaden**
- BIOL 107.** Zinc fluxes in control of gamete maturation, cell cycle, and fertilization. **A.R. Bayer**, E.L. Que, F.E. Duncan, T.K. Woodruff, T.V. O'Halloran
- BIOL 108.** SHH transcription factors Gli-1 and Gli-3R: Modulators of retina regeneration. **B.D. Center**, K. Barbosa, A. Luz-Madrugal, K. Del Rio-Tsonis
- BIOL 109.** Mutation of yeast hexokinase I for structure-function analysis. **G. Geibel**, **J. Diaz**, E. Munk, W. Haggren, S.B. Braun-Sand
- BIOL 110.** Structures of complexes of G-quadruplex DNA with drug like molecules. **H. Ranpura**, P.H. Bolton
- BIOL 111.** Role of biochemical composition and extracellular polymeric substances on forward osmosis membrane fouling during algae separation. **W. Fang**
- BIOL 112.** Identification of cellular targets in *Saccharomyces cerevisiae* of K20, an antifungal derived from kanamycin. **A. LeRoy**, J. Takemoto, C.T. Chang, D.N. Heaton
- BIOL 113.** DNA-mediated redox signaling by UvrC. **M.A. Grodick**, R.M. Silva, A. Zhou, J.K. Barton
- BIOL 114.** Structure of the periplasmic sensor domain of the histidine kinase CusS shows unusual metal ion coordination at the dimeric interface. **T. Affandi**, A.V. Issaian, S.A. Roberts, M.M. McEvoy
- BIOL 115.** Synthesis of photoresponsive single stranded DNA aggregates via click chemistry. **S.K. Rastogi**, R. Gu, J. Lamas, X. Li, S. Zauscher, W.J. Brittain
- BIOL 116.** Withdrawn.
- BIOL 117.** Development of an electrochemical microRNA sensor. **J. Philippe**, S. MacArdele, M.C. Buzzeo
- BIOL 118.** Electrochemical reactivity of selenocystine. **H. Wang**, E. Karnaukh, L.M. Walker, M.C. Buzzeo
- BIOL 119.** Withdrawn.
- BIOL 120.** Unraveling the dynamics of the EF1 hand upon Ca²⁺ binding in neurocalcin delta. **Y. Yang**, A. Krishnan, J. Viviano, V. Venkataraman
- BIOL 121.** Alteration of the reaction profile of serine racemase via site-directed mutagenesis: Identification of an apparent "hotspot" with regard to reaction manifold. **D.L. Nelson**, G.A. Applegate, D.B. Berkowitz
- BIOL 122.** Hydrogen-bonded interaction of perfluorooctanoic acid with DNA. **D. Meng**, H. Zhang
- BIOL 123.** Mechanistic investigation of hydrolytic decompositions of Roussin's black and Roussin's red salts in aqueous acidic and basic solutions. **T. Drummond**, P. Maragh, T. Dasgupta
- BIOL 124.** Neuroprotective effect of Buyang Huanwu Decoction in ischemic stroke mice by proteomics study. **H. Chen**, Y. Shen, Y. Chen, Y. Lin
- BIOL 125.** Seeing double: Evolution may utilize multiple parallel paths to optimize new protein folds. **T.N. Szyszka**, V. Kumirow, M. Cordes
- BIOL 126.** Investigating the redox properties of human DNA primase. **E. O'Brien**, M. Holt, A. Ehlinger, W.J. Chazin, J.K. Barton
- BIOL 127.** Peptide inhibitors of coagulation factor complex assembly. **N. Kastelewitz**, H.H. Yin
- BIOL 128.** Functional characterization of a polyketide synthase (PKS) dehydratase domain using chemical probes. **Y. Li**, G. Dodge, R. Feick, J. Smith, C.C. Aldrich
- BIOL 129.** Electron transfer and DNA replication: Assessing the functional role of the yeast DNA polymerase δ [4Fe-4S]²⁺ cluster. **P.L. Bartels**, J.L. Stodola, P.M. Burgers, J.K. Barton
- BIOL 130.** Active site explorations of carotenoid oxygenases via integration of spectroscopy, crystallography, and enzymology. **E.R. Farquhar**, X. Sui, P. Kiser, M.P. Hendrich, K. Palczewski, M.R. Chance
- BIOL 131.** Influence of the role of dehydroshikimate dehydrogenase in production of β -carboxyglutamic acid from D-glucose using an *Escherichia coli* heterologous host. **G. Canales**, K.B. Finney, L. Harrington, R. Jha, K. Hotta, D. Fox, A.T. Koppisch
- BIOL 132.** Ionic liquids as a matrix for delivery of chemically diverse antibiotics to bacterial biofilms. **K.S. Lovejoy**, N.V. Warrington, T. Kern, **K.L. Merrett**, P. Manchen, P. Phillips, K. Ong, N. Nieto, R.J. Vierling, C.L. Meyers, R.E. Del Sesto, D. Fox, A.T. Koppisch
- BIOL 133.** Biological and mechanical properties of cartilage proteoglycans. **F. Horkay**, I. Horkay Szakaly, E.K. Dimitriadis, I.L. Morgan, P.J. Basser
- BIOL 134.** Highly selective RNA-based sensor for quick and easy detection of lead. **S. DasGupta**, J.A. Piccirilli
- BIOL 135.** Fluorescence microspectroscopy assessment of the in vitro dimerization of BACE1-GFP fusion protein in cultured cells. **S. Gardeen**, J.L. Johnson, A.A. Heikal
- BIOL 136.** Progress toward multisite incorporation of noncanonical amino acids into coat proteins of M13 bacteriophage. **D.G. Schwark**, M.A. Schmitt, J.D. Fisk
- BIOL 137.** Posttranslational modification of tumor suppressor protein par-4. **W. Chen**, A.K. Swain, K. Ponniah, J. Ramchandani, M.M. Tomovic, M.S. Warden, S.M. Pascal
- BIOL 138.** Protein photo-oxidation: The effects of singlet oxygen on protein function. **M.F. Eatwell**, J.D. Thoenke
- BIOL 139.** Detection of enzyme activities with diamagnetic catalyCEST MRI contrast agents. **S. Sinharay**, J. Cardenas-Rodriguez, M. Pagel
- BIOL 140.** Systematic engineering and synergistic binding of PEG-ylated ligands on phage for the detection of prostate cancer cells. **K. Mohan**, G.A. Weiss
- BIOL 141.** Soybean lipoxygenase activity measured by lipid-coated gold nanoparticle biosensors. **Y. Cai**, S.M. Budy, S.M. Reed, M.K. Knowles
- BIOL 142.** Novel biomarkers for HIV-1 disease progression. **T. Taylor**, A. Ghorpade, K. Borgmann, A. Pandya
- BIOL 143.** Developing an enzymatic switch from HSV-thymidine kinase as a potential cancer therapeutic. **N. Shelat**, M.A. Ostermeier
- BIOL 144.** Investigating the structural impact of the antimicrobial peptide combi-2 in model membranes. **B.M. Almarwani**, A. Sunda-Meya, N. Pamburu
- BIOL 145.** Optimal conditions for expression and purification of recombinant U-specific MC1 ribonuclease. **N.P. Lesner**, P.A. Limbach, B. Addepalli
- BIOL 146.** Investigation into the energetic processes of peptide bond formation on prebiotic earth. **C.M. Nevin**, K. Cody, G. Hassell, T. Hughes, D.F. Moriarty, K.P. Rhoads, A. Weatherax
- BIOL 147.** Design of ionic liquid materials for transdermal delivery and pathogen neutralization. **R.E. Del Sesto**, D. Fox, A.T. Koppisch, A. Newsham, M. Jones, B. Hammonree, A. Palacios, K.S. Lovejoy, T. Kern, M. Zakrewsky, S. Mitragotri
- BIOL 148.** Inhibiting β -ketoacyl acyl carrier protein synthases in *Staphylococcus aureus*. **C. Gu**, K. Kapilashrami, G.R. Bommineni, N. Nesbitt, P.J. Tonge
- BIOL 149.** Reaction of Zn-proteome with diethylamine NONOate (DEA-NO): Measurement of labilized zinc by TSQ, Zinquin and FluoZin-3 is sensor dependent. **M. Karim**
- BIOL 150.** Development and qualification of cell culture bioreactor scale-down models. **P. Yeung**, C. Okediadi, P. Lanter, B. Figueroa
- BIOL 151.** Exploring the role of a distant domain dynamics on substrate binding of *Escherichia coli* prolyl-tRNA synthetase. **M.P. Mocol**, S. Bhattacharyay, S. Hati
- BIOL 152.** Exploring the intrinsic dynamics of proteins involved in metabolic pathways using coarse-grained normal mode analysis. **R.D. McMunn**, S. Bhattacharyay, S. Hati
- BIOL 153.** EGFR tyrosine kinase targeted compounds: Synthesis, in vitro antitumor activity, and molecular modeling studies of new series of benzothiazole and pyrimido[2,1-b]benzothiazole derivatives. **M. Gabr**, N. El Gohary, E. El Bendary, M. El Kerdawy

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.

- BIOL 154.** Dynamic regulation of p97 ATPase activity by p37 and p47 is impaired in pathogenic p97 IBMPFD/ALS mutants. **X. Zhang, L. Gui, T. Chou, D. Wong, D. Moen**
- BIOL 155.** Calorimetric studies of therapeutic compounds binding to modified DNA. **R.E. McKnight, L.T. Marr**
- BIOL 156.** Quantitative analysis of the cellular internalization of Engrailed-2 homeoprotein. **L. Molina, L. Carlier, F. Burlina, O. Lequin, S. Sagan**
- BIOL 157.** Monitoring nanoparticle self-assembly using a bifurcated fluorescent aptamer. **D. Marashi, T.A. Rogers, L. Jaeger, W.W. Grabow**
- BIOL 158.** Design, synthesis, and evaluation of small molecule probes for caspase-1. **C.E. Karver, M. Kawarski, T. Hageman**
- BIOL 159.** Structural and energetic determinants of adhesive binding specificity in type I cadherins. **H. Song, J. Vendome, K. Felsovalyi, Z. Yang, W.L. Hubbell, L. Shapiro, B.H. Honig**
- BIOL 160.** Staphyloferrin B: Total synthesis, structure activity relationship studies, and bioactivity. **J. Lybaek Hoj Madsen, E.M. Nolan**
- BIOL 161.** Building new protein mimics for siRNA delivery. **B.M. deRonde, L.M. Minter, G.N. Tew**
- BIOL 162.** Small molecules as chemical biology probes of chlamydial effector molecules: Efforts toward the development of an antichlamydial therapeutic. **K. Alser, D.G. McCafferty**
- BIOL 163.** Light harvesting DNA-protein biosensor. **M. Naganbabu, M. Skwierczynski, M.P. Bruchez**
- BIOL 164.** Blue dyes: Blue-red tandem dyes as bright fluorogenic biosensors. **M. Naganbabu, Y. Wang, J. Kurish, M.P. Bruchez**
- BIOL 165.** Interaction of pyrazinamide and structural analogs with reverse micelle membrane models. **B. Peters, Z. Arhouna, F. Fontes, C. Morris, A. Pena, D. Crick, D.C. Crans**
- BIOL 166.** Sense codon reassignment: Toward multisite incorporation of multiple non-canonical amino acids. **W. Biddle, M.A. Schmitt, J.D. Fisk**
- BIOL 167.** Thermodynamic determination of RNA duplex stability in magnesium solutions. **N. Meyer, B. Znosko**
- BIOL 168.** Investigation of radiolabeled holo-intrinsic factor in the detection of the cubilin receptor. **J. Workinger**
- BIOL 169.** Withdrawn.
- BIOL 170.** Oxidation of p53 via DNA-mediated charge transport. **K.N. Schaefer, W.M. Geil, J.K. Barton**
- BIOL 172.** Withdrawn.
- BIOL 173.** New nucleoside antibiotics synthesis via an enzyme catalyzed amide-ester exchange reaction. **X. Liu, S.G. Van Lanen, K.D. Green, S. Garneau-Tsodikova**
- BIOL 174.** Solution structure of a 2:1 complex of anticancer drug XR5944 with TFF1 estrogen response element: Insights into DNA recognition by a bis-intercalator. **C. Lin, R.I. Mathad, N. Sidell, D. Yang**
- BIOL 175.** Understanding single-molecule protein dynamics with carbon nanocircuits. **M. Iftikhar**
- BIOL 176.** Survival mechanism of blood typing IgM antibodies sorbed into paper. **L. Guan, R. Cao, J. Tian, W. Shen**
- BIOL 177.** Determination of *trans*-resveratrol and its metabolites in rat serum and liver using liquid chromatography with high resolution time of flight-mass spectrometry. **K. Kusler, J. Rousova, M. Leadbetter, D.S. Lijanage, N. Dongari, E. Sauter, A.V. Novikov, A. Kubatova**
- BIOL 178.** Buckminster fullerene effect on cytochrome P450 mediated metabolism. **C. Bostick, T.S. Tracy, W.D. Tish, P.M. Gannett**
- BIOL 179.** Investigating the link between environmental exposure and dry eye syndrome. **A. Alhalwani**
- BIOL 180.** Cr(VI) reduction by *Acinetobacter* sp. HK-1 with the assistance of a novel quinone/graphene oxide composite. **H. Zhang, H. Lu**
- BIOL 181.** Examining the effect of 2-aminoanthracene exposure in Sprague Dawley dams from gestation through postnatal period. **S.L. Whitby, D. Hunter, W. Yau, E.W. Howerth, W.E. Gato**
- BIOL 182.** DFT study elucidates proximal pocket hydrogen bond influence on mechanism of compound I formation in chloroperoxidase. **A.D. Pardillo, O. Morozov, D.C. Chatfield**
- BIOL 183.** Concentration and time dependent accumulation of Creighton silver nanoparticles in Vero 76 cells. **S.A. Paluri, N.H. Lam, I.E. Pavel Sizemore**
- BIOL 184.** O-GlcNAc modification blocks the aggregation and toxicity of the Parkinson's disease associated protein α -synuclein. **N.P. Marotta, Y. Lin, B. Zaro, M.R. Pratt**
- BIOL 185.** Withdrawn.
- BIOL 186.** Bioorthogonal approach to chemical virology. **S.M. Jensen, J.C. Jewett**
- BIOL 187.** Highly potent and selective metalloinhibitors for SH3 domains based on rhodium(II) metallopeptides. **F. Vohidov, Z.T. Ball**
- BIOL 188.** Streptomycin: An unusual lasso peptide antibiotic from the understudied halophilic actinomycete *Streptomonospora alba*. **J.J. Tietz, M. Metele, J.O. Melby, P.M. Blair, L. Zhu, I. Livnat, K. Severinov, D.A. Mitchell**
- BIOL 189.** Interaction between the antimicrobial peptide Leucocrocin and model membranes. **A. Stone, A. Sunda-Meya, N. Phambu**
- BIOL 190.** Characterization of the hexose-1-phosphate transferase from the *Vibrio vulnificus* capsular polysaccharide biosynthesis pathway. **K.M. Erickson, M.A. Chahoud, J.M. Hazel, J. Troutman**
- BIOL 191.** Linking airborne biological particles and ice nuclei in a rural, marine environment near Ucluelet, British Columbia. **J. Li, R. Mason**
- BIOL 192.** Site-specific protein-PEG-like/zwitterionic polymer conjugates by in situ atom transfer radical polymerization: A comparative study. **S. Bhattacharjee, X. Li, W. Liu, A. Chilkoti**
- BIOL 193.** Structural characterization of the N-terminal domain of *Plasmodium falciparum* copper P-ATPase. **J. Kisaka, D.L. Huffman**
- BIOL 194.** Promising thermostable alternative scaffold protein for M13 phage display. **N. Zhao, M.A. Schmitt, J.D. Fisk**
- BIOL 195.** Withdrawn.
- BIOL 196.** Improve blood typing performance within paper substrate through cellulose network structure design. **L. Li, X. Huang, W. Liu, W. Shen**
- BIOL 197.** In vitro model for measuring efficacy of GABAergic medicines in the treatment of bipolar disorder by studying expression of the protein GAD₆₇. **S.N. Frank, A. Jacoby**
- BIOL 198.** Novel G-quadruplex formed in the proximal P1 promoter of bcl-2 gene is a gene suppressor. **B. Onel, M. Carver, D. Yang**
- BIOL 199.** Mechanistic Investigation of chelation-assisted copper-catalyzed click chemistry. **A. Tuley, E. Vatanev, W. Liu**
- BIOL 200.** Role of proximal thiolate ligand in chloroperoxidase catalysis. **E. Shersher, X. Wang, A. Bolhassani**
- BIOL 201.** Modified p27^{CRP1} promoter-reporters in the context of cancer stem cells. **A.M. Cabreriza, S.K. Szwed, L. Bouchez, M.J. Sever**
- BIOL 202.** How nature makes vitamin B₁₂: The last unsolved biosynthetic module. **D.J. Diaz, S.H. Abdelwahed, T.P. Begley**
- BIOL 203.** Curacin biosynthesis: A model for unexpected dehydratase domain activity. **W. Fiers, G. Dodge, R. Fecik, D.H. Sherman, J. Smith, C.C. Aldrich**
- BIOL 204.** Employing mass spectrometry: The proteomic discovery of chlamydomonas reinhardtii's nutritional metal metabolism. **D. Jarrett, M. Miethke, D. Shirasaki, R.R. Loo, S.S. Merchant, J.A. Loo**

- BIOL 205.** Examination of latent structure in an intrinsically disordered protein and the thermodynamics of its binding to a target molecule. **A. Zidell, S.A. Showalter**
- BIOL 206.** Chemical tools to study ubiquitin and ubiquitin-like activating E1 enzymes. **A.V. Statsyuk, H. An**
- BIOL 207.** Azinomycin biosynthesis: Probing the mechanism of azabicyclic biosynthesis. **K. Nepal, S. Mori, D. Simkhada, V. Sharma, G.T. Kelly, C. Bryant, D. Delgado, Y. Rezenom, C. Watanabe**
- BIOL 208.** Discovery of lead macrocycle series from DNA-encoded libraries. **W. Connors**
- BIOL 209.** Regulation of metabolic enzymes by lysine succinylation. **O.D. Nelson, S. Sadhukhan, H. Lin**
- BIOL 210.** Study of iron metal oxides and metal-organic frameworks against Chinese hamster ovarian cell lines. **S. Bashir, B. Martinez, X. Du, J.L. Liu**
- BIOL 211.** Synthesis, characterization, and antibacterial bioassay and molecular modeling studies of novel (E)-N-(5-chloro-2-(2-oxoazetidin-1-yl)benzylidene)benzohydrazide derivatives. **P. Tigulla, P. Sureka, B. Ram, B. Balaram, V. Srinivasarao**
- BIOL 212.** Thiol-X reactions in action: Making oligonucleotide analogs in a click. **S. Pattanayak, W. Xi, T. Gong, C.J. Kloxin, C. Bowman**
- BIOL 213.** Understanding catalytic outcome in a model monoterpene synthase: mutational analysis of (4S)-limonene synthase. **N. Sridivya, E.M. Davis, R.B. Croteau, B.M. Lange**
- BIOL 214.** Toward cellular and tissue selective inhibition of histone deacetylases (HDAC): Development of cellular- and isoform-selective HDAC probes. **P.A. Petukhov, T. Hanigan, I. Kastrati, J. Frasar**
- BIOL 215.** Building a high definition breast tissue classifier: Applications in FT-IR histopathology. **S. Leslie, S. Mittal, D. Mayerich, A. Balla, R. Bhargava**
- BIOL 216.** Withdrawn.
- BIOL 217.** Use of CRISPR-Cas 9 to develop a human embryonic stem cell line carrying the Trp64Arg mutation of the β 3 adrenergic receptor. **J. Luna-Torres**
- BIOL 218.** Examining the importance of backbone hydrogen bonding in the RGD-integrin interaction: Consequences for engineering degradable cell-adhesive biomaterials. **K. Eckes, K. Baek, N.A. Hummell, L.J. Suggs**
- BIOL 219.** Discovery and characterization of human sORF-encoded polypeptides (SEPs). **J. Ma, A. Saghatelian**
- Interfacial Biomolecular Recognition**
Sponsored by COLL, Cosponsored by BIOL†

MONDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 4

The Chemistry & Biology of Non-Natural Nucleic Acids

N. Richards, *Organizer, Presiding*

- 8:30 BIOL 220.** Exploring the sequence space from expanded genetic alphabets. **L. Zhang, Z. Yang, K.M. Bradley, S. Hoshika, M. Kim, H. Kim, C. McLondon, C. Liu, W. Tan, S.A. Benner**
- 9:15 BIOL 221.** Structural characterization of non-natural ZP base pairs in duplex DNA. **M.M. Georgiadis, W.F. Kellelt, I. Singh, S. Hoshika, S.A. Benner, N.G. Richards**
- 10:00 BIOL 222.** Crystallization and structure of a functional riboswitch bearing an unnatural base pair. **A. Hernandez, S. Hoshika, H. Kim, M. Kim, S.A. Benner, J.A. Piccirilli**

- 10:45 BIOL 223. Award Address** (Nobel Laureate Signature Award for Graduate Education in Chemistry Sponsored by Avantor Performance Materials). Expansion of the genetic alphabet. **F.E. Romesberg**

MONDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 4

New Approaches to Investigating Chromatin Modifying Enzymes: Structure and Function

J. Meier, *Organizer, Presiding*

- 2:30 BIOL 224.** Protein methyltransferase inhibitors as personalized cancer therapeutics. **R. Copeland**
- 3:05 BIOL 225.** ChIP-less analysis of chromatin states and quantifying histone PTMs using data-independent acquisition mass spectrometry. **Z. Su, K. Krautkramer, J. Dowell, J. Denu**
- 3:40 BIOL 226.** Chemical probes to antagonize readers and writers methyl marks. **C. Arrowsmith**
- 4:15 BIOL 227.** Targeting MLL1 complex assembly for inhibition of H3K4 methyltransferase activity. **Y. Dou**
- 4:50 BIOL 228.** Unconventional chemical tools to interrogate protein methyltransferases. **M. Luo**

TUESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 4

Putting Chemical Biology in Context

Z. Gartner, *Organizer, Presiding*

- 8:30 BIOL 229.** Building small molecules to probe or perturb complex biological systems. **L.D. Lavis**
- 9:05 BIOL 230.** Chemistry-directed stem cell pluripotency and differentiation. **L.L. Kiessling**
- 9:40 BIOL 231.** Discovery of a class of endogenous mammalian lipids with anti-diabetic and anti-inflammatory effects. **A. Saghatelian, M.M. Yore, I. Syed, P.M. Moraes-Vieira, T. Zhang, M.A. Herman, E.A. Homan, J. Lee, S. Chen, O. Peroni, A. Hammarstedt, U. Smith, T.E. McGraw, B.B. Kahn**
- 10:15 BIOL 232.** Nucleic acids as chemical probes of cell-cell interactions. **Z. Gartner**
- 10:50 BIOL 233.** Fluorogenic fluorescent probes reveal that the Hsp70-40-nucleotide exchange factor folding pathway hastens transthyretin folding and alters the resulting structure, rendering it more kinetically stable. **X. Zhang, J.W. Kelly, A. Baranczak, P. Liu**
- Interfacial Biomolecular Recognition**
Sponsored by COLL, Cosponsored by BIOL†

TUESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 4

ACS Chemical Biology Award Symposium

L. Kiessling, *Organizer, Presiding*

- 2:30 BIOL 234.** Inositol pyrophosphates provide a link between metabolism and signaling. **D. Fiedler**
- 3:15 BIOL 235.** Chemical-proteomic strategies to investigate reactive cysteines. **E. Weerapana**
- 4:00 BIOL 236.** Use of chemical genetics to study mRNA splicing. **K.M. Shokat**
- 4:45 BIOL 237.** Engineering proteins for selective catalysis. **H. Yang, C. Zhang, P. Srivastava, K. Ellis-Guardiola, J.C. Lewis**

WEDNESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 4

In Vivo We Trust: Small Molecule Phenotypic Screening in Animals

R. Peterson, Organizer, Presiding

8:30 BIOL 238. Reverse genetic analysis of restless legs syndrome in *Drosophila*. N. Donelson, K. Trinh, S. Sanyal

9:00 BIOL 239. Fly approach to cancer therapeutics. R. Cagan

9:30 BIOL 240. Using *C. elegans* to identify novel small molecules that alter fat and feeding. K. Ashrafi

10:00 Intermission.

10:15 BIOL 241. P7C3 and an unbiased approach to drug discovery for neurodegenerative diseases. J. Ready

10:45 BIOL 242. Zebrafish screen identifies compounds that protect against chemotherapy-induced heart failure. Y. Liu, A. Asnani, L. Zou, V.L. Bentley, M. Yu, Y. Wang, G. Dellaire, K.S. Sarkar, H.H. Chen, D.E. Sosnovik, J.T. Shin, D.A. Haber, J.N. Berman, W. Chao, R. Peterson

11:15 BIOL 243. Developmental vitamin D availability regulates hematopoietic stem cell production and expansion. M. Cortes, M. Chen, S.Y. Liu, W. Kwan, D.L. Stachura, T. Schlaeger, D. Traver, G.Q. Daley, W. Goessling, T.E. North

Interfacial Biomolecular Recognition

Sponsored by COLL, Cosponsored by BIOL†

WEDNESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 4

Graduate Student & Postdoctoral Symposium

V. Bandarian, Organizer, Presiding

2:30 BIOL 244. Novel genetic interactions with cell-envelope targeting antibiotics using ultrahigh density transposon libraries in *Staphylococcus aureus*. M. Santiago, T. Meredith, S. Walker

2:45 BIOL 245. General approach to analysis of phosphatase activity in biological samples. J.R. Beck, A. Lawrence, A.S. Tung, E.N. Harris, C.I. Stains

3:00 BIOL 246. Reconstitution and in-vitro activation of the prokaryotic pentameric ligand-gated ion channel ELIC. O.S. Shafaat, R. Rusinova, J.R. Winkler, O.S. Andersen, H.B. Gray, D.A. Dougherty

3:15 BIOL 247. Nonenzymatic isomerization of acinetobactin, a siderophore from pathogenic *Acinetobacter baumannii*. J.A. Shapiro, T.A. Wenciewicz

3:30 BIOL 248. Controlling the phosphoproteome: Ligand-gated split-kinases and split-phosphatases. J. Castillo-Montoya, K. Camacho-Soto, B. Tye, L. Ogunleye, I. Ghosh

3:45 Intermission.

3:55 BIOL 249. Dual small-molecule rheostat for precise control of protein concentration in mammalian cells. Y. Lin, M. Pratt

4:10 BIOL 250. Repair of oxidized DNA in nucleosome core particles. E.D. Olmon, S. Delaney

4:25 BIOL 251. Omics-based discovery of the rimosamides: A new class of nonribosomal peptide-polyketide hybrids. R.A. McClure, J.R. Doroghazi, A.W. Goering, Y. Chen, W.W. Metcalf, R.J. Thomson, N.L. Kelleher

4:55 BIOL 252. Withdrawn.

Interfacial Biomolecular Recognition

Sponsored by COLL, Cosponsored by BIOL†

BMGT

Division of Business Development and Management

K. Allen and J. L. Bryant, Program Chairs

OTHER SYMPOSIA OF INTEREST:

Industrial Innovations in Polymer Chemistry (see POLY, Mon)

Best Practices for Success with SBIR & STTR Grants (see SCHB, Sun)

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of Terry L. Brewer (see SCHB, Mon)

Chemical Angel Network: Chemists Investing in Chemical Companies (see PROF, Mon)

Chemical Tales of Success: Helpful Tips for Younger Chemists (see YCC, Tue)

SOCIAL EVENTS:

Reception: PNNL 50th Anniversary Reception 5:00 PM: Sun

Reception and Book Signing: Award for Industrial Chemistry 5:30 PM: Mon

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Crystal Ballroom B/C

Crystal Ballroom B/C

ACS Award in Industrial Chemistry: Symposium in Honor of Thomas J. Colacot

Cosponsored by ANYL and I&EC

J. L. Bryant, Organizer

S. Chandrasekaran, Presiding

8:00 Introductory Remarks.

8:05 BMGT 1. Metal-mediated and metal-catalyzed coupling for incorporation of fluorine into aromatic molecules. J.F. Hartwig

8:35 BMGT 2. Metal catalyzed carbonylation reactions through reversible oxidative addition. M. Lautens

9:05 BMGT 3. Understanding and design of organopalladium reactivity with experimental and computational tools. F. Schoenebeck

9:35 Intermission.

9:43 Remarks.

9:45 BMGT 4. Carbon-carbon and carbon-heteroatom bond forming reactions in continuous flow. T. Noël

10:30 BMGT 5. Applications of Pd and Ni catalysis to Pfizer's portfolio. J. Magano

11:00 BMGT 6. Cross-coupling without redox changes at the metal – enantioselective dimerization of alkenes. T. RajanBabu

11:30 BMGT 7. Asymmetric C-C bond formation in outer sphere Pd catalyzed processes. B.M. Trost

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Crystal Ballroom B/C

Crystal Ballroom B/C

ACS Award in Industrial Chemistry: Symposium in Honor of Thomas J. Colacot

Cosponsored by ANYL and I&EC

J. L. Bryant, Organizer

J. A. Gladysz, Presiding

1:15 Introduction of Plenary Address.

1:25 BMGT 8. On the magical power of d-block transition metals as exemplified by ZACA (Zr-catalyzed asymmetric carboalumination of alkenes) – lipase-catalyzed acetylation – transition metal-catalyzed cross-coupling for highly enantioselective synthesis of various types of chiral organic compounds. E. Negishi, S. Xu, A. Oda, Y. Matsueda, H. Li, T.P. Bobinski

2:15 Intermission.

2:30 BMGT 9. Photoinduced, copper-catalyzed coupling reaction. G.C. Fu

3:00 BMGT 10. Connecting directed ortho metalation – transition metal catalyzed chemistries. V.A. Snieckus

3:30 BMGT 11. Important catalytic transformations for drug development. C. H. Senanayake

4:00 BMGT 12. ppm-Level Pd-catalyzed cross-couplings in water at room temperature. B. H. Lipshutz

4:30 Introductory Remarks of Award Recipient.

4:40 BMGT 13. Award Address (ACS Award in Industrial Chemistry sponsored by the ACS Division of Business Development & Management and the ACS Division of Industrial & Engineering Chemistry). Story of Pd-catalyzed coupling: The reactions of the 21st century. T. Colacot

5:25 Concluding Remarks.

Innovations in Macromolecular Network Chemistry

Industrial Innovations in Polymer Chemistry

Sponsored by POLY, Cosponsored by BMGT

CARB

Division of Carbohydrate Chemistry

E. Rozners, Program Chair

OTHER SYMPOSIA OF INTEREST:

Frontiers in Glycoscience (see CELL, Mon, Tue)

Ronald Breslow Award for Achievement in Biomimetic Chemistry (see ORGN, Sun)

Cellulose in Solid State and Solution - Structure, Chemistry and Reaction Mechanisms (see CELL, Sun, Mon, Tue, Wed)

ACS Chemical Biology Award Symposium (see BIOL, Tue)

Application of Computational Chemistry to Biomass Chemistry and Utilization (see CELL, Sun, Mon)

The Chemistry & Biology of Non-Natural Nucleic Acids (see BIOL, Mon)

BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Sun

SUNDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1C

Wolfrom Award Symposium

N. L. Pohl, E. Rozners, Organizers

J. C. Paulson, Presiding

9:30 CARB 1. Building on Wolfrom's legacy: From the Chemurgy of yesterday to the renewables of today. K.B. Hicks, A.A. Boateng, C.A. Mullen, Y. Eikasabi, A.T. Hotchkiss, M.P. Yadav

10:10 CARB 2. Cranberries: From polyphenols to polysaccharides. C. Khoo

10:50 CARB 3. Bioactive pectic oligosaccharides. A.T. Hotchkiss

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1C

Isbell Award and Gin New Investigator Award Symposium

N. L. Pohl, E. Rozners, Organizers

J. C. Paulson, Presiding

1:00 CARB 4. Recent studies on the synthesis of glycans from mycobacteria and campylobacters. T.L. Lowary

1:30 CARB 5. Synthesis of heparan sulfate oligosaccharides and glycopeptide. X. Huang, S.B. Dulaney, Y. Xu, K. Yoshida, B. Yang, W. Yang, J. Liu

2:00 CARB 6. Therapeutic in vivo synthesis by glycoconjugates. K. Tanaka

2:30 Intermission.

2:50 CARB 7. Split personality of human O-GlcNAc transferase. S. Walker

3:20 CARB 8. Photocrosslinking approach to discover O-GlcNAc-interacting proteins. A. Rodriguez, S. Yu, B. Li, J.J. Kohler

3:50 CARB 9. Chemical probes for the functional analysis of O-GlcNAc modifications. M. Pratt

MONDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1C

Glycomimetic Compounds: An Untapped Source of Novel Therapeutics

J. Magnani, Organizer, Presiding

9:00 CARB 10. Hexosamine mimetics designed to reverse the Warburg Effect. K.J. Yarema

9:30 CARB 11. Selectin antagonists: Acyclic ethers with a define conformational bias. Y. Guindon, C. Mickael, G. Tambulet, M. Prévost

10:00 CARB 12. Toward the development of selective DC-SIGN antagonists. A. Bernardi

10:30 Intermission.

11:00 CARB 13. Design and discovery of GMI 1070 (Rivipansel), a novel pan-selectin antagonist for the treatment of vaso-occlusive crisis in sickle cell disease. J.M. Peterson, A. Sarkar, J.T. Patton, M. Rahman, N. Karasany, B. Ernst, J.L. Magnani

11:30 CARB 14. New NMR tools for unraveling the conformation, dynamics, and recognition properties of glycomimetics. J. Jimenez-Barbero

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1C

Glycomimetic Compounds: An Untapped Source of Novel Therapeutics

J. Magnani, Organizer, Presiding

1:30 CARB 15. Galectin-ligand analogs and mimetics in intracellular vesicle damage and in angiogenesis. U.J. Nilsson, H. Leffler, N. Panjwani

2:00 CARB 16. Druggability of lectins, using the example of a bacterial adhesin. B. Ernst, P. Frei, J. Bezencon, D. Eris, S. Rabbani, P. Zihlmann, R. Preston, B. Fiege

2:30 CARB 17. Well-defined antibody-drug conjugates (ADCs) through site-specific conjugation. G. Boons

3:00 Intermission.

3:30 CARB 18. Isoform selective inhibition of tumor-associated carbonic anhydrase IX using carbohydrate-based sulfamates for the treatment of several cancers. B. P. Mahon, J. Ladwig, L. Bornaghi, D. Vullo, S. Poulsen, C.T. Supuran, R. McKenna

4:00 CARB 19. Synthesis and properties of polyfluorinated carbohydrates. B. J. Linclau

4:30 **CARB 20.** Computational design of glycomimetic inhibitors — prospects and limitations. **M. Frank, P. Nyholm**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E. Rozners, *Organizer*

8:00 - 10:00

32-33, 35-38, 43, 45-49, 51-52, 57-60, 62. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1C

Protein Glycosylation: Simulation, Synthesis, Characterization & Application

G. Beckham, *Organizer*

Z. Tan, *Organizer, Presiding*

9:15 **CARB 21.** Sugars and proteins: Building glycoproteins. **B.G. Davis**

9:40 Discussion.

9:45 **CARB 22.** New tools in glycoprotein chemical synthesis. **X. Li**

10:10 Discussion.

10:15 **CARB 23.** Synthesis of homogeneous glycoproteins and application to biochemical studies and biosimilar comparability analysis. **T.J. Tolbert**

10:40 Discussion.

10:45 Intermission.

11:05 **CARB 24.** Site-specific investigation of O-GlcNAc modifications using synthetic proteins. **M. Pratt**

11:30 Discussion.

11:35 **CARB 25.** Chemical synthesis as a tool to study protein glycosylation. **Z. Tan, X. Guan**

12:00 Discussion.

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1C

Protein Glycosylation: Simulation, Synthesis, Characterization & Application

Z. Tan, *Organizer*

G. Beckham, *Organizer, Presiding*

1:45 **CARB 26.** Intracellular traffic of cell surface mimetic quantum dots-anchored glycopeptides. **S. Nishimura, R. S. Tan, K. Naruchi, M. Amano, H. Hinou**

2:10 Discussion.

2:15 **CARB 27.** Protein glycosylation in the baculovirus-insect cell system. **D. L. Jarvis**

2:40 Discussion.

2:45 **CARB 28.** Manipulating protein stability by glycosylation. **Y. Levy**

3:10 Discussion.

3:15 Intermission.

3:35 **CARB 29.** Impact of glycosylation upon protein conformational tendencies. **W. G. Noid**

4:00 Discussion.

4:05 **CARB 30.** Computational study of glycosylphosphatidyl-Inositol (GPI) anchor fragments embedded in phospholipid membranes. **M. Wehle, R. Lipowsky, P.H. Seeberger, G. Brezesinski, C. Stefanii, D. Varon-Silva, M. Santer**

4:30 Discussion.

TUESDAY EVENING

Section A

Colorado Convention Center
Hall C

General Posters

E. Rozners, *Organizer*

7:00 - 9:00

CARB 31. Withdrawn.

CARB 32. Synthesis and antibacterial activity of antibiotic-functionalized graphite nanofibers. **R. M. Giuliano, M. Rotella, A. Briegel, J. Hull, A.F. Lagalante**

CARB 33. Encapsulation and release of an active enzyme utilizing cobalt crosslinked chitosan nanoparticles. **J.B. Lampe, G. Castillo, C.S. Morrison, D. Nguyen, R.J. Cavazos, R.A. Petros**

CARB 34. Reduction of flammability of cotton fabrics treated with phosphoryl piperazine derivatives. **T. Nguyen, S. Chang, B. Condon, R. Slopek, E. Graves**

CARB 35. Synthesis of hyaluronic acid-based phototherapeutics. **R. A. Guerrieri, E. Xu, R. D. Dolewski, R.G. Barkley, J.V. Ruppel, N.L. Snyder**

CARB 36. Synthesis of meso-substituted porphyrin and carboxyphthalocyanine bacteriochlorin conjugates. **G.T. Mukosera, R.D. Dolewski, J.V. Ruppel, N.L. Snyder**

CARB 37. Progress on the total synthesis of *Aspergillus fumigatus* galactosylamino-glycans for diagnostic and therapeutic applications. **E.J. Baker, N.L. Snyder**

CARB 38. Progress on the synthesis of *N*-acetylglucosamine (LacNAc) probes for studying binding differences carbohydrate recognition domains of galectins-1, -3 and -9. **C. Tao, N.L. Snyder**

CARB 39. Carbohydrate-based small molecules with immunostimulatory properties. **C.E. Marzabadi, V. Basava, C. Bitsakis, E. Hanawa**

CARB 40. Synthesis of wooden based resource derived furanic diol and polymerization of PU via various isocyanate. **B. Kim, S. Kim, J. Cho**

CARB 41. Selective hydrogenation of biomass-derived sugars using supported Ru nanoparticles based catalysts. **J. Hwang, A.A. Dabbawala**

CARB 42. Hydrothermal treatment of eucalyptus using acidic ionic liquid as catalyst toward a biorefinery concept. **J. Xu, R. Sun**

CARB 43. Carbohydrate polymer-coating chemistry for cellulose based bioassays. **R. Cao, L. Guan, M. Li, W. Shen**

CARB 44. Synthesis of fluorogenic probes for selective biomass degradation by fungi. **Q. Zhang, X. Peng, M. Grilley, J. Takemoto, C.T. Chang**

CARB 45. Synthesis and stability study of DNA duplexes with 1'-carboxamide residues. **W. Dong, S.A. Woski**

CARB 46. Semisynthetic approach to cancer vaccines utilizing mimetics of natural and unnatural Tn antigens. **S. Nishat, A.A. Shaik, P.R. Andreana**

CARB 47. Chemical synthesis and O-glycosidic linkage conformation in a ¹³C-labeled βMan(1→4)βXyl(1→4)βMan(1→4)βXylOCH₃ tetrasaccharide: Effects of linkage structure and context. **W. Zhang, A.S. Serianni**

CARB 48. Quantitative evaluation of D-galactose-lectin binding properties via development of diversely presented carbohydrate surfaces. **B. Meng, K. Tschersch, M.D. Best, D.C. Baker**

CARB 49. Lipase-mediated modification of peracylated macrolactonic sophorolipids. **A. Sembaveya, J.A. Carr**

CARB 50. Optimization of autohydrolysis of bamboo for the production of low-DP xylo-oligosaccharides using response surface methodology. **X. Xiao, J. Bian**

CARB 51. Facile synthesis of nested fragments of high-mannose *N*-glycans with lightly protected glycosyl acceptors. **Q. Pan, S. Zhao, W. Zhang, Z. Zhang, A.S. Serianni**

CARB 52. Synthesis of 2-amino sugar building blocks and application for glycodiversification studies. **C.M. Rojas, A. Brown, G. Ezeude, M. Miller, A. Scharnow, A. Oviatt**

CARB 53. Novel catalytic approach for the regioselective oxidation of carbohydrates under mild conditions. **W. Muramatsu**

CARB 54. Using potatoes as a carbohydrate based additive in road salt. **R. Byrnes, D. Szlosek, G. Smith, J. Walters, R. Tanous, D.A. Arris**

CARB 55. Amide-linked RNA: Synthesis, structure, and RNA interference activity. **E. Rozners, D. Mutisya, C. Selvam, P. Tanui, B.D. Lunstad, S.D. Kennedy, P.S. Pallan, A. Haas, D. Leake, M. Egli**

CARB 56. Modification of glucose for targeted cellular delivery. **H. Jacobs, Z.J. Witzczak**

CARB 57. Targeted study of bacterial glycoproteins using metabolic oligosaccharide engineering. **D.H. Dube, E. Clark**

CARB 58. Development of a cyclooctyne-based photodynamic antibiotic for targeting *Helicobacter pylori*'s surface sugars. **D.H. Dube, I. Kline**

CARB 59. Analysis of *Helicobacter pylori* strains deficient in protein glycosylation. **D.H. Dube, S. Mikami, H. Carol**

CARB 60. Synthesis of chitosan beads enclosed magnetic Fe₃O₄ nanoparticles endorsed several applications from environmental remediation to bio-nanocomposite integration in biomedicine interdisciplinary fields. **V. Fernandez-Alos, A. Padilla, C. Castro-Alvarado, F.R. Roman**

CARB 61. Hybrid ceramide-glycosgenin triterpene saponin as a vaccine adjuvant. **V. Pathak, A.K. Pathak**

CARB 62. Cell-surface engineering with biomimetic materials: Mucins and the cancer glycoalyx. **J. Kramer, C.R. Bertozzi**

CARB 63. Structural characterization of a newly discovered trisaccharide in banana fruit ethanol extract. **M.A. Madson**

CARB 64. Effect of conjugation and microwave treatment on structure and functional characteristics of gum karaya (*Sterculia urens*). **H. Mirhosseini, E. Shekarforoush**

CARB 65. Synthesis, characterization, and application of soy protein flour-based additive to increase the dry strength of recycled and virgin paper furnish. **A. Salam, L. Lucia, H. Jameel**

CARB 66. Structural insight into glycosylated human Notch1 EGF12 analogs. **S. Hayakawa, H. Hinou, S. Nishimura**

CARB 67. Metabolism of four metabolic chemical reporters and their relative selectivity for different glycoproteins. **A. Batt, M. Pratt**

CARB 68. Changes in metabolic chemical reporter structure yield a selective probe of O-GlcNAc modification. **K.N. Chuh**

CARB 69. Efficient method for the incorporation of molecular probes at multiple/specific sites in RNA: Levulinyl protection for 2'-ACE[®], 5'-silyl oligoribonucleotide synthesis. **M.O. Delaney**

CARB 70. Aldehyde bearing triterpene saponins as vaccine adjuvants. **V. Pathak, A. K. Pathak**

CARB 71. Xanthan: Conformation, degradation, and hydrophobic modification. **I. Jenssen, A. Ulset, H. Schols, A. Roy, F. Renou, B. Christensen**

CARB 72. Alkali pretreatment of cellulose I to cellulose II with thiourea as an additive. **V. Uniyal, P. Gupta, S. Naithani**

CARB 73. Immunomodulation of the linear b-(1,3)-glucan fr*Saccharomyces cerevisiae* through activation of mitogen-activated protein kinases and nuclear factor-κB in murine RAW264.7 macrophages. **X. Xu**

CARB 74. O-mannosylated glycan induced conformational alteration of α-D-strogylican fragment. **H. Hinou, S. Nishimura**

CARB 75. Efficient and α-selective glycosylation using 3-iodo Kdo (3-deoxy-D-manno-oct-2-ulosonic acid) fluoride donors. **B. Pokorny, P. Kosma**

CATL

Division of Catalysis Science and Technology

V. Schwartz, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller (see I&EC, Tue)

Computational Pyrolysis and Upgrading of Bio-oils (see COMP, Wed)

ENFL Distinguished Researcher Award: Symposium in Honor of James Burrington (see ENFL, Mon, Tue)

Catalysis for Unconventional Energy Sources (see ENFL, Sun, Mon)

C1 Catalytic Chemistry (see ENFL, Tue, Wed)

Elucidation of Mechanisms & Kinetics on Surfaces (see COLL, Wed)

SUNDAY MORNING

Section A

Colorado Convention Center
Room 107

Electrocatalysis and Photocatalysis

Electrocatalysis

S. Ren, *Organizer*

K. Leonard, *Organizer, Presiding*

8:40 **CATL 1.** Anodized silver plate electrode for carbon dioxide reduction. **L.Q. Zhou, C. Ling, H. Jia**

9:00 **CATL 2.** Nanostructured Zn electrodes for electrochemical carbon dioxide reduction. **J. Rosen, F. Jiao**

9:20 **CATL 3.** Mechanistic analysis of electrochemical oxygen reduction and development of economical silver alloy catalysts for low temperature fuel cells. **A. Holewinski, S. Lincic**

9:40 Intermission.

10:00 **CATL 4.** Molecular catalyst for water oxidation that binds to metal oxide surfaces and exhibits high activity without ligand degradation. **G.W. Brudvig, S.W. Sheehan, J. Thomsen, U. Hintermair, R.H. Crabtree, C.A. Schmuttenmaer**

10:40 **CATL 5.** Synthesis of a fibrous MnOx catalytic film on FTO by dual-session cyclic voltammetry. **H. Yuan, R.Y. Ofoli**

11:00 **CATL 6.** Mechanistic insight into water reduction provided by labile ligand variation at Rh(III) in Ru(II), Rh(III), Ru(II) supramolecular photocatalysts. **H.M. Rogers, K.S. Brewer**

11:20 **CATL 7.** Perfluorinated phthalocyanines and other ligands for efficient co-catalyzed electrooxidation of water. **V.O. Rodionov, N. Morlanes, B. Chen, K. Takanabe**

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.

11:40 CATL 8. Exploring earth-abundant chalcogenides and phosphides for catalytic hydrogen generation from water. Y. Sun

Section B

Colorado Convention Center
Room 109

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis Challenges and Opportunities for Renewable Energy Catalysis

J. A. Keith, A. J. Morris, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 CATL 9. Learning from nature how to make solar fuels. G.W. Brudvig

9:10 CATL 10. Solar fuels: Thermodynamics, candidates, tactics, and figures of merit. S. Bernhard, A.C. Brooks, M. Li, H.N. Kagalwala, D.N. Chirdon

9:40 CATL 11. Wavefunction embedding methods for the study of renewable energy catalysis. T.F. Miller

10:10 Intermission.

10:30 CATL 12. Withdrawn.

10:50 CATL 13. Theoretical modeling of excited-state processes for renewable energy: What do we need to make an impact? A. Krylov

11:20 CATL 14. Decoding the zeolite genome and its application in understanding the active sites in the selective catalytic reduction of NO_x using NH₃ in Cu-SSZ13. F. Goeltl, R. Bulo, I. Hermans, P. Sautet

Section C

Colorado Convention Center
Room 111

New Catalysis Through Ligand Design Energy and Catalysis

Financially supported by RSC Journal of Chemical Science

J. S. Figueroa, *Organizer*

A. S. Veige, *Organizer, Presiding*

8:10 Introductory Remarks.

8:12 CATL 15. From light-triggered hydride transfer to photo(electro)catalysis. A.J. Miller, C.L. Pitman, S.M. Barrett, K.R. Brereton, S.A. Slattery, R.L. McCoy

8:34 CATL 16. Water splitting with cobalt and nickel complexes: Core vs. ligand design. F. Evangelisti, R. Moré, F. Hodel, S. Luber, G.R. Patzke

8:56 CATL 17. New ligands for multifunctional bimetallic catalysts. B.M. Cossairt, S. Flowers, D. Henckel

9:18 CATL 18. Small molecule activation by platinum complexes containing bulky tin groups. B. Captain, A. Koppaka, L. Zhu, V. Yempally, G.C. Fortman, D. Isrow, C.D. Hoff

9:40 CATL 19. Oxazolonylborate metal compounds and catalysis. A.D. Sadow

10:02 Intermission.

10:17 CATL 20. Closing a cycle: Silver-heteroatom bonds in the heterolysis of dihydrogen. J.P. Sadighi, B. Tate, J.T. Nguyen, J. Bacsa, A.D. Royappa

10:39 CATL 21. Nucleophilic CH activation of benzene and methane with Rh and Ir complexes in strongly basic solvents. B.G. Hashiguchi, M.M. Konnick, R.A. Periana

11:01 CATL 22. Pincer ligand variations in catalysis of dehydrogenative borylation of terminal alkynes. O. Ozerov, C. Lee, J. Zhou, N. Bhuvanesh

11:23 CATL 23. Improved catalysts for the telomerization of butadiene with methanol. J. Briggs, J. Klinckenberg, J. Patton, H. Launay, M. Van Engelen, H. Hagen, D.C. Rosenfeld

11:45 CATL 24. Hemilabile N,O-chelating ligands: Dynamic coordination modes for promoting reactivity and hydroaminoalkylation catalysis. L. Schafer, E. Chong, J. Lauzon, M.W. Drover

Section D

Colorado Convention Center
Room 108

Symposium in Honor of Jens Rostrup-Nielsen

J. Hansen, *Organizer*
B. H. Davis, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 CATL 25. Review of patent literature relating to synthesis gas production and Fischer-Tropsch tail gas processing aimed at the cost effective enhancement of the GTL process efficiency. A.P. Steynberg

8:50 CATL 26. Branching pattern in Fischer-Tropsch synthesis. H. Schulz

9:25 CATL 27. Improving Pt/zirconia WGS catalysts through doping by Y and electronic promotion with Na. G. Jacobs, M. Martinelli, W.D. Shafer, U. Graham, B.H. Davis

10:00 Intermission.

10:15 CATL 28. Sulfur passivated reforming for production of syngas with low H₂/CO ratio. N.R. Udengaard

10:50 CATL 29. Catalytic aspects of fuel processing for fuel cells and power to gas. J.B. Hansen

11:25 CATL 30. First-principles study of Co-based catalysts for syngas conversion. W. Li

Catalysis for Un-conventional Energy Sources

Fuel Cell, Solar Cell and Solar Fuel

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 107

Electrocatalysis and Photocatalysis Photocatalysis

S. Ren, *Organizer*

K. Leonard, *Organizer, Presiding*

1:30 CATL 31. Using photoelectrochemistry to investigate visible light active photocatalytic materials. J. Byrne, J.W. Hamilton

1:50 CATL 32. ZnO-SnO₂ photocatalyst: An in-depth study on morphologies affect on photocatalytic activity. D.A. Ramirez, L. Hope-Weeks

2:10 CATL 33. Investigations of the role of surface metal catalysis and near surface nonmetal dopants in the photocatalytic activity of TiO₂. C. Muhich, Y. Zhou, J.Y. Westcott, A. Holder, A.W. Weimer, C. Musgrave

2:30 CATL 34. Synthesis and limits of p-CuBi₂O₇ nanocrystals as visible light photocatalyst for hydrogen evolution from water. G. Sharma, J. Wang, F.E. Osterloh

2:50 Intermission.

3:10 CATL 35. Electrochemical synthesis of ternary oxide photoelectrodes for use in solar water splitting. T. Kim, D. Kang, K. Choi

3:50 CATL 36. Nanohybrids based on semiconductors and Co₃O₄ or semiconductors/ photosensitizers for photoassisted water oxidation and fuel generation. O. Yehezkeili, D. de Oliveira, A. Harguindey, J. Cha

4:10 CATL 37. Charge carrier dynamics of photoexcited Co₃O₄ in methanol: Extending high harmonic transient absorption spectroscopy to liquid environments. L. Baker, C. Jiang, S.T. Kelly, J.M. Lucas, J. Vura-Weis, M.K. Gilles, P. Alivisatos, S.R. Leone

4:30 CATL 38. Can we accurately model the key electronic properties of semiconductor for photocatalysis? P. Sautet, T. Le Bahers, M. Harb, K. Takahashi

4:50 CATL 39. Overall photocatalytic water splitting using small organic shuttles. J. Sommers, N. Alderman, C.J. Viasus, C.H. Wang, S. Gambarotta

Section B

Colorado Convention Center
Room 109

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis Challenges and Opportunities for Renewable Energy Catalysis

J. A. Keith, A. J. Morris, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 CATL 40. New strategies for catalytic process design: Oxidative methane coupling with soft oxidants. T.J. Marks, M. Peter

2:10 CATL 41. Mechanistic insights into catalytic conversion methane over supported catalysts. M. Neurock

2:40 CATL 42. Significance of catalyst/support interactions for Pt nanoparticles on amorphous silica supports using density functional theory. C. Ewing, M.J. Hartmann, G. Veser, J.J. McCarthy, K. Johnson, D. Lambrecht

3:00 Intermission.

3:20 CATL 43. Plasmon-enhanced chemistry. G.C. Schatz

3:50 CATL 44. Plasmon-enabled hot carrier photocatalysis. N.J. Halas

4:20 Concluding Remarks.

Section C

Colorado Convention Center
Room 111

New Catalysis Through Ligand Design New Frontiers in Catalysis

Financially supported by Exxonmobil

A. S. Veige, *Organizer*

J. S. Figueroa, *Organizer, Presiding*

1:20 Introductory Remarks.

1:22 CATL 45. Development of molecular catalysts for the production of polyolefins. J. Klosin

1:44 CATL 46. Micromanaging metal catalysts with structurally tunable acyclic carbene ligands. L.M. Slaughter, A.A. Ruch, S. Handa

2:06 CATL 363. Terminal olefin-selective self-metathesis of 1,4-dienes using homogeneous Mo and W catalysts. K.M. Wampler, J. Uy, S.A. Cohen

2:28 CATL 47. Carbazole-based coordination polymers to incorporate Lewis base functionality. D.R. Manke

2:50 CATL 48. Ligand design toward functional materials. J.M. Blackwell

3:12 Intermission.

3:27 CATL 49. Synthesis and reactivity of a molecular titanium nitride. D.J. Mindiola

3:49 CATL 50. Reactivity of a dianionic 14⁻electron Pd(0) complex supported by charged carboranyl phosphine ligands. V. Lavallo

4:11 CATL 51. Synthesis, characterization, and hydrogenation catalysis of a rhodium *NNN*-pincer complex. P.G. Hayes, M.M. Hänninen, C.S. MacNeil

4:33 CATL 52. Selective ethylene oligomerization. O.L. Sydora

4:55 CATL 53. Tailoring bimetallic catalysts with metal-metal interactions for small-molecule activation. C.C. Lu, R. Siedschlag, R.C. Cammarota, L.J. Clouston, K.D. Vogiatzis, V. Bernales, L. Gagliardi

5:17 Concluding Remarks.

Section D

Colorado Convention Center
Room 108

Symposium in Honor of Jens Rostrup-Nielsen

B. H. Davis, *Organizer*

J. Hansen, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CATL 54. Importance of methane formation in determining overall selectivity of Fischer-Tropsch synthesis over cobalt-based catalyst. B. Todic, W. Ma, G. Jacobs, B.H. Davis, D. Bukur

2:05 CATL 55. Structure-stability relationships for supported copper and nickel catalysts. K.P. De Jong

2:35 CATL 56. Precious metal catalytic reforming of biosyngas. J. Abbott, A. Steele

3:05 Intermission.

3:20 CATL 57. Coke management on zeolites: The benefits of hierarchization. J. Gilson, L. Lakiss, Z. Qin, V. Valtochev, K. Thomas, A. Vicente, C. Fernandez, F. Ngoye, S. Laforge, C. Canaff, Y. Poulloux, L. Pinard

3:50 CATL 58. Gas loop design incorporating water electrolysis. A. De Klerk

4:20 CATL 59. Catalyst and process parameters for the gasification of rice husk with pure CO₂ and the gasification kinetics. Z. Chen, L. Zhang

Catalysis for Un-conventional Energy Sources

Biofuel and CO₂ Utilization

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

MONDAY MORNING

Section A

Colorado Convention Center
Room 107

Surface Chemistry and Catalysis on Oxides Oxide-Model Catalysts

Y. Xu, *Organizer*

W. Huang, Z. Wu, *Organizers, Presiding*

8:10 Introductory Remarks.

8:15 CATL 60. Energetics of catalytically-relevant adsorbates on well-defined oxide surfaces. C.T. Campbell

8:50 CATL 61. Oxidation reactions on PdO(101). J.F. Weaver

9:25 CATL 62. CO oxidation over a Pt/Fe₂O₃(001) model catalyst: Watching Mars-van Krevelen at work. R. Blum, J. van der Hoeven, P. de Jongh, M. Schmid, U. Diebold, G. Parkinson

9:45 CATL 63. Water Interaction with model iron oxide surfaces. S. Schauermann, P. Dementyev, K. Dostert, C.P. O'Brien, H. Freund

10:05 Intermission.

10:15 CATL 64. Model catalyst design: A material science perspective at the atomic level. H. Freund

10:50 CATL 65. Electron transfer between single gold nanocrystals and oxide supports during hydrogen adsorption: A surface plasmon spectroscopy study. S.S. Collins, M. Cittadini, C. Pecharomán, A. Martucci, P. Mulvaney

11:10 CATL 66. Electron transfer reactions at single crystal oxide surfaces as monitored by electron paramagnetic resonance spectroscopy: Alkaline earth oxide surfaces as exploratory examples. T. Risse, N. Richter, D. Cornu

11:30 CATL 67. Determining the enantiomeric excess of epoxides at oxide surfaces using vibrational sum frequency generation. F. Geiger

11:50 CATL 68. Enantioselectivity of chiral metal films grown on chiral oxide surfaces. S.F. Yuk, A.R. Asthagir

Section B

Colorado Convention Center
Room 109

Electrocatalysis and Photocatalysis Electrocatalysis

K. Leonard, *Organizer*

S. Ren, *Organizer, Presiding*

8:20 CATL 69. Tuning core/shell nanoparticles for catalysis optimization. S. Sun

9:00 CATL 70. Effect of measurement protocol and impurity levels on the oxygen reduction reaction activity of Pt/C using rotating disk electrode. K. Shinozaki, J.W. Zack, S. Pilypenko, R.M. Richards, B.S. Pivovar, S.S. Kocha

‡ Cooperative Cosponsorship

- 8:50 CATL 135.** Hydrocarbon oxidation reactivity in iron metal-organic frameworks. **D. Xiao**, E.D. Bloch, J.A. Mason, W. Queen, M.R. Hudson, N. Planas, P. Verma, D.G. Truhlar, L. Gagliardi, C.M. Brown, J.R. Long
- 9:20 CATL 136.** Catalytic conversion of methane to methanol and acetic acid on singly dispersed oxide species on internal surface of ZSM5. **F. Tao**, D. Xiao, A. Frenkel
- 9:50 CATL 137.** Ethylene epoxidation on metal-substituted silica mesopore catalysts: A combined experimental and theoretical investigation. **P.D. Patel**, W. Yan, A. Ramanathan, B. Subramaniam, B. Laird, W. Thompson
- 10:20** Intermission.
- 10:35 CATL 138.** General mechanistic role of reactive oxygen for the activation of alkanols, alkenes, and alkanes on dispersed metal clusters. **Y. Chin**, W. Tu, P. Lachkov
- 11:05 CATL 139.** Withdrawn.
- 11:35 CATL 140.** Biocatalytic polymer membrane system for selective partial oxidation of methane to methanol. **J. Stolaroff**, S.E. Baker, C. Blanchette, J.M. Lenhardt
- 12:05** Concluding Remarks.

Section B

Colorado Convention Center
Room 109

Surface Chemistry and Catalysis on Oxides Oxide-Synthesis and Catalysis

Z. Wu, *Organizer*
W. Huang, Y. Xu, *Organizers, Presiding*

- 8:10 CATL 141.** Controllable synthesis and catalytic property of ceria-based nano- and mesoporous materials. **C. Yan**
- 8:45 CATL 142.** Structure sensitivity and reaction pathways in oxygenate reactions catalyzed by CeO₂. **A.K. Mann**, Z. Wu, D.R. Mullins, S.H. Overbury
- 9:20 CATL 143.** Advanced nanomaterials: Synthesis and catalytic applications. **M. Gawande**, R.S. Varma, L. Kvitik, R. Zboril
- 9:40 CATL 144.** On the surface dependent acid-base property of ceria nanoshapes. **Z. Wu**, A.K. Mann, S.H. Overbury
- 10:00** Intermission.
- 10:10 CATL 145.** Rod-shaped metal oxides: Structural control and catalytic properties. **W. Shen**
- 10:45 CATL 146.** Electronic and reaction study of doped CeO₂ with Fe cations for hydrogen production from water. **Y. Alsalik**, H. Idriss
- 11:05 CATL 147.** Withdrawn.
- 11:25 CATL 148.** Controlling the selectivity of metal oxide catalysts using silanes and phosphonates for polyol dehydration. **L. Ellis**, D.K. Schwartz, J.W. Medlin
- 11:45 CATL 149.** Surface modification of silica-supported Ti(IV) and Nb(V) oxides for understanding reactivity and stability in the epoxidation of alkenes with H₂O₂. **N.E. Thornburg**, R.E. Franks, J.M. Notestein

Section C

Colorado Convention Center
Room 111

Symposium in Honor of Jens Rostrup-Nielsen

B. H. Davis, *Organizer*
J. Hansen, *Organizer, Presiding*

8:30 Introductory Remarks.

- 8:35 CATL 150.** Role of alkali in heterogeneous catalysis for gas cleaning in stationary and mobile applications. **P. Haghighi Moud**, J. Granstrand, S. Dahlin, M. Nilsson, K. Andersson, L. Pettersson, **K. Engvall**

- 9:05 CATL 151.** Electron microscopy advances for catalysis. **S. Helveg**

- 9:35 CATL 152.** Fischer-Tropsch synthesis: A time resolved study evidences changes in the product distribution during the initial steps on cobalt catalysts. **G. Melaei**, W. Ralston, W. Liu, G.A. Somorjai

10:05 Intermission.

- 10:20 CATL 153.** Withdrawn.

- 10:50 CATL 154.** Effect of metal on the reduction and reoxidation characteristics of ceria under ethanol steam reforming conditions. **U.S. Ozkan**, H. Sohn, I. Soykal, J.T. Miller, F. Tao

- 11:20 CATL 155.** Fischer-Tropsch synthesis in coal-to-liquids: Old technology with a bright future? **J.W. Niemantsverdriet**

Section D

Colorado Convention Center
Room 108

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Jingguang G. Chen

Heterogeneous Catalysis
D. Esposito, J. R. Kitchin, *Organizers*
M. A. Barteau, *Presiding*

- 8:30 CATL 156.** Oxygen removal and chain growth pathways in the catalytic upgrading of oxygenates. **E. Iglesia**

- 9:00 CATL 157.** Alkane activation over molybdenum carbide nanoparticles supported on nonacidic zeolites. **E.P. Schreiner**, S. Teketel, R.F. Lobo

- 9:30 CATL 158.** Single-atom-catalysts: New opportunities in selective hydrogenation reactions. **T. Zhang**

10:00 Intermission.

- 10:15 CATL 159.** Spectator or Intermediate? Simultaneous MS/FTIR studies of methanol catalysis. **C. Mims**, C.H. Peden, C.T. Campbell, Y. Yang, J.H. Kwak

- 10:45 CATL 160.** Metal catalysts on silica: issues and opportunities. **S. Soled**, S. Miscoe, J.E. Baumgartner

- 11:15 CATL 161. Award Address** (George A. Olah Award in Hydrocarbon or Petroleum Chemistry sponsored by the George A. Olah Award Endowment). Carbide and bimetallic catalysts for hydrocarbon transformation reactions. **J.G. Chen**

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller

Sponsored by I&EC, Cosponsored by CATL

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Room 107

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

Oxidation and Oxidative Coupling
J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

1:30 Introductory Remarks.

- 1:35 CATL 162.** Insights into confinement effects in methane-to-methanol conversion over Fe-SSZ-13. **F. Goeltl**, C. Michel, P. Andrikopoulos, I. Hermans, P. Sautet

- 2:05 CATL 163.** Methane to methanol conversion on copper-containing small-pore aeolites. **B. Ipek**, M.J. Wulfers, S. Teketel, J.P. Smith, K.S. Booksh, R.F. Lobo

- 2:35 CATL 164.** Ethylene epoxidation in metal-substituted mesopore catalysts: Multiscale insights from experiment and molecular simulation. **J.L. Kern**, K.G. Steenbergen, W. Yan, A. Ramanathan, B. Subramaniam, W. Thompson, B.B. Laird

3:05 Intermission.

- 3:20 CATL 165.** Methane coupling reaction in an oxysteam stream via an OH radical pathway. **K. Takanabe**

- 3:50 CATL 166.** Effects of transition metal doping in TiO₂ nanowire catalysts for oxidative coupling of methane. **R.T. Yunarti**, J. Ha, D. Suh, J. Choi, Y.J. Hwang

- 4:20 CATL 167.** Efficient removal of formaldehyde by layered double hydroxides at room temperature. **F. Liu**, P. Zhang

- 4:50 CATL 168.** Withdrawn.

5:20 Concluding Remarks.

Section B

Colorado Convention Center
Room 109

Surface Chemistry and Catalysis on Oxides Metal-Oxide Interface: Oxidation Reactions

W. Huang, Z. Wu, Y. Xu, *Organizers*
X. Gong, S. H. Overbury, *Presiding*

- 1:20 CATL 169.** Identification of reaction sites for the oxidation of NO on a mixed Fe+Cr oxide surface. **M.A. Henderson**, M.H. Engelhard

- 2:30 CATL 171.** Selectivity changes at interfaces between Pt and oxide nanoparticles in catalytic alcohol oxidation. **K. An**, G.A. Somorjai

- 2:50 CATL 172.** Remarkable enhancement of dichloromethane oxidation over potassium-promoted Pt/Al₂O₃ catalysts. **J. Lu**

3:10 Intermission.

- 3:20 CATL 173.** Reactivity of water and hydroxyls on oxide surfaces. **W. Huang**

- 3:55 CATL 174.** On the interface confinement effect in the oxide-on-metal inverse catalysts. **Q. Fu**

- 4:30 CATL 175.** Catalysis by HBEA zeolite in aqueous media: The impact of water on reaction pathways and catalyst performance. **A. Vjunov**, J.L. Fulton, D.M. Camaioni, M.A. Derewinski, J.A. Lercher

- 4:50 CATL 176.** Toward improved catalytic low-temperature CO removal in H₂ rich streams. **J. Saavedra**, C.J. Pursell, B.D. Chandler

- 5:10 CATL 177.** Direct simulation evidence of generation of oxygen vacancies at the golden cage Au₁₀ and TiO₂(110) interface for CO oxidation. **L. Li**, X.C. Zeng

Section C

Colorado Convention Center
Room 111

Symposium in Honor of Jens Rostrup-Nielsen

J. Hansen, *Organizer*
B. H. Davis, *Organizer, Presiding*

1:20 Introductory Remarks.

- 1:25 CATL 178.** Hot electron surface chemistry at oxide-metal interfaces: The foundation of acid-base catalysis. **G.A. Somorjai**

- 1:55 CATL 179.** Enhanced activity and selectivity of Fischer-Tropsch synthesis catalysts in water/oil emulsions. **D.E. Resasco**

- 2:25 CATL 180.** Insights into emission and capture of atoms during Ostwald ripening. **A.K. Datye**, T.R. Johns, C. Carillo, S. Challa, A. DeLaRiva, B. Kiefer, C.H. Kim, M.P. Balogh, J.W. Niemantsverdriet

- 2:55 CATL 181.** Withdrawn.

3:25 Intermission.

- 3:40 CATL 182.** Critical role of isolation effect in solid solution catalysts for CO₂ reforming of methane. **Y.H. Hu**

- 4:10 CATL 183.** Coking- and sintering-resistant core-shell nanoparticles for dry reforming of methane. **N. Almata**, P. Lavelle, K. Takanabe, J.M. Basset

- 4:40 CATL 184.** ECUST coal gasification updates: New projects and operations experience. **J. Xu**

5:10 Concluding Remarks.

Section D

Colorado Convention Center
Room 108

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis

Solid State and Heterogeneous Conversions Processes
J. A. Keith, A. J. Morris, *Organizers, Presiding*

1:30 Introductory Remarks.

- 1:40 CATL 185.** Ab initio approaches to modeling catalysis on solid oxide fuel cell cathodes. **D.D. Morgan**

- 2:10 CATL 186.** Oxygen reduction mechanisms on perovskite oxides and the effects of dissimilar interfaces. **B. Yildiz**

- 2:40 CATL 187.** Investigating CuO catalyzed oxidation of glucose to gluconic acid using an integrated computational and experimental approach: Insights into the role of lattice oxygen. **Q. Thang Trinh**, P. N. Amiampong, Y. Yang, **S. Mushrif**

3:00 Intermission.

- 3:20 CATL 188.** Promotion and poisoning of hydrogen evolution by co-adsorbed CO on transition-metal electrodes. **Y. Zhang**, V. Sethuraman, R. Michalsky, A.A. Peterson

- 3:40 CATL 189.** Critical role of water in catalytic CO oxidation over Au/TiO₂ catalysts: Part 1 — experiment. **J. Saavedra**, H. Doan, C.J. Pursell, L. Grabow, **B.D. Chandler**

- 4:10 CATL 190.** Critical role of water in catalytic CO oxidation over Au/TiO₂ catalysts: Part 2 — theory. **H. Doan**, J. Saavedra, C.J. Pursell, B.D. Chandler, **L. Grabow**

4:40 Concluding Remarks.

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller

Sponsored by I&EC, Cosponsored by CATL

TUESDAY EVENING

Section A

Colorado Convention Center
Hall C

General Poster Session

I. I. Soykal, *Organizer*

6:00 - 8:00

- CATL 191.** Growth of carbon nanofibers synthesized from electrocracking of gas on a Ni/Al₂O₃ catalyst: Thermodynamic and kinetic analyses. **A.S. Ismail**

- CATL 192.** Influence of ligand substitution on electronic properties in bis(diphosphine) nickel (II) catalysts used in hydrogen catalysis. **T.L. Brown**, A. Pitts-Mccoy, J. Niklas, O. Poluektov, K. Mardis

- CATL 193.** Characterization of amine-treated zeolites by methanol chemisorption. **A.D. D'Amico**, C. Baker, J.L. Gole, J.I. Brauer, S. Graham, J.Z. Hu, J.C. Kerwin, M.G. White

- CATL 194.** Metal-oxide sites for facile methane dissociation. A. Trincherio, A. Hellman, H. Grönbeck

- CATL 195.** Hydrodesulphurization of the DBT using low ratio nickel-molybdenum sulfide catalysts. **I.A. Montemayor**, J.S. Soliner, D.F. Gonzalez, J.G. Parsons

- CATL 196.** Direct oxidative carboxylation of olefins for the synthesis of cyclic organic carbonates. **A. Sahe**, R.M. Rioux

- CATL 197.** Chiral carbazolic porous framework as asymmetric heterogeneous organocatalyst. **X. Zhang**, A. Kormos, J. Zhang

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.

- CATL 198.** High pressure STM studies on carbon monoxide adsorption on copper and cobalt sites. **Y. Hao, B. Eren, M. Salmeron, G.A. Somorjai**
- CATL 199.** Highly efficient visible light-induced active oxygen generation by carbazolic porous organic frameworks and their use in organic synthesis. **J. Luo, J. Zhang**
- CATL 200.** Hydrodesulfurization of dibenzothiohene using tungsten, cobalt and nickel. **D.F. Gonzalez, K. Williams, J.S. Solner, J.G. Parsons**
- CATL 201.** Hydrodesulphurization of DBT using CoMoS₂ catalyst. **J.S. Solner, D.F. Gonzalez, J.G. Parsons**
- CATL 202.** Water's effect on the nucleation and growth of nickel nanoparticles on ceria thin films. **E.W. Peterson, J. Zhou**
- CATL 203.** Secretive world of copper substituted zeolites in NH₃-SCR investigated by EPR. **A. Godiksen, S.B. Rasmussen, T.V. Janssens, H. Falsig, L.F. Lundegaard, P. Moses, F. Giordano, E. Borfecchia, K. Lomachenko, C. Lamberti, S. Bordiga, P. Beato, S. Mossin**
- CATL 204.** Withdrawn.
- CATL 205.** Structure and catalytic activity of Mo and Cr nanoparticle in ZSM-5 for natural gas conversion to aromatics. **J. Gao, Y. Zheng, J. Jehng, Y. Tang, J. Gallagher, J.T. Miller, I.E. Wachs, S. Podkolzin**
- CATL 206.** Methanol conversion to dimethyl ether over Fe-embedded graphene. **A. Thivasathit, J. Sirirajansre, P. Khongpracha, C. Warakulwit, J. Limtrakul**
- CATL 207.** Role of acid strengths and confinement effects on the conversion of propan-2-ol: MFI zeolites vs. Keggin polyoxometalates. **S. Choomwattana, J. Sirirajansre, J. Limtrakul**
- CATL 208.** Preparation of di- and triglycerol using acetate salts. **J. Lee, T. Han, S. Park, M. Cheong**
- CATL 209.** Preparation of di- and triglycerol using heterogeneous catalysts. **J. Lee, S. Park**
- CATL 210.** Cross-selectivity in the catalytic decarboxylative ketonization. **A. Ignatchenko, V. Marino, J. DeRaddo**
- CATL 211.** Condensation of ketones with carboxylic acids: Extending kinetic scheme for the mechanism of ketonic decarboxylation. **T. DiProspero, H. Patel, A. Ignatchenko**
- CATL 212.** Efficient catalytic conversion of cellulose into levulinic acid by sulfonated hyperbranched poly(arylene oxindoles) with chloro substituents. **F. Yu, J. Thomas, S. Van de Vyver, M. Smet, W. Dehaen, B.F. Sels**
- CATL 213.** Photocatalytic production of H₂O₂ and its further utilization for Baeyer-Villiger oxidation. **L. Liu, A. Corma**
- CATL 214.** Synthesis, characterization of Ag/SiO₂ and Ag/Co₃O₄ hierarchically porous monoliths and evaluation for hydrogenation of dyes. **Y. Hakat, T. Kotbagi, M.G. Bakker**
- CATL 215.** Evaluation of Ag/SiO₂ and Ag/Co₃O₄ Hierarchically porous monoliths for epoxidations. **Y. Hakat, T. Kotbagi, M.G. Bakker**
- CATL 216.** Aerobic oxidation reaction catalyzed by graphene oxide. **J. Park, F. Raza, D. Yim, J. Kim**
- CATL 217.** Zeolite-templated Ni nanostructure for methanol oxidation reaction. **D. Aldhayan**
- CATL 218.** Preparation of C60 nanowiskers – WO₃ nanocomposites and kinetics for photocatalytic degradation of organic dyes. **K.H. Kim, H.S. Park, J.W. Ko, W.B. Ko**
- CATL 219.** Investigation of structure, composition, and catalytic activity of AuPd bimetallic nanoparticles of variable Au/Pd ratio. **T.A. G. Silva, E. Teixeira-Neto, L.M. Rossi**
- CATL 220.** Picking up the pace: Improving oxygen evolution reaction catalysts. **M. Hinojos, S. Jin, L. Li**
- CATL 221.** Preparation of SAPO-34 by vapor-phase crystallization. **W. Wang, H. Liu, W. Yang**
- CATL 222.** Silver nanoparticle-functionalized 2D nanosheets as a plasmonic photocatalyst for reduction of nitroaromatic compounds. **H. Lee, J. Park, F. Raza, D. Yim, J. Kim**
- CATL 223.** Investigation of metal xanthates as latent thermal epoxy resin curing catalysts. **T.C. Vagvala, S.S. Pandey, Y. Ogomi, S. Hayase**
- CATL 224.** Multiwalled carbon nanotubes supported palladium-iridium alloy nanoparticles with enhanced electrocatalytic activity for the formic acid oxidation. **F. Wang, F. Wang, J. Bao, H. Liu**
- CATL 225.** Sb-doped SnO₂ supported platinum catalyst with high stability for proton exchange membrane fuel cells. **M. Dou, M. Hou, F. Wang**
- CATL 226.** Nitrogen-doped hierarchical porous carbon fabricated from food waste as the support material for Pt electrocatalyst toward the oxygen reduction reaction. **F. Wang, Y. Huang, H. Liu, Y. Cao**
- CATL 227.** Comparison of hydrogen peroxide decomposition in the presence of N₂, H₂ and C₂H₄ over supported Pd catalysts. **T. Chen, E. Kertalli, A. Nijhuis, S.G. Podkolzin**
- CATL 228.** Effect of Hydrogen and Propylene Presence on Hydrogen Peroxide Decomposition over Pd. **T. Chen, E. Kertalli, A. Nijhuis, S.G. Podkolzin**
- CATL 229.** Learning from microbial systems to develop biomimetic catalysts for hydrocarbon oxidation. **S.S. Yu, S.I. Chan**
- CATL 230.** Hydrodesulfurization of thiophene using phosphomolybdic acid and nickel substituted phosphomolybdic acid as catalyst. **A.M. Alsalmeh, M.H. Siddiqui**
- CATL 231.** Catalytic ozone membrane reactor for treatment of EDCs in water. **T. Corbet, L. Li, Y. Li, W. Han, K. Yeung**
- CATL 232.** Role of surface chemistry on the photoactivity of C-doped TiO₂ derived from TiC. **W. Ching, S.A. Ferdousi, K.L. Yeung**
- CATL 233.** Pd@V-P oxide core-shell nanoparticles supported on MWCNTs as selective electrocatalyst for the ORR. **H. Liu, J. Bao, F. Wang**
- CATL 234.** Homogenous Ir-catalyzed asymmetric hydrogenation of pyridinium Salts: High throughput experimentation approach, scope and preliminary mechanistic studies. **Y. Huang, Y. Chen, Y. Liu, S.W. Kraska, I.W. Davies, M. Chang, S. Liu, X. Zhang**
- CATL 235.** Hydrogen generation via sodium borohydride hydrolysis using graphene supported platinum-cobalt catalysts prepared by microwave-assisted synthesis. **K. Antanaviciute, A. Matuseviciute, L. Tamasauskaite-Tamasuniunite, I. Stalioniene, A. Zieliene, L. Naruskevicius, B. Simkunaite-Stanyniene, E. Norkus**
- CATL 236.** N-Heterocyclic carbene-based materials for CO₂ activation. **E. Kaley, E. Finney**
- CATL 237.** Graphene supported PtAuCeO₂ nanocomposites as electrocatalysts for fuel cells. **M. Urbonas, L. Tamasauskaite-Tamasuniunite, V. Kepeniene, A. Matuseviciute, R. Kondrotas, R. Juskenas, V. Pakstas, E. Norkus**
- CATL 238.** Aqueous phase CO₂ reduction with sodium borohydride: An ab initio molecular dynamics and nudged-elastic band mechanistic study. **M.C. Groenenboom, K.A. Grice, J.A. Keith**
- CATL 239.** Tandem isomerization-decarboxylation of unsaturated fatty acids to olefins via Ruthenium metal-as-ligand catalysts. **R.E. Murray, E.L. Walter, K.M. Doll**

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 107

Novel Catalytic Materials for Renewable Fuels/Chemicals

M. Foston, J. C. Hicks, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 **CATL 240.** Supported metal catalysts for lignin hydrogenolysis. **S.L. Scott, Z. Jones, X. Wu**

8:40 **CATL 241.** Lignin depolymerization by rhodium phosphine complexes and water-stable Lewis acids. **R. Jastrzebski, B.M. Weckhuysen, P.C. Bruijninx**

9:00 **CATL 242.** Designing active and stable Ru catalysts for the aqueous-phase hydrogenation levulinic acid. **J. Bond, O.A. Abdelrahman**

9:20 **CATL 243.** Promotion of activity and selectivity by alkanethiol monolayers for Pd-catalyzed benzyl alcohol hydrodeoxygenation. **C. Lien, J.W. Medlin**

9:40 **CATL 244.** Direct catalytic conversion of Ethanol stream to hydrocarbon blend-stock: Approaches to increase liquid hydrocarbon production. **Z. Li, E. Casbeer, B.H. Davison, C.K. Narula**

10:00 Intermission.

10:10 **CATL 245.** One-pot conversion of Kraft lignin into high-valued small-molecular chemicals over nanostructured molybdenum based catalyst. **Y. Li**

10:30 **CATL 246.** Mechanism and kinetics of acetic acid ketonization over zeolites. **S. Crossley, A. Gumdiyala, . Godavarthy**

10:50 **CATL 247.** Catalytic pathways and periodic trends for the hydrogenation of acetic acid in aqueous phase. **J. Shangquan, Y. Chin**

11:10 **CATL 248.** Nitrate-Intercalated Layered double-hydroxide catalysts for lignin depolymerization. **J.S. Kruger, N.S. Cleveland, M.J. Biddy, G. Beckham**

11:30 **CATL 249.** Effects of Bronsted acid strength and site environment for C=C bond formation and hydrogen transfer reactions. **F. Lin, Y. Chin**

Section B

Colorado Convention Center
Room 109

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

Hydrogenation and Dehydroaromatization

J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **CATL 250.** Mechanistic insights into the activation of CO and hydrocarbon chain growth in Fischer Tropsch synthesis. **M. Neurock, D. Hibbitts, B. Loveless, C. Buda, T. Lawlor, E. Dybeck**

8:50 **CATL 251.** Quantum mechanical analysis of CO₂ and CO hydrogenation on metal-doped Cu(111) surfaces. **Y. Santiago-Rodriguez, M. Curet-Arana**

9:20 **CATL 252.** Catalytic light olefin upgrading: Using natural gas for gasoline quality improvement. **P. He, H. Song**

9:50 **CATL 253.** Natural gas to chemicals via reactive separation. **P. Chitta**

10:20 Intermission.

10:35 **CATL 254.** Topsøe aromatics synthesis catalysts. **L.J. Lemus-Yegres, B. Temel, X. Yang, F. Joensen, P.H. Nielsen**

11:05 **CATL 255.** Structure and regeneration of Mo/ZSM-5 catalysts for natural gas conversion. **J. Gao, Y. Tang, I.E. Wachs, S.G. Podkolzin**

11:35 **CATL 256.** High selectivity of zinc and phosphorus modified ZSM-5 for MTA. **J. Qiao, J. Teng, Y. Wang, W. Yang**

12:05 Concluding Remarks.

Section C

Colorado Convention Center
Room 111

Surface Chemistry and Catalysis on Oxides

Metal-Oxide Interface: Others

W. Huang, Y. Xu, *Organizers*

Z. Wu, *Organizer, Presiding*

Q. Fu, *Presiding*

8:10 **CATL 257.** Role of surface oxygen vacancies in heterogeneous Au catalysis. **J. Behm**

8:45 **CATL 258.** Role of TiO₂ defects and the Ru/TiO₂ interface on the conversion of phenolics. **S. Crossley, T. Omotso**

9:05 **CATL 259.** Investigation of Pd-Cu single atom alloy catalysts for selective hydrogenation of acetylene in ethylene. **X. Cao, A. Mirjalili, W. Xie, B. Jiang**

9:25 **CATL 260.** Selective hydrogenation of phenol catalyzed by palladium on high surface ceria at room temperature and ambient pressure. **N. Nelson, A.D. Sadov, I.I. Slowing**

9:45 Intermission.

9:55 **CATL 261.** Importance of the metal-oxide interface in catalysts for the water-gas shift and methanol synthesis. **J. Rodriguez, D.J. Stacchiola, P. Liu, S.D. Senanayake, J. Graciani, J.F. Sanz**

10:30 **CATL 262.** Kinetically stabilized Pd@Pt core-shell nanocubes with thin Pt layers for enhanced catalytic hydrogenation performance. **P. Zhang, S. Zhou**

10:50 **CATL 263.** Investigating the function of metal oxide promoters on supported Rh catalysts for syngas conversion to oxygenates through surface and interface modification. **N. Yang, S. Fleischman, P. Wang, S.F. Bent**

11:10 **CATL 264.** Preparation of 3D ordered macroporous SiO₂-supported K₂MnCeO₄ catalysts for soot combustion. **X. Yu, Z. Zhao**

11:30 **CATL 265.** Modeling acrolein hydrogenation on constrained platinum nanoparticles. **C. Engelhardt, D. Ellis, K.R. Poeppelmeier, R. Kennedy**

Section D

Colorado Convention Center
Room 108

Theoretical and Experimental Synergies at the Frontiers of Renewable Catalysis

CO₂ Reductions

J. A. Keith, A. J. Morris, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 **CATL 266.** Design principles for reversible CO₂ chemistries. **W.F. Schneider, T. Lee**

9:10 **CATL 267.** Electrocatalytic conversion carbon dioxide to fuels promoted by 1,3-dialkylimidazolium based ionic liquids. **J. DiMaggio, J. Medina-Ramos, R.C. Pupillo, J. Rosenthal**

9:40 **CATL 268.** Toward electrochemical carbon dioxide reduction by porous coordination networks. **W. Maza, S. Ahrenholtz, A.J. Morris**

10:00 Intermission.

10:20 **CATL 269.** Hydrogen evolution in the context of electrochemical CO₂ reduction. **R.J. Nielsen, S. Johnson, Y. Lam, W.A. Goddard, D.W. Shaffer, J. Yang**

10:50 **CATL 270.** Thermodynamic considerations in the design of molecular electrocatalysts for selective CO₂ reduction. **J. Yang, D.W. Shaffer, S. Poteet, J. Ritter**

11:20 **CATL 271.** First-principles quantum chemical investigations on the selectivity of borohydride for carbon dioxide and bicarbonate reduction in protic conditions. **M.C. Groenenboom, K.A. Grice, J.A. Keith**

WEDNESDAY AFTERNOON

Colorado Convention Center
Room 107

Novel Catalytic Materials for Renewable Fuels/Chemicals

M. Foston, J. C. Hicks, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **CATL 272.** Synthesis of glycal-based bolaamphiphiles tethered to cobalt-Schiff base complexes for catalyst delivery to lignocellulose biomass. **J.J. Bozell, C. Nijjob, B.K. Long**

1:55 **CATL 273.** Anion catalysis: A novel pathway for C-O activation. **M. Emmert**

2:15 **CATL 274.** Role of defect sites in the hydrolysis of cellulose over activated carbon catalysts. **G. Foo, C. Sievers**

- 1:55 CATL 340.** Nanostructured nickel and cobalt phosphides as electrocatalysts for the hydrogen evolution reaction. E.J. Popczun, R.E. Schaak, C.G. Reed
- 2:15 CATL 341.** Withdrawn.
- 2:35 CATL 342.** Theoretical investigation of thermodynamic and kinetic properties of dihydropyridines in the catalytic reduction of CO₂ and various unsaturated functional groups. Y. Kuo, C. Lim, A. Holder, J.T. Hynes, C. Musgrave
- 2:55 Intermission.**
- 3:05 CATL 343.** Gold nanowires as an efficient and durable catalyst for CO₂ reduction. W. Zhu, Y. Zhang, H. Zhang, H. Lv, Q. Li, A.A. Peterson, S. Sun
- 3:25 CATL 344.** Design of visible light activated TiO₂ photocatalysts from first principles simulations. M. Nolan
- 3:45 CATL 345.** Carbon negative, renewable energy compatible electrochemical process for converting CO₂ and water into CO and H₂. D. Kauffman, C. Matranga, D. Alfonso, J. Thakkar, R. Jin

Section B

Colorado Convention Center
Room 109

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

CO₂ Activation

J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

1:30 Introductory Remarks.

- 1:35 CATL 346.** Electrochemical reduction of CO₂ to fuels. A.T. Bell
- 2:05 CATL 347.** CO₂ splitting in a packed-bed dielectric barrier discharge reactor. K.J. Nordheden, A.M. Banerjee, J. Billinger, S.M. Stagg-Williams, B. Subramaniam
- 2:35 CATL 348.** Carbon depositions and kinetic study over Ni-based catalysts in steam-CO₂ reforming of methane. Y. Park, Y. Kim, D. Moon
- 3:05 Intermission.**
- 3:20 CATL 349.** Functionality and topology dependence of CO₂/CH₄ adsorption and selectivity in zeolitic imidizolate frameworks (ZIFs). B.B. Laird
- 3:50 CATL 350.** Conversion of CH₄ and CO₂ into acetic acid on zinc-modified H-ZSM-5 zeolite. W. Wang, J. Wu, S. Yu
- 4:20 CATL 351.** Simultaneously converting carbonate/bicarbonate and biomass to value-added carboxylic acid salts by aqueous-phase hydrogen transfer. H. Lin, J. Su
- 4:50 CATL 352.** Engineering Co-exposed (001) and (101) facets and defects in TiO₂ nanocrystals for enhanced CO₂ photoreduction. L. Liu
- 5:20** Concluding Remarks.

Section C

Colorado Convention Center
Room 111

General Papers

V. Schwartz, *Organizer*
A. K. Mann, *Organizer, Presiding*

1:30 Introductory Remarks.

- 1:35 CATL 353.** Colloidal supported metal nanoparticles (CSMNPs) as novel intermediate nanocatalysts for the Suzuki and Heck reactions. R. Narayanan, K. Gude
- 1:55 CATL 354.** Model nanoparticle and zeolite catalysts for high selectivity hydrocarbon reforming. N. Musselwhite, S. Alayoglu, K. Na, K. An, G.A. Somorjai
- 2:15 CATL 355.** Stability and phase transfer of catalytically-active nanoparticle suspensions. I. Sriram, K. Jeerage
- 2:55 CATL 356.** Cu and CoCu surfaces in equilibrium with CO at Torr pressures. B. Eren, M. Salmeron, G.A. Somorjai
- 3:15 Intermission.**
- 3:30 CATL 357.** Identify the active species in ligand and base-free Cu-catalyzed aerobic homo-coupling of alkynes. L. Liu, A.L. Perez, A. Corma

- 3:50 CATL 358.** Metal-ligand cooperation in methanol/water dehydrogenation. M. Trincado
- 4:10 CATL 359.** New composite catalyst for trioxane production: Dramatic salt effect on trioxane synthesis. L. Yin, Y. Hu, Z. Yang, J. Qi
- 4:30 CATL 360.** Surface-bound ligands modulate chemoselectivity and activity of a bimetallate nanoparticle catalyst. V.O. Rodionov, B. Vu, K. Bukhriakov
- 4:50 CATL 361.** Controlled synthesis of Pd-NiO@SiO₂ mesoporous core-shell nanoparticles and their enhanced catalytic performance for *p*-chloronitrobenzene hydrogenation with H₂. S. Zhou, H. Liu, K. Tao
- 5:10 CATL 362.** TP³⁺- and V-doped TiO₂ quantum dots loaded on MCM-41 for photocatalytic degradation of organic dyes and isomerization of norbornadiene. L. Pan, J. Zou, S. Wang, Z. Huang, L. Wang, X. Zhang

CELL

Division of Cellulose and Renewable Materials

C. Frazier, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Next Generation Smart Materials (see POLY, Sun, Mon, Wed, Thu)

Water Our Most Critical Resource (see AGFD, Wed, Thu)

Biofuels & Sustainable Energy: Biomass Pretreatment & Hydrolysis (see BIOT, Tue, Wed, Thu)

Colorado Biotechnology: The Science of Colorado's Craft Beer, Wine & Spirits Industries (see BIOT, Sun)

Nanoscale Spectroscopic and Microscopic Characterization (see PMSE, Tue, Wed)

SOCIAL EVENTS:

Dinner, 6:30 PM, Tue

BUSINESS MEETINGS:

CELL Division Business Meeting, 5:00 PM: Wed

CELL Division Executive Committee Meeting, 5:00 PM: Sat

SUNDAY MORNING

Section A

Colorado Convention Center
Room 403

Cellulose in Solid State and Solution – Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Structural Aspects of Cellulose and NMR Studies
F. Liebner, L. Lucia, A. Potthast, *Organizers*
P. Kosma, J. Ralph, *Presiding*

8:00 Introductory Remarks.

- 8:05 CELL 1.** Thomas Rosenau, playful explorer of the mysteries of cellulose. A.D. French
- 8:35 CELL 2.** Imperfections in higher plant cellulose: Crystal stacking faults and structure of crystal-crystal interfaces. C. Driemeier
- 9:05 CELL 3.** Fabrication and characterization of cellulose nanoanemone. T. Kondo
- 9:35 CELL 4.** Cellulose nanocrystals: New preparation routes, and the relationship to the structure of native cellulose. E. Kontturi
- 10:05 Intermission.**
- 10:20 CELL 5.** Structural characteristics influencing the reactivity of isolated cellulose I. T. Larsson
- 10:50 CELL 6.** Identifying different hydroxyl populations in cellulose by ¹H MAS NMR. E. Lindh, C. Terenzi, I. Furó, L. Salmén

- 11:20 CELL 7.** High-resolution solution-State NMR of wood and pulp in ionic liquid electrolytes. A.J. Holding, V. Mäkelä, K.J. Helminen, I. Kilpeläinen, A.W. King
- 11:50 CELL 8.** NMR analysis of periodate-oxidation products of 5-*N*-acetylneuraminic acid methyl glycosides and 2,8-polyisalic acid (PSA). P. Kosma

Section B

Colorado Convention Center
Room 404

Functional Lignocellulosics and Nanotechnology

I. Filpponen, S. Spirk, *Organizers*
T. Nypelö, M. S. Peresin, *Organizers, Presiding*

8:00 Introductory Remarks.

- 8:05 CELL 9.** Picking foams from cellulose nanofibrils. L. Wagberg, N. Tchang Cervin
- 8:35 CELL 10.** Inhibition of alphavirus infection with tyrosine sulfate mimetic cellulose nanocrystals. J.O. Zoppe, V. Ruottinen, J. Ruotsalainen, S. Rönkkö, L. Johansson, A. Hinkkanen, K. Järvinen, J. Seppälä
- 8:55 CELL 11.** Modification of nanocellulose with natural molecules: A green perspective for cellulose based materials with active properties. A. Garcia, A. Gandini, N. Belgacem, J. Bras
- 9:15 CELL 12.** Size exclusion nanocellulose based paper filter for virus removal. A. Mhraryan
- 9:35 CELL 13.** Antibacterial surface modification of nanocellulosic materials. J. Henschen, J. Illergård, P. Larsson, M. Ek, L. Wågberg
- 9:55 Intermission.**
- 10:15 CELL 14.** Tuning the properties and yield of cellulose nanocrystals in the production space. J. Zhu
- 10:35 CELL 15.** Properties of nanocellulose from wood pulp and bacterial cellulose obtained by different methods. L. Vikele, I. Sable, L. Rozenberga, R. Treimane, A. Treimanis, P. Semjonovs
- 10:55 CELL 16.** Nanocrystalline cellulose from agricultural waste for optical devices. L. Steiner, A.G. Dumanli, D. Reid, M. Duer, S. Vignolini
- 11:15 CELL 17.** Characterisation and reinforcing properties of cellulose nanocrystals esterified in water. B. Dhuiege, G. Sèbe
- 11:35 CELL 18.** Control of the surface properties of cellulose nanocrystals by transesterification of vinyl esters. J. Brand, G. Sèbe
- 11:55 CELL 19.** One step polymer grafting of poly(methyl methacrylate) from cellulose nanocrystals for composite applications. S. Kedzior, L. Graham, E.D. Cranston

Section C

Colorado Convention Center
Room 405

Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser

Green Chemicals from Lignocellulosics
G. Garnier, S. Kelley, *Organizers*
T. G. Rials, *Organizer, Presiding*

8:00 Introductory Remarks.

- 8:05 CELL 20.** Mechanisms of biogenic formaldehyde generation in wood. G.E. Frazier, G. Wan, M. Tasooji, H. Wise
- 8:35 CELL 21.** Amphipathic lignin derivatives for enzymatic saccharification and fermentation of lignocellulosics. Y. Yamamoto, N. Cheng, K. Igarashi, K. Koda, Y. Uraki
- 9:05 CELL 22.** Homogeneous tosylation of agarose as an approach towards functional bio-based materials. M. Gericke, T.J. Heinze
- 9:35 Intermission.**
- 9:50 CELL 23.** From sustainable chemical blocks to fuel: Synthesis of hydrocarbons from isoprene and acrolein. Z. Tong, F. Wang

- 10:20 CELL 24.** Development of an efficient polymer analogous reaction in ionic liquids and its application to chemical modification of lignocellulose. R. Kakuchi, Y. Shibata, M. Yamaguchi, K. Takahashi

10:50 CELL 25. Fundamental approaches to multiscale, multiphase phenomena in cellulose pyrolysis chemistry. C. Krumm, A. Paulsen, P.J. Dauenhauer

11:20 CELL 26. Valorization of lignin to renewable fuels and chemicals through biological funneling and chemical catalysis. D. Vardon, M. Franden, C. Johnson, E. Karp, M. Guarnieri, J. Linger, P. Pienkos, T.J. Strathmann, G. Beckham

Section D

Colorado Convention Center
Room 406

Lignin Biosynthesis, Characterization and Modifications

Lignin Biosynthesis and Biotechnical Conversion
T. Tamminen, *Organizer*
C. Crestini, *Organizer, Presiding*

- 8:00 CELL 27.** β-O-4 -type quinone methides in lignin biosynthesis and in pulping. J. Sipilä, A. Haikarainen, P. Nousiainen, M. Muuronen
- 8:30 CELL 28.** Molecular models of milled-wood lignin. P. Schifffels, H. Lange, C. Crestini
- 9:00 CELL 29.** Mechanical properties of bamboo nanofibers: An atomic simulation study. S. Yousefian, N. Rahbar
- 9:30 CELL 30.** Impact of changes in the lignin synthetic pathway on cell wall architecture. J. Liu, J.C. Cusumano, J. Kim, C. Chapple, L. Makowski
- 10:00 Intermission.**
- 10:15 CELL 31.** Diastereoselective fungal ligninolysis. D.J. Yelle, A.N. Kapich, C. Houtman, F. Lu, V. Tymokhin, R.C. Fort, J. Ralph, K. Hammel
- 10:45 CELL 32.** Exquisite sensitivity of Acridine Orange to lignocellulosic oxidation and mechanistic investigation. P. Kitiin, J. Worpel, J. Houtman, K.E. Hammel, C.G. Hunt, C.J. Houtman
- 11:15 CELL 33.** Lipoxygenase: A new oxidative enzyme for lignin biorefinery. C. Crestini, H. Lange, P. Gianni, E. Bartzoka
- 11:45 CELL 34.** Quantitation of S/G ratio in woods using 1064 nm FT-Raman spectroscopy. U.P. Agarwal, S. Ralph

Section E

Colorado Convention Center
Room 407

Application of Computational Chemistry to Biomass Chemistry and Utilization

Synthesis and Molecular-level Interactions of Cellulose
S. C. Chmely, T. J. Elder, *Organizers*
P. Ramakrishnan, *Presiding*

- 8:00 CELL 35.** Synthesizing cellulose. B.C. Knott, M.F. Crowley, M. Himmel, J. Zimmer, G. Beckham
- 8:30 CELL 36.** QM/MM and MD study on catalytic mechanism of bacterial CESA. H. Yang, J. Lee, J. Zimmer, Y.G. Yingling, J.D. Kubicki
- 9:00 CELL 37.** Molecular dynamics simulation study of the AxCeSD octamer complexed with cellulose chains. T. Yui, T. Uto, Y. Ikeda, K. Tajima, M. Yao
- 9:30 CELL 38.** Molecular basis for cellulose twist. M.F. Crowley, L. Bu, M. Himmel
- 10:00 Intermission.**
- 10:10 CELL 39.** DFT calculations on the thermodynamics of PCW component interactions. J.D. Kubicki, V. Gibilittera, T. Weiss, H. Watts, L. Petridis, P. Langan, L. Zhong
- 10:40 CELL 40.** Can crystal structure conformations help validate conformational analyses of isolated molecules? A.D. French
- 11:10 CELL 41.** Hydration control of the mechanical and dynamical properties of cellulose. L. Petridis, H.M. O'Neill, M. Johnsen, B. Fan, E. Mamontov, J.K. Maranas, R. Schulz, P. Langan, J.C. Smith

11:40 **CELL 42.** Modeling graphene-cellulose-water interactions. S.J. Eichhorn, R.A. Bryce, R. Alqus

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 403

Cellulose in Solid State and Solution – Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Plant Cell Walls and Biorefineries

F. Liebner, L. Lucia, A. Potthast, *Organizers*
H. Sixta, A. Van Heiningen, *Presiding*

1:30 **CELL 43.** Recent progress on oxygen delignification of softwood Kraft pulp. A. Van Heiningen

2:00 **CELL 44.** BLN hot water extraction process – taking forest biomass fractionation to a totally new level. S. Willför, L. Vähäsalo, S. von Schoultz

2:30 **CELL 45.** Full utilization of wood in the future pulp mill bio-refinery. P. Aexgård

3:00 **CELL 46.** Influence of pectinase treatments on the dissolution abilities of cellulose pulps in NaOH-water. P.R. Navard, N. Dos Santos, J. Puls, B. Saake

3:30 **Intermission.**

3:45 **CELL 47.** Nanoporous cellulose: A new form of cellulose with novel properties. R.H. Atalla, R.S. Atalla

4:15 **CELL 48.** New model of plant cell wall cellulose elementary fibril. U.P. Agarwal

4:45 **CELL 49.** Effect of cellulose polymorphism on the TEMPO-based oxidation and further grafting by amidation. D. Da Silva Perez, Y. Habibi, A. Guillemain, J. Puteaux, L. Heux

5:15 **CELL 50.** Porosity development of dissolving pulp during mechanical and enzymatic processing. S. Grönqvist, T. Hakala, T. Kämpuri, M. Vehviläinen, T. Liittä, T. Maloney, A. Suurnäkki

Section B

Colorado Convention Center
Room 404

Functional Lignocellulosics and Nanotechnology

T. Nypelö, M. S. Peresin, S. Spirk, *Organizers*
I. Filpponen, *Organizer, Presiding*
T. Tammelin, *Presiding*

1:30 **CELL 51.** Functionalising micro/nanofibrillated cellulose with TEMPO-based approaches: From laboratory to pilot scale. D. Da Silva Perez, A. Guillemain, S. Tapin-Lingua, V. Meyer, B. Fabry, P. Huber

1:50 **CELL 52.** Structurally colored films using nanocellulose fiber. S.J. Eichhorn, P. Vukusic, D. Hewson, J.C. Grunlan, P. Tzeng

2:20 **CELL 53.**

Architecture and properties of hybrid cellulose nanocrystals/Gibbsite nanoplatelets multilayered films. C. Martin, R. Barker, E.D. Cranston, L. Heux, B. Jean

2:40 **CELL 54.** Functional cellulose nanocrystals for ATRP and click chemistry-preparation and characterization. A. Carlmark, A. Boujemaoui, S. Mongkhontreerat, E.E. Malmström

3:00 **CELL 55.** Surfactant and polymer-enhanced CNC Pickering emulsions, gels, and oil powders. Z. Hu, R.H. Pelton, E.D. Cranston

3:20 **Intermission.**

3:40 **CELL 56.** Cellulose nanocrystals with CO₂-switchable aggregation and redispersion properties. H. Wang, J. Bouchard, P.G. Jessop, P. Champagne, M.F. Cunningham

4:00 **CELL 57.** Nanocellulose composites for electronic paper displays. A.G. Dumanli, H. Yuan, U. Steiner

4:20 **CELL 58.** Withdrawn.

4:40 **CELL 59.** Composite fibers from cellulose nanofibril emulsions. T. Nypelö, C.A. Carrillo, O.J. Rojas

5:00 **CELL 60.** Structure and properties of carboxylated nanocellulose with various counter-ions. M. Shimizu, T. Saito, A. Isogai

5:20 **CELL 61.** Thermoresponsive TOCN films: Influence of PNIPAm on film properties. N. Lavoine, J. Bras, T. Saito, A. Isogai

Section C

Colorado Convention Center
Room 405

Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser

Fundamentals of Cellulosic Materials

S. Kelley, T. G. Rials, *Organizers*
G. Garnier, *Organizer, Presiding*

1:30 **CELL 62.** Contributions of computational chemistry to understanding cellulose. A.D. French

2:00 **CELL 63.** Pros and cons of various cellulose crystallinity estimation methods: 380-Raman, ¹³C NMR, and Segal-WAXS. U.P. Agarwal

2:30 **CELL 64.** Interactions between rod-shaped nanoparticles and polymer chains in aqueous solutions. H. Oguzlu, Z. Khalili, Y. Boluk

3:00 **CELL 65.** Synthesis and properties of fatty acid esters of technical lignins for biorefinery applications. K. Koivu, H. Sadeghifar, P. Nousiainen, D. Argyropoulos, J. Sipilä

3:30 **Intermission.**

3:45 **CELL 66.** Single step functionalization of cellulose to produce bacterial cellulose-reinforced derivatised all-cellulose nanocomposites. K. Lee, A. Bismarck

4:15 **CELL 67.** Polymer-grafting or adsorption of amphiphilic block copolymers – different approaches to compatibilization in CNF-based nanocomposites. E.E. Malmström, C. Bruce, L. Fogelström, M.K. Johansson, A. Carlmark

4:45 **CELL 68.** Cellulose surfaces modified by latex particles prepared via RAFT-mediated emulsion polymerization. A. Carlmark, L.K. Carlsson, E.E. Malmström, L. Wagberg, J. Engström, F. Hatton, M. Jawerth, C. Freire, F. D'Agosto, M. Lansalot

5:15 **CELL 69.** Model cellulose surfaces to characterize (bio)polymer interaction: Designing the interphase. G. Garnier, J. Su, C. Garvey, W. Batchelor, W. Raverty

Section D

Colorado Convention Center
Room 406

Lignin Biosynthesis, Characterization and Modifications

Lignin Characterization

C. Crestini, *Organizer*
T. Tamminen, *Organizer, Presiding*

1:30 **CELL 70.** Why “laboratory standard” is not good enough in GPC-analyses of Lignins. H. Lange, F. Rulli, C. Crestini

2:00 **CELL 71.** Enzyme surface hydrophobicity predicts enzyme adsorption to lignin films. D. Sammond, J. Yarbrough, E. Mansfield, Y.J. Bomble, M. Resch, J.J. Bozell, M.E. Himmel, M.F. Crowley

2:30 **CELL 72.** Comparing different approaches to measure molar mass of lignin: SEC, DOSY and AsFIFFF. I. Sulaeva, I. Sumerskii, M. Bacher, G. Zinovyev, U. Henniges, T. Rosenau, A. Potthast

3:00 **CELL 73.** Exploring the use of pulsed field gradient (PFG) NMR to extract molecular weight distributions of lignin. J.O. Thomas, C.F. Clewett, T.M. Alam

3:30 **Intermission.**

3:45 **CELL 74.** Analysis of lignin hydroxyl groups by NMR spectroscopy. E.A. Capanema

4:15 **CELL 75.** Characterization of alkaline lignin by thermal desorption and pyrolysis methods. K. Voeller, A. Kubatova, E.I. Kozliak

4:45 **CELL 76.** Low-field NMR study of interactions between lignin and cellulase. M. Li, J. Yang, M. Tu, T.J. Elder

5:15 **CELL 77.** Facile quantification of biomass Lignin using acidic lithium bromide (ALB) method. N. Li, J. Alexander, X. Pan

Section E

Colorado Convention Center
Room 407

Application of Computational Chemistry to Biomass Chemistry and Utilization

Cellulose Degradation and Conversion

S. C. Chmely, T. J. Elder, *Organizers*
P. Ciesielski, *Presiding*

1:30 **CELL 78.** Solvation dynamics and energetics of hydride transfer reactions in cellulose biomass conversion. S. Mushrif, C. BK, J.J. Varghese

2:00 **CELL 79.** Frequency filtration to obtain realistic thermal vibrations in crystal from molecular dynamics. Y. Ogawa, Y. Nishiyama, K. Mazeau

2:30 **CELL 80.** Mechanism of alkyl and alkaline earth chloride-enhanced hydrolysis of cellulose in acid solutions. P. Chen, B. Rabideau, A.E. Ismail

3:00 **CELL 81.** Computational targets for reaction pathways and energetics of cellulose conversion to fuels and chemicals. P.J. Dauenhauer

3:30 **Intermission.**

3:40 **CELL 82.** Interference trinity: Lignins' role in biomass recalcitrance explored through petascale simulation. J.V. Vermaas, X. Qi, R. Schulz, L. Petridis, J.C. Smith

4:10 **CELL 83.** Unmasking the mystery base employed by the *T. reesei* Cel6A cellulase. H. Mayes, B. Knott, M.F. Crowley, A.W. Goetz, J. Ståhlberg, L.J. Broadbelt, G. Beckham

4:40 **CELL 84.** Role of water on metal catalyst performance for ketone hydrogenation: A joint experimental and theoretical study on levulinic acid conversion into gamma-valerolactone. C. Michel, J. Zafrañ, A.M. Ruppert, J. Matras-Michalska, M. Jedrzejczyk, J. Grams, P. Sautet

5:10 **CELL 85.** Multiscale modeling of the interfacial structure in xylan/cellulose nanocomposites. K. Mazeau, P. Perre, I. Li, X. Frank

SUNDAY EVENING

Section F

Colorado Convention Center
Hall C

Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser

Posters

G. Garnier, S. Kelley, T. G. Rials, *Organizers*

6:00 - 8:00

CELL 86. Macroalgae as filler in thermoplastic composites: Opportunities and weaknesses. M. Bulota, T. Budtova

CELL 88. Where are the *gauche-gauche*-CH₂OH groups in cellulose I materials? U.P. Agarwal

CELL 90. Study of nitrogen fixation by condensation of urea on hydrothermally treated corn cob. J.A. Cordoba Arias, E. Salcedo Pérez, R. Manriquez Gonzalez, E. Delgado

CELL 93. Analysis of recalcitrant lignin structures to understand the impact of alkaline hydrothermal pretreatment on enzyme digestibility. L. Xiao, Y. Bai, X. Chen, Z. Xue, R. Sun

CELL 94. Synthesis and characterization of novel green wood adhesives from biorefinery lignin. P.S. Dongre, M. Driscoll, J. Smith, T. Amidon, B. Bujanovic

CELL 96. Properties of regenerated bamboo fibers prepared from raw materials with different hemicellulose content. J. Chen, K. Wang, F. Xu, R. Sun

CELL 99. Structural characterization of annealed bacterial cellulose by SFG, FTIR and XRD. Y. Weng, K. Kafle, S.H. Kim, J.M. Catchmark

CELL 101. Microwave-assisted carbonization of bamboo by wet torrefaction in diluted acid. M. Li, Y. Shen, J. Sun, C. Chen, X. Li, R. Sun

CELL 102. Production of furfural from hemicelluloses in biphasic system by highly efficient and recyclable magnetic solid acid from glucose. Y. Bai, L. Xiao, X. Chen, R. Sun

CELL 105. Systematic evaluation on degradation products during hydrothermal pretreatment of sweet sorghum basis for biorefinery. S. Sun

CELL 107. Sustainable bitumen. T. Slaghek, D.V. Vliet, I. Haaksman, C. Giesen

CELL 110. Physical and structural changes in cellulose microfibrils responsible for enzymatic hydrolysis rate deactivation studied by FTIR, XRD, XPS and SFG. K. Kafle, C. Lee, H. Shin, S.H. Kim, S. Park

CELL 111. Impact of fractionation time on thermal and chemical properties of organosolv lignins. J. Tao, O. Hosseinaei, P. Kim, D.P. Harper, J.J. Bozell, T.G. Rials, N. Labbe

CELL 112. In situ catalytic fast pyrolysis of lignin for production of phenols using oxide catalysts. V. Nair, V. R

CELL 115. All-cellulose composites from partial hydrolysis oxidation and thermal crosslinking. N. Guigo, A. Codou, L. Heux, N. Sbirrazzuoli

Section F

Colorado Convention Center
Hall C

General Posters

Cosponsored by CARB

C. E. Frazier, *Organizer*

6:00 - 8:00

CELL 87. Use of micro-structured cellulose from soybean hulls as coating additives for paper. A. Ferrer, C.L. Salas, T.W. Theysen, O.J. Rojas

CELL 89. Bioinspired xyloglucan-containing films as responsive smart materials. A. Villares, C. Moreau, B. Cathala

CELL 91. Cellulose nanoparticles from new sources – agricultural wastes: Apple tree (*Malus domestica*) pruning residues and pea (*Pisum sativum*) stalks. A. Garcia, A. Gandini, J. Labidi, N. Belgacem, J. Bras

CELL 92. Hybrid composites with microcrystalline cellulose, lignin, and polyethylene. A. Treimanis, M. Laka, J. Ganster, J. Erdmann, L. Ziegler

CELL 95. Sulfite pretreatment of post-enzymatic hydrolysis softwood residue to enhance saccharification and produce lignosulfonates. B. Jeuck, O.J. Rojas, H. Jameel

CELL 97. Process simulation of biomass fast-pyrolysis into transportation fuels: Model sensitive to variations in biomass chemical composition. C.E. Aizpuru, H. Kim, H. Jameel, M. Wright, S.S. Kelley, S. Park

CELL 98. Characterization and evaluation of the lignin from one-pot HDA process for chemical transformation of biomass into hydrocarbons. C. Yoo, S. Zhang, H. Kim, J. Zeng, J. Ralph, Z. Tong, X. Pan

CELL 100. Study on the characteristics of two marine oil-degraded yeasts and their utilization for carbon source spectrum of crude oil. C. Ma, J. Liu, N. Ma, X. Mou, N. He

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

- CELL 103.** Novel production of furfural from biomass based on hot water extracted pentoses. **C.D. Wood**, B. Bujanovic, T. Amidon
- CELL 104.** Cooxidant-free TEMPO-mediated oxidation of highly crystalline *Cladophora* nanocellulose. **D.O. Carlsson**, J. Lindh, L. Nyholm, M. Stromme, A. Mhramyan
- CELL 106.** Potential for enhancement of enzymatic hydrolysis of sugar maple (*Acer saccharum*). **M.A. Uygut**, M. Zelic, C.D. Wood, **D.B. Corbett**, P.S. Dongre, B. Bujanovic
- CELL 108.** Structures of carboxylated cellulose fibers – fates of S1, S2, and S3 layers. **G. Sim**, M.N. Alam, L. Godbout, T.G. van de Ven
- CELL 110.** Development of 3 drug combination formulations with cellulose esters for the effective oral treatment of HIV. **H. Arca**, D. Dahal, K.J. Edgar
- CELL 113.** Magnetic responsive hybrid paper materials that react to external magnetic fields. **H. Wang**, M. Biesalski
- CELL 114.** Effect of different ratio of CMC and Eu(III) on the fluorescence properties and structures of CMC/Eu nanocomposites. **B. Wang**, J. Ye, J. Xiong
- CELL 116.** One-pot formation of 2,3-dialdehyde cellulose (DAC) beads. **J. Lindh**, D.O. Carlsson, C. Ruan, M. Stromme, A. Mhramyan
- CELL 117.** Interactions between cellulose surfaces and cellulases from different origins studied by QCM. **J. Song**, Y. Li, O.J. Rojas
- CELL 118.** Isolation and structural analysis of novel sulphur-free lignin fraction from non-wood plant materials. **J. Sipila**, J. Kontro, P. Nousiainen, Y. Mälikki
- CELL 119.** Vibrational sum-frequency-generation (SFG) spectroscopy study of cellulose microfibril orientation and assembly in onion epidermis and reaction woods. **K. Kafle**, X. Xi, R. Shi, C. Lee, A. Mittal, S. Park, B.R. Tittmann, V. Chiang, D. Cosgrove, Y. Park, S.H. Kim
- CELL 120.** Determination of the molecular weight distribution of highly oxidized dialdehyde cellulose by size exclusion chromatography. **I. Sulaeva**, T. Rosenau, A. Potthast, **K. Klinger**
- CELL 121.** Nanofibrillation of dried pulp in NaOH solutions and their regenerations. **K. Abe**
- CELL 122.** Characterization of cellulose nanofibrils sheet mixed with synthetic or natural pulp fiber. **K. Sim**, H. Youn, J. Lee, H. Lee
- CELL 123.** Theoretical models of electron transfer processes in LPMOs and model peptide systems. **L. Berstis**, M.F. Crowley, G. Beckham
- CELL 124.** Continuous hydrolysis of carboxymethyl cellulose with cellulase aggregates trapped inside membranes. **L. Nguyen**, K. Yang
- CELL 125.** Novel materials from wood component. **L.K. Carlsson**, P. Martirez, M. Helander, A. Lopez Cabezas, O. Schmidt
- CELL 126.** Production of nanocellulose through hydrolysis without mineral acids using sub-critical water. **L. Pereira Novo**, A. Garcia, A. da Silva Ouwelo, N. Belgacem, J. Bras
- CELL 127.** New nanohybrid materials from sugar cane bagasse: The role of acid hydrolysis. **L. Diaz**, R. Hernandez Ortiz, M. Tete, E. Mata, E. Sosa, R. Atencio
- CELL 128.** Imaging cellulose nanocrystals by transmission electron spectroscopy. **M. Kaushik**, W. Chen, T.G. Van De Ven, A.H. Moores
- CELL 129.** Evaluation of various parameters in the production of whey protein concentrate-based films. **M. Viquez**, M. Molina Cordoba, M. Esquivel Alfaro, M. Montero Calderon
- CELL 130.** Immobilization of *glucosyl oxidase* in cellulose supports. **M.L. Auad**, R.A. Ballester, O. Nordness, M. Arugula, A.L. Simonian
- CELL 131.** Thermal protection of vitamins B1, B2, B3, B6 and B12 with bacterial nanocellulose. **M. Osorio Delgado**, D. Sanchez, J. Velásquez-Cock, R. Zuluaga Gallego, P. Gañán, C. Jiménez, O.J. Rojas, L. Velez-Acosta, B. Gómez, C. Castro Herazo

- CELL 132.** Effects of time, temperature, and pH on the Interconversion of cellulose I to cellulose II. **M. Islam**, C.J. Huntley, W.E. Collier, M.L. Curry
- CELL 133.** Polymeric functionalized beads from alginate for targeted release of auxin into water. **M. Li**, G. Buschle-Diller, T.J. Elder
- CELL 134.** Moisture and solvent responsive cellulose/SiO₂ nanocomposite materials. **M. He**, B. Duan, L. Zhang
- CELL 135.** Paper-based microfluidics for typing of primary and secondary human blood groups in "text". **M. Li**, W. Then, J. Tian, W. Shen
- CELL 136.** In vitro synthesis of cellulose under various conditions. **P.A. Penttilä**, J. Sugiyama, T. Imai
- CELL 137.** Method for studies of oxidoreductase catalyzed oxidation of synthetic lignin in presence of co-oxidants. **P. Nousiainen**, J. Kontro, H. Manner, A. Hatakka, J. Sipila
- CELL 138.** Regenerated cellulose fiber from ionic liquid-waste cotton solution by dry-jet wet spinning. **S. Asaadi**, M. Hummel, H. Sixta
- CELL 139.** Evaluation of nanocelluloses as flooding additives for the petroleum industry. **S.N. Molnes**, K. Syverud, S. Strand, K.G. Paso
- CELL 140.** Modification and optimization of cellulose nanocrystal-latex interactions. **S. Kedzior**, Z. Dastjerdi, M.A. Dubé, E.D. Cranston
- CELL 141.** Structural stability of the molecular chain sheets composing the crystal structures of cellulose allomorphs: A theoretical study. **T. Uto**, T. Yui
- CELL 142.** Characterization of noncrystalline regions in regioselectively methylated cellulose films using vapor-phase deuteration and generalized 2D correlation infrared spectroscopy. **Y. Hishikawa**, T. Kondo
- CELL 143.** Density functional theory calculations on concerted lignin pyrolysis mechanisms. **T.J. Elder**, A. Beste
- CELL 144.** Effect of urea as an additive in the alkali pretreatment of cellulose I to cellulose II. **V. Niyal**, P. Gupta, S. Naithani
- CELL 145.** Iridescent 3D structures produced by evaporation of droplets of cellulose nanocrystal suspensions. **X. Mu**, D.G. Gray
- CELL 146.** 3D nanofiber scaffolds of bacterial cellulose and chitosan generated from solution blowing spinning using an airbrush. **X. Yin**, L.A. Lucia, A. Nandgaonkar
- CELL 147.** Hydrophobic functionalization of jute fabric via enzymatic grafting of octadecylamine. **X. Fan**, A. Dong, Q. Wang, P. Wang, J. Yuan
- CELL 148.** Textile fibers from recycled waste materials. **Y. Ma**, S. Asaadi, M. Maattanen, A. Sarkkilahti, M. Hummel, A. Harlin, H. Sixta
- CELL 149.** Hemicellulose-based hydrogel containing Ag nanoparticles for antibacterial application. **Y. Guan**, F. Peng, R. Sun
- CELL 150.** Antibacterial cellulose acetate films containing N-halamine modified nanocrystalline cellulose. **Y. Liu**, X. Ren, G. Buschle-Diller
- CELL 151.** Direct chemical modification and separation of biomass components using ionic liquids based organocatalysts. **Y. Shibata**, R. Kakuchi, K. Takahashi
- CELL 152.** Preparation of butyl levulinate through the acid catalyzed solvolysis of cellulose using a single reaction process. **Y. Hishikawa**, M. Yamaguchi, S. Kubo, T. Yamada
- CELL 153.** Effect of molecular weight and chain length on surface and interfacial tension, emulsification and cleaning properties of polysaccharide-based surfactants derived from pectin. **Z. Mohd Aris**, V. Bavishi, N. Tchirkova, R. Nagarajan

MONDAY MORNING

Section A

Colorado Convention Center
Room 403

Cellulose in Solid State and Solution – Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau Advances in Lignin Chemistry and Analysis of Polysaccharides

F. Liebner, L. Lucia, A. Potthast, *Organizers*
D. O. Klemm, M. Tenkanen, *Presiding*

- 8:00 CELL 154.** Update on Zip-lignins™: Lignins designed for deconstruction. **J. Ralph**, F. Lu, S.D. Karlen, D. Padmakshan, M. Regner, R. Smith, H. Kim, Y. Zhu, J. Rencoret, J. Grabber, C.G. Wilkerson, J.C. Sedbrook, S. Mansfield
- 8:30 CELL 155.** Cross-coupling and oxidation of novel lignin monomers with conventional monolignols. **T.J. Elder**, J. Ralph
- 9:00 CELL 156.** Recent advances in lignin chemistry. **M. Balakshin**
- 9:30 CELL 157.** Multistep lignin degradation method for the isolation of lignin-carbohydrate-complex (LCC) bonding sites. **D. Ando**, F. Nakatsubo, T. Takano, H. Yano
- 10:00 Intermission.**
- 10:15 CELL 158.** Determination of molecular mass and molecular mass distribution of TEMPO-oxidized celluloses (TOCs) and TOC nanofibrils (TOCNs) using SEC-MALLS. **R. Hiraoki**, Y. Ono, T. Saito, A. Isogai
- 10:45 CELL 159.** Recent advances in biorefinery process stream analysis. **A. Potthast**
- 11:15 CELL 160.** Mass spectrometry analysis of structural details in O-acetylglucuronoxylans. **S. Chong**, P. Tuomänen, M. Juvonen, M. Derba-Maceluch, E. Mellerowicz, **M. Tenkanen**
- 11:45 CELL 161.** Cellulose degradation during deformation processing and analytics. **T. Roeder**, G. Kilba, W. Milacher, G. Kraft, A. Potthast, T. Rosenau

Section B

Colorado Convention Center
Room 404

Functional Lignocellulosics and Nanotechnology

T. Nypelö, S. Spirk, *Organizers*
I. Filpponen, M. S. Peresin, *Organizers, Presiding*

- 8:00 CELL 162.** Functionalization of nanocelluloses by supramolecular motifs to combine competing properties. **J.R. McKee**, E. Appel, E. Janacek, H. Tenhu, E. Kontturi, O.A. Scherman, **O.T. Ikkala**
- 8:30 CELL 163.** Controlling the elastic modulus of cellulose nanofibril hydrogels – scaffolds with potential in tissue engineering. **K. Syverud**, S.R. Pettersen, K.J. Draget, G. Chinga-Carrasco
- 8:50 CELL 164.** Aerogels and foams from cellulose nanocrystals as superabsorbents, shape recovery materials, and templates. **X. Yang**, Z. Hu, **E.D. Cranston**
- 9:10 CELL 165.** Biocompatible cellulose-based cell scaffolds: Generation of interconnected micron-size pores embedded in frameworks of nanoporous PMMA-reinforced cellulose struts. **N. Pircher**, D. Fischhuber, L. Carbajal Galan, C. Strauß, J. Nedelec, C. Kasper, T. Rosenau, F. Liebner
- 9:30 CELL 166.** Photoactive materials for wound care purposes based on bacterial cellulose. **H. Hettegger**, S. Sortino, A. Potthast, T. Rosenau
- 9:50 Intermission.**
- 10:10 CELL 167.** Functionalization of cellulose nanofibril surfaces to enhance crystallization and mechanical properties of poly-l-lactide. **S. Fujisawa**, T. Saito, A. Isogai
- 10:30 CELL 168.** Phase behavior of water-in-oil emulsions stabilised solely by hydrophobised bacterial cellulose nanofibrils. **K. Lee**, J. Blaker, R. Murakami, J.Y. Heng, A. Bismarck
- 10:50 CELL 169.** Withdrawn.

- 11:10 CELL 170.** Silver nanoparticles synthesis mediated by cellulose nanocrystals: Role of surface chemistry in nucleation phenomena. **K. Uddin**, A.R. Lokanathan, J. Laine, O.J. Rojas

- 11:30 CELL 171.** Nanocomposites from holocellulose and silver with enhanced antimicrobial activity. **L. Fu**, F. Deng, M. Ma

Section C

Colorado Convention Center
Room 405

Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser

Advanced Materials from Lignocellulosics

G. Garnier, T. G. Riels, *Organizers*
S. Kelley, *Organizer, Presiding*

- 8:00 CELL 172.** Biobased materials from lignocellulosic fibers: A brief overview. **E. Frollini**, B. Rodrigues, E. Ramires, F. de Oliveira, I. Razera, R. Passos de Oliveira Santos
- 8:30 CELL 173.** Efficient adsorbents based on nanoporous carbon fibers from cellulosic precursors. **D. Berek**, I. Novak, K. Munka
- 9:00 CELL 174.** Curing behavior and bond performance of wood adhesive from enzymatic hydrolysis residues of lignocellulosic biomass. **I. Hafez**, H. Yang, W.T. Tze
- 9:30 CELL 175.** Electrospinning of lignin based composite nanofibers with nanocrystalline celluloses. **M. Cho**, F.K. Ko, S.H. Renneckar
- 10:00 Intermission.**
- 10:15 CELL 176.** Preparation and properties of composite Lyocell fibers using hemicelluloses as regulator. **J. Chen**, Y. Guan, K. Wang, F. Xu, R. Sun
- 10:45 CELL 177.** Repeated homogenization, a route for decreasing the energy consumption in the nanofibrillated cellulose manufacturing process? **A. Naderi**, T. Lindström
- 11:15 CELL 178.** Recent advances in cellulose ester performance and applications. **J.D. Goodrich**
- 11:45 CELL 179.** Biopolymer modification: Converting biopolymers into processable thermoplastics. **W.G. Glasser**
- 12:15 Concluding Remarks.**

Section D

Colorado Convention Center
Room 406

Lignin Biosynthesis, Characterization and Modifications

Degradative Routes for Lignin Valorisation

C. Crestini, T. Tamminen, *Organizers*
R. Gosselink, *Presiding*

- 8:00 CELL 180.** Willow as a potential source of lignin raw material. **T. Tamminen**, A.M. Koskinen, T. Vuorinen
- 8:30 CELL 181.** New multiplexed assay for lignin depolymerization. **M. Kent**, I. Avina, N. Rader, V. Chavez, M. Busse
- 9:00 CELL 182.** Sub- and supercritical water liquefaction of alkali lignin in presence of carbon dioxide and ammonia. **A. Numan-Al-Mobin**, C. Lynde, P. Kolla, D.J. Dixon, A. Kubatova, A. Smirnova
- 9:30 CELL 183.** Lignin oxidation depolymerization using graphene oxide as a metal-free catalyst. **J. Zeng**, Z. Tong
- 10:00 Intermission.**
- 10:15 CELL 184.** Catalytic hydrogen-free conversion of lignin in key aromatics. **R. Gosselink**
- 10:45 CELL 185.** Metal-organic frameworks as selective catalysts for carbon-oxygen bond cleavage in lignin model compounds. **V. Stavila**, K. Leong, R. Parthasarathi, K. Sale, R. Davis, M. Allendorf
- 11:15 CELL 186.** Comparative separation and characterization of lignin by catalytic hydrothermal pretreatment with metal chlorides. **M. Wu**, X. Zhang, R. Sun
- 11:45 CELL 187.** Correlating structural features of lignin with physical properties: Toward a descriptive-predictive database. **H. Lange**, O. Sevastyanova, C. Crestini

8:30 CELL 312. Synergistic templated self-assembly of cellulose nanocrystals (CNCs) in thin block copolymer films. **D. Grolman, J. Gilman, A. Karim**

9:00 CELL 313. New concepts for molecular engineering of macroscopic adhesion between cellulose surfaces. **A. Trager, S. Pendergraph, A. Carlmark, L. Wagberg**

9:30 CELL 314. Improved interfacial bonding in cellulosic biocomposites with humins-based furanic resins. **N. Guigo, J. Pin, A. Mija, L. Vincent, N. Sbirrazzuoli, J.C. van der Waals, E. de Jong**

10:00 Intermission.

10:15 CELL 315. Spray-dried microencapsulation of tea tree oil with a complex of methyl cellulose/chitosan/alginate. **J. Chen, X. Yin, X. Wang, J. Chen, L. Zhu, L.A. Lucia**

10:45 CELL 316. Photocatalytic and biocatalytic degradation of dye solution using laccase and titanium dioxide loaded on bacterial cellulose. **A. Nandgaonkar, Q. Wang, W. Krause, Q. Wei, L. Lucia**

11:15 CELL 317. Enzymatic bio-fuel cells based on bacterial cellulose (BC)/MWCNT/laccase (Lac) and bacterial cellulose / MWCNT/ glucose oxidase (GOD) electrodes. **Q. Wang, A. Nandgaonkar, L. Lucia, Q. Wei**

11:45 CELL 318. Improved antibacterial coatings with Nanotitania and cyclic N-halalmine. **X. Ren, J. Li, L. Li, T. Huang**

Section D

Colorado Convention Center
Room 406

Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America

Composites and Nanomaterials

J. Campos-Teran, O. El Seoud, D. Petri, O. J. Rojas, Organizers
M. L. Auad, Organizer, Presiding
R. Christoph, J. Vega-Baudrit, Presiding

8:00 CELL 319. Renewable resources as precursors of biobased thermosetting resins. **M.L. Auad, B. Sibaja**

8:25 CELL 320. Sisal pulp as raw material for magnetic hybrid films and sugars. **E. Frollini, L. Varanda, A. de Oliveira, Á. Faceto, B. Rodrigues, D. Furlan, D. de Moraes, J. Kaschuk**

8:50 CELL 321. Biopolymers from tomato agro-industrial residual wastes. **M.B. Gómez-Patiño, J. Méndez-Méndez, M. Jaramillo-Flores, J. Campos-Terán, D. Arrieta-Baez**

9:15 CELL 322. Formation and characterization of 10,16-dihydroxyhexadecanoic acid thin films extracted from tomato residues. **J. Hernández-Ortiz, M.B. Gómez-Patiño, C. Ramos-Torres, D. Arrieta-Baez, J. Campos-Terán**

9:40 Intermission.

9:55 CELL 323. Functional lignins used as curing agent in fiber-reinforced epoxy-materials. **M.A. Biesalski, M. Baaske, S. Mehrlase, R. Klein, S. Valkonen, M. Duetsch**

The use of any device to capture images (e.g., camera 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.

10:20 CELL 324. Deconstructing a natural fiber: Physicochemical and structural properties of cellulose nanofibrils and nanocrystals from Colombian fique plants. **S.A. Ovalle-Serrano, L.F. Jaimes-Cote, C.P. García-Villamizar, F.N. Gómez-Jaimes, C. Blanco-Tirado, M.Y. Combariza**

10:45 CELL 325. Collection and evaluation of blended polypropylene banana tree rachis fibers (Musa AAA). **R. Zamora**

11:10 CELL 326. Surface active materials from functionalized fique's nanocrystalline cellulose. **F.N. Gómez-Jaimes, M.M. González-Bernal, C.F. Medina-Sandoval, J. Valencia, M.Y. Combariza, C. Blanco-Tirado**

11:35 CELL 327. QCM/SPR to study the oxidation and removal of unsaturated fatty acids from NFC and PET surfaces by lipooxygenase treatment. **A. H.M. Tayeb, O.J. Rojas, C.L. Salas, K.D. Wing**

12:00 Concluding Remarks.

Section E

Colorado Convention Center
Room 407

Cellulose Dissolution: New Solvents and Mechanisms

N. Abidi, E. L. Quitevis, Organizers, Presiding

8:00 Introductory Remarks.

8:05 CELL 328. Recent developments in solvents for cellulose. **T.J. Heinz**

8:35 CELL 329. Interactions between cellulose and small molecules. **R. Liu, C. Zhang, Z. Liu, Z. Jiang, Y. Huang**

9:05 CELL 330. Mechanism and kinetics of advantaged biofuels synthesis from D-fructose. **T. Flannelly, S. Dooley, J. Leahy**

9:35 CELL 331. Biphasic process using molten salt hydrates for chemical transformation of lignocellulosic biomass into furan-based chemicals. **C. Yoo, S. Zhang, X. Pan**

10:05 Intermission.

10:20 CELL 332. Homogeneous saccharification of lignocellulosic biomass in molten salt hydrates. **N. Li, X. Pan**

10:50 CELL 333. Energetically favored alternative hydrogen bond of cellulose II and cellulose III'. **P. Chen, Y. Ogawa, Y. Nishiyama, M. Bergensträhle-Wohlert, K. Mazeau**

11:20 CELL 334. Probing particle - particle interactions in swollen cellulose nanocrystal thin films by surface plasmon resonance spectroscopy. **M.S. Reid, M. Villalobos, E.D. Cranston**

11:50 CELL 335. On the combination of NaOH activation and DMAc/LiCl dissolution of cellulose from cotton fibers during different stages of fiber development. **S.P. Liyanage, N. Abidi**

12:20 Concluding Remarks.

Polymeric Biomaterials

Sensors and Medical Devices

Sponsored by PMSE, Cosponsored by CELL

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 403

ACS Award for Affordable Green Chemistry: Symposium in Honor of John Frye, Todd Werpy, and Alan Zacher

Cosponsored by MPPG

C. E. Frazier, L. A. Lucia, Organizers, Presiding

1:30 Introductory Remarks.

1:35 CELL 336. Chemical functionalization and characterization of crystalline cellulose derived from agricultural waste products. **C.J. Huntley, K.D. Crews, M.L. Curry**

2:00 CELL 337. Isomerization of glucose to fructose by magnetic organic basic catalysts in aqueous media. **Q. Yang, T. Runge**

2:25 CELL 338. Direct thermal processing of cellulose plasticized with ionic liquids and its composites as polymer electrolytes. **J. Wu, Y. Liao, Y. Ye, X. Zhou, B. Brycki, X. Xie**

2:50 CELL 339. Fabrication and characterization of cellulose functional materials using ionic liquid 1-ethyl-3-methylimidazolium acetate (EmimAc). **J. Pang, X. Zhang, Q. Zhang, M. Wu, R. Sun**

3:15 CELL 340. Flexible route for solely biomass-derived *p*-xylene and terephthalic acid. **F. Wang, Z. Tong**

3:40 Intermission.

3:55 CELL 341. Cellulose nanocrystals as reinforcing agent in melt-spinning of polypropylene. **X. Lu**

4:20 CELL 342. Continuous hydrothermal liquefaction of cellulosic and lignocellulosic biomass. **J. Billing, A. Schmidt, T. Hart, G. Maupin, R.T. Hallen, D.C. Elliott**

4:45 CELL 343. Overview of the catalyst and process research and development efforts related to the PNNL glycerol to propylene glycol process. **J. Frye, A. Zacher, T. Werpy**

5:15 CELL 344. Award Address (ACS Award for Affordable Green Chemistry sponsored by The Dow Chemical Company and endowed by Rohm and Haas). Scale up challenges of first of a kind renewable chemicals. **T. Werpy, J. Frye, A. Zacher**

5:45 Concluding Remarks.

Section B

Colorado Convention Center
Room 404

Functional Lignocellulosics and Nanotechnology

I. Filpponen, S. Spirk, Organizers
T. Nypelö, M. S. Peresin, Organizers, Presiding

1:30 CELL 345. Withdrawn.

1:50 CELL 346. Defined cellulose-polymer hybrid materials by synthesis under homogeneous reaction conditions. **M.W. Ott, M. Biesalski**

2:10 CELL 347. Carbon dot (CD) modified cellulose nanocrystals (CNC) for biosensing and -imaging. **J. Guo, I. Filpponen, O.J. Rojas**

2:30 CELL 348. Carbon quantum dots from biomass: Synthesis and functionalization. **X. Wang, Z. Liang, R. Sun**

2:50 Intermission.

3:10 CELL 349. Inkjet printed paper-based sensing device for colorimetric determination of contaminants in drinking water. **P. Gasparic, A. Kornherr, S. Hribenik, K. Stana-Kleinschek**

3:30 CELL 350. Improving the redispersability of cellulose nanofibrils. **E.I. Filpponen, A. Anttila, O.J. Rojas**

3:50 CELL 351. Carboxymethylated lignin (CML) in liquid and solid foams. **S. Li, O.J. Rojas**

4:10 Concluding Remarks.

Section C

Colorado Convention Center
Room 405

Smart and Responsive Composites from Renewable Building Blocks

Advanced Nanoreactor Systems/New Paradigms to Smart Material Chemistry & Engineering

Cosponsored by PMSE

Y. Habibi, Q. Lin, Organizers
L. A. Lucia, Organizer, Presiding

1:30 CELL 352. Cellulose nanocrystals as 2D chiral inducers: Enantioselective catalysis and transmission electron microscopy 3D characterization. **M. Kaushik, C. Benoit, C.M. Cirtiu, A.H. Moores**

2:00 CELL 353. Reinforcing piezoelectric films with cellulose nanocrystals. **M. Shir Mohammad, J. Simonsen, J. Nairn**

2:30 CELL 354. Two-stage separation and alignment of cellulose nanocrystals. **Y. Hu, N. Abidi**

3:00 Intermission.

3:15 CELL 355. Life cycle assessment of high performance nanocellulose-reinforced advanced fibre composites. **H. Martin, S. Evangelisti, P. Lettieri, K. Lee**

3:45 CELL 356. Regioselective preparation of curdlan derivatives aminated at the C-6 position for biomedical applications. **R. Zhang, K.J. Edgar**

4:15 CELL 357. Macroscopic cellulose probes for contact adhesion. **S.A. Pendergraph, C. Carrick, L. Wagberg, A. Carlmark, M.K. Johansson, G. Klein, A. Trager**

4:45 Concluding Remarks.

Section D

Colorado Convention Center
Room 406

Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America

Fundamental Aspects in Processing and Energy

M. L. Auad, J. Campos-Teran, O. El Seoud, O. J. Rojas, Organizers
D. Petri, Organizer, Presiding
S. Madrigal, Presiding

1:30 CELL 358. Determination of useful parameters to decide the suitability of a biomass to be used as raw material for thermochemical processes. **A. Puente-Urbina**

1:55 CELL 359. Performance of a low-cost portable carbonizer for the valorization of lignocellulosic wastes. **E. Perez**

2:20 CELL 360. New organic composites for FDM applications. **R. Christoph, J. Vega-Baudrit**

2:45 CELL 361. Strategies for the utilization of cellulosic residues generated from the pineapple cultivation. **M. Esquivel Alfaro, G. Moreno Cento, D. Rojas Fonseca, K. Ramirez Amador, G. Jiménez Villalta**

3:10 Intermission.

3:25 CELL 362. Carbonize it or not? A simple test method for biomass materials. **J.F. Quesada-Kimzey**

3:50 CELL 363. Emulsified systems containing cellulose nanofibrils (CNF). **C.A. Carrillo, T. Nypelö, O.J. Rojas**

4:15 CELL 364. Adsorption of inorganic photo-active nanoparticle/enzyme hybrid systems on surfaces modified with cellulose obtained from natural and industrial residues: A QCM study. **I. Iñárritu, A. Topete, R. López-Simeon, E. Torres, J. Campos-Teran**

4:40 CELL 365. Drying kinetics as a convenient method to determine relative diffusivity of water in woody biomasses. **A. Puente-Urbina, J. Morales-Aymerich, Y. Kim, J.F. Mata**

5:05 Panel Discussion.

5:30 Concluding Remarks.

Section E

Colorado Convention Center
Room 407

Cellulose Dissolution: New Solvents and Mechanisms

Ionic Liquids

N. Abidi, E. L. Quitevis, Organizers, Presiding

1:30 Introductory Remarks.

1:35 CELL 366. Enzymatic pretreatment to improve cellulose solubility in a green solvent of NaOH/urea. **L. Zhang, T. You, L. Zhang, F. Xu**

2:05 CELL 367. Development and characterization of compatible cellulose and cellulose blended with soy protein membranes using a novel solvent system. **E.F. Douglass, R. Kotek**

2:35 CELL 368. Withdrawn.

3:05 CELL 369. Effective dissolution of cellulose for making electrically-responsive films. **S. Acharya, Y. Hu, N. Abidi**

3:35 Intermission.

3:50 CELL 370. Cellulose/PVA composite films prepared by NaOH/urea solvent: Structure and properties. **M. Xu, H. Ge, X. Wang**

4:20 CELL 371. Facile ionic liquid-mediated technology for cellulose nanocrystals production directly from wood. **H. Abushammala, I. Krossing, M.G. Laborie**

4:50 CELL **372**. Ionic liquids: Not always innocent solvents for cellulose. M.T. Clough, K. Geyer, P. Hunt, S. Son, U. Vagt, T. Welton

5:20 CELL **373**. How ionic liquids effect glucose and cellobiose solvation: Insights from enhanced sampling molecular dynamics techniques. V.S. Bharadwaj, T. Ashurst, T. Schutt, C.M. Maupin

5:50 Concluding Remarks.

Polymeric Biomaterials

Instructive Tissue Engineering Matrices

Sponsored by PMSE, Cosponsored by CELL

THURSDAY MORNING

Section A

Colorado Convention Center
Room 403

Conservation Science of Cellulosic Materials - Recent Developments

Degradation of Paper: Analysis and Approaches to Prevent It

A. Potthast, *Organizer*
U. Henniges, *Organizer, Presiding*

8:00 CELL **374**. Degradation of paper under adverse environmental conditions: Modeling considerations. J. Tétreault, P. Bégin, A. Dupont

8:30 CELL **375**. Ancient paper as a multicomponent system: A novel approach to the kinetics of its degradation. S. Zaccaron, P.F. Calvini, R. Ganzerla

9:00 CELL **376**. Cellulose as a detector for assessing storage materials for cultural heritage objects. E. Breitung, M. Wiggins, L. Nguyen

9:30 CELL **377**. Durability and permanency of formulated traditional Malay black ink on European handmade paper upon accelerated aging tests. R. Abdul Razak, R. Othman, M. Barkeshli

10:00 Intermission.

10:15 CELL **378**. Withdrawn.

10:45 CELL **379**. Paper strengthening and desacidification by polyaminoalkylalkoxyisilane copolymer networks: A model study. C. Piovesan, A. Dupont, O. Fichet, I. Fabre-Francke, B. Lavédrine, H. Chéradame

11:15 CELL **380**. Parylene coatings for cultural heritage paper strengthening. L. Pei, M. Pollei, S. Jordan-Mowery, J.W. Batty

11:45 CELL **381**. Paper deacidification using polysaccharide and alkaline nanoparticles. T. Mohan, L. Amornkitbamrung, R. Kargl, S. Hribernik, K. Stana-Kleinschek, V. Ribitsch

Section B

Colorado Convention Center
Room 404

Research on Renewable Materials: US and EU Perspectives

Development and Implementation of Bioeconomy Strategies/Initiatives for Collaborative Research and Innovation

P. R. Navard, *Organizer*
P. E. Fardim, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **382**. European Union policy and initiatives for developing the bioeconomy sector. P.R. Navard

8:35 CELL **383**. Renewable materials research in the U.S. Forest Service: A perspective. W.L. Nieh

9:05 Intermission.

9:20 CELL **384**. Biobased industries initiative: Realizing the European bioeconomy potential. P. van Leeuwen, P.R. Navard

9:50 CELL **385**. Biomass raw materials-related issues on bioeconomy strategies, research and development, and industrial implementation. D. Da Silva Perez

10:20 CELL **386**. Network with COST Action FP1205: Innovative applications of regenerated wood cellulose fibers. Å. Östlund, D. Jones

10:50 CELL **387**. Horizon 2020: EU research and innovation program. K. Stana-Kleinschek

Section D

Colorado Convention Center
Room 406

Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America

Applications

M. L. Aua, O. El Seoud, D. Petri, O. J. Rojas, *Organizers*

J. Campos-Teran, *Organizer, Presiding*
E. Torres, *Presiding*

8:00 CELL **388**. Preparation and characterization of antimicrobial cellulose beads. D. Petri, L.S. Blachechen, P.E. Fardim

8:25 CELL **389**. Secondary liposomes stabilized by the electrostatic deposition of chitosan-tannin composites as potential delivery systems for proteins. S. Madrigal-Carballo, J. Araya-Matey, E. Alfaro-Viquez, D. Esquivel-Alvarado, C.G. Krueger, J.D. Reed

8:50 CELL **390**. Chitosan-Collagen hybrid 3D-scaffolds as potential biomaterials for tissue engineering. P. Cubero-Mora, E. Alfaro-Viquez, D. Esquivel-Alvarado, M. Esquivel-Alfaro, S. Madrigal-Carballo

9:15 CELL **391**. Effect of fiber orientation in bacterial cellulose scaffold on cellular response: Adhesion, proliferation, differentiation of equine mesenchymal stem cells. R.S. Benson

9:40 Intermission.

9:55 CELL **392**. Tannin-chitosan composite nanoparticles as alternatives to antibiotics. C.G. Krueger, E. Alfaro-viquez, S. Madrigal-Carballo, J.D. Reed

10:20 CELL **393**. Bacterial cellulose research experience between Colombia, Finland, and the US. C. Castro Herazo, R. Zuluaga Gallego, J. Arboleda, H. Orelma, L.O. Morales, P. Gañán, O.J. Rojas

10:45 CELL **394**. Improved thermal stability of polylactic acid (PLA) film using β -cyclodextrin inclusion complex with PLA. K. Rodriguez, Y. Kim, Y. Byun

11:10 CELL **395**. Biotechnological valorization of waste sludge in a food industry: Design and evaluation process at lab scale. J.M. Naranjo, W. Osorio viana, A. Merchan, L. Gomez

11:35 CELL **396**. Functionalization of bacterial nanocellulose membranes with *Triticum vulgare* for wound dressing applications. M. Osorio Delgado, I. Oriz, J. Velásquez-Cock, R. Zuluaga Gallego, O.J. Rojas, M.S. Peresin, P. Gañán, C. Castro Herazo

12:00 Concluding Remarks.

Section E

Colorado Convention Center
Room 407

Cellulose Dissolution: New Solvents and Mechanisms

Ionic Liquids

N. Abidi, E. L. Quitevis, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL **397**. NMR spectroscopy, relaxometry, diffusion, and rheological studies of cellulose in the ionic liquid 1-butyl-3-methylimidazolium chloride. M.E. Ries, T. Budtova, A. Radhi

8:35 CELL **398**. Dissolution, regeneration, and characterization of cellulose and cellulose/chitin in ionic liquid. P.T. Wansapura, N. Abidi, T. Jackson, Y. Hu, E.L. Quitevis

9:05 CELL **399**. Dissolution of cellulose and exfoliation of graphene by aralkylimidazolium-based ionic liquids. E. Gurung, K. Mendoza, G. Tamas, R. Bari, T. Jackson, P.T. Wansapura, M. Green, N. Abidi, E.L. Quitevis

9:35 CELL **400**. Application of two-stage ionic liquid-mediated system for cellulose nanocrystals (CNCs) production. J. Mao

10:05 Intermission.

10:20 CELL **401**. Synthesis of ionic liquids for pretreatment of lignocellulosic waste. A. Camacho-Dávila, V. Martínez-Burciaga, G.I. Israel-Orozco, S. Rubio-Perea, G. González-Sánchez, L. Ballinas-Casarrubias, L. Villanueva

10:50 CELL **402**. From paper pulp to dissolving pulp to textile fibres with ionic liquids using IONCELL-P&F. A.M. Stepan

11:20 CELL **403**. Optimization of a low temperature lignocellulosic pretreatment process using ionic liquids. C. Schall, S. Vashghhani Farahani

11:50 Concluding Remarks.

Polymeric Biomaterials

Instructive Tissue Engineering Matrices

Sponsored by PMSE, Cosponsored by CELL

THURSDAY AFTERNOON

Section A

Colorado Convention Center
Room 403

Conservation Science of Cellulosic Materials - Recent Developments

Paper Conservation: Transition Metal Ions and Specific Topics

U. Henniges, *Organizer*
A. Potthast, *Organizer, Presiding*

1:30 CELL **404**. Removal of the aqueous washing treatment aid ionic fixative from paper. J. Roller

2:00 CELL **405**. Analysis of paper surviving from a tragic scene. K. Ahn, T. Zweckmair, A. Schedl, A. Potthast

2:30 CELL **406**. Dyes used by Iranian masters in paper dyeing process based on Persian medieval recipes. M. Barkeshli

3:00 Intermission.

3:15 CELL **407**. Damage caused by iron ions or pigments (Prussian blue) during aging of Japanese paper. K. Kida, M. Inaba, A. Potthast, N. Hayakawa

3:45 CELL **408**. Stabilization of green copper based pigments. J. Malešič, J. Kolar, M. Anders

4:15 CELL **409**. Electron paramagnetic resonance as a probe for metal ions and radicals in paper. A. Zoleo, M. Bronzato

4:45 Concluding Remarks.

Section B

Colorado Convention Center
Room 404

Research on Renewable Materials: US and EU Perspectives

Clusters and Networks for Research and Innovation

P. E. Fardim, *Organizer*
P. R. Navard, *Organizer, Presiding*

1:30 CELL **410**. Withdrawn.

2:00 CELL **411**. Biomass supply chain innovation: A case study. S. Jackson

2:30 CELL **412**. European Polysaccharide Network of Excellence (EPNOE). P.E. Fardim, J. van Dam

3:00 Intermission.

3:15 CELL **413**. Sun Grant Initiative: Bringing a regional focus to a national opportunity. T.G. Rials

3:45 CELL **414**. Interregional Scientific/Industrial Centre (BIO)-Polymers-Materials-Technologies for Economy, POLINTEGRA, as a model of cooperation between business and science. D. Ciechanska

4:15 CELL **415**. Finnish bioeconomy cluster. P.E. Fardim, M. Leskela

4:45 CELL **416**. 4D product: Integration over time is the only way to understand sustainability. M.E. Jones

5:15 Concluding Remarks.

CHED

Division of Chemical Education

W. Jones, I. Levy, and A. Marsh, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Active Learning in the Undergraduate Analytical Chemistry Curriculum (see ANYL, Tue)

Diversifying STEM: Uniting through our Differences for a Brighter Scientific Future (see CMA, Mon)

Environmental Chemistry: Pedagogical Models and Practices (see ENV/R, Wed, Thu)

SOCIAL EVENTS:

High School-College Interface Luncheon (Tickets Required), 12:00 PM, Sun

Division Reception, 5:30 pm, Sun

STRETCH Your Students' Polymer Knowledge - For pre-college educators, 4:30 PM, Mon

SUNDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Silver

High School Program

Cosponsored by SOCED

Financially supported by ACS Education Division

S. B. Mitchell, *Organizer, Presiding*

8:00 Registration.

8:30 Introductory Remarks.

8:40 CHED **1**. Demonstrations guaranteed to get oohs and ahhs! How to turn ordinary activities into unforgettable learning experiences. S. Spangler

10:10 CHED **2**. Writing across the curriculum: Concept journals as a means to teach the metric system. S.B. Mitchell

10:30 Intermission.

10:50 CHED **3**. A few insights into classroom and lab safety. H.W. Gendreau

11:10 CHED **4**. Spectroscopy of natural resources. D. McGraw

11:30 CHED **5**. Spark student's interest in chemistry with resources from the American Chemical Society. K.M. Kaleuati, M. Gmurczyk

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research

New and Noteworthy in 2013-2014

D. M. Bunce, M. N. Stains, *Organizers*

S. Pazični, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **6**. Replicating peer-led team learning in cyberspace: Research, opportunities, and challenges. P. Varma-Nelson, J. Smith, S.B. Wilson, J. Banks, L. Zhu

9:10 CHED **7**. Insights into how students learn from molecular visualizations through the lens of variation theory. R.M. Kelly

9:45 Intermission.

10:00 CHED **8**. Looking for links: Examining student responses in creative exercises for evidence of linking chemistry concepts. L. Ye, S.E. Lewis

10:35 CHED **9**. Argumentation and participation patterns in general chemistry peer-led sessions. U. Kulatunga, R.S. Moog, J.E. Lewis

11:10 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Spruce

Current Practice and Research Using ACS Exams

T. Holme, *Organizer*
K. L. Murphy, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 10. Cultivation of creative thinking ability in the course of Food Engineering Operations. D. Lin, M. Luo, B. Pu

8:55 CHED 11. Seven courses, two exams: Designing the ACS Inorganic Chemistry Exams for a diverse undergraduate curriculum. B.A. Reisner

9:15 CHED 12. ACS examination in organic chemistry at Hampton University. C.M. Bump, E.M. Ndiip, G.C. Nwokogu, M.K. Waddell

9:35 CHED 13. Assessment of nontraditional students in organic chemistry. R.D. Barrows

9:55 Intermission.

10:10 CHED 14. Creating the Exams Data Analysis Spreadsheet (EDAS) as a tool to help instructors conduct customizable analyses of student ACS exam data and compare the results to national normative statistics. A. Brandriet, T. Holme

10:30 CHED 15. Use of American Chemical Society examinations as assessment tools. S.M. Socol

10:50 CHED 16. Chemical thinking: Exploring the impact of a new general chemistry curriculum. V. Talanquer, J.R. Pollard

11:10 CHED 17. Exploring the use of the Anchoring Concepts Content Map as a programmatic assessment tool. C.J. Luxford, T. Holme

11:30 Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel
Denver

Undergraduate Research Papers**Organic Chemistry**

Cosponsored by SOCED

C. V. Gauthier, *Organizer*
J. V. Ruppel, N. L. Snyder, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 18. Synthetic investigation and application of a substituted 4,6-dimethylcyclohexene compound. W.P. Miller, K. Cetto Bales, S. Franke McDevitt

8:45 CHED 19. Chemistry for chiral skeletons: Building chiral fragments from enantiopure 1,2-amino alcohols. J.C. Serrano, Z.V. Boskovic, S. Ferrara, L. Furst, S.O. Figueroa, D.K. Crews, A. Guerrero, C. Brackeen, S.D. Nelson, S. Dandapani, A.J. Phillips, S.L. Schreiber

8:55 CHED 20. Evaluation of a new rhomnoidic donor containing a sulfonyl directing group for the formation of beta-rhomnoidic linkages. E.J. Medici, E.D. Anderson, N.L. Snyder

9:05 Intermission.

9:15 CHED 21. Regioselective opening of propenylbenzene oxides via intramolecular N-H activation. C. Tutwiler, C.J. Monceaux

9:25 CHED 22. Novel hydroxyproline methodology involving an auxiliary salicylaldehyde capture followed by imine-induced intramolecular rearrangement to achieve chemoselective ligations at difficult proline site. G.G. Simpson, K. Ha, A. Katritzky

9:35 CHED 23. Why does the acetaldehyde enolate favor reaction at the O atom during gas-phase nucleophilic substitution? Contributions by resonance and inductive effects. C. Seitz, J.M. Karty

9:45 Intermission.

9:55 CHED 24. Investigating the mechanism of cyanoacrylate polymerization in latent fingerprint development. E.M. Persson, K. McCarthy, A.S. Dutton

10:05 CHED 25. Methods towards the synthesis of Stachybotrin D. W. Teh, D.C. Bromfield Lee

10:15 CHED 26. Rapid synthesis of N-(2-hydroxybenzyl)acetamide. K.A. Dockter, L.I. Bobyleva, M.M. Bobylev

10:25 CHED 27. Synthesis of trehalose-based oligosaccharides for medicinal applications. E.A. Palumbo, N.L. Snyder

10:35 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel
Columbine

From Cornerstone to Capstone: Culminating Experiences in the Undergraduate Chemistry Curriculum that Foster Integration and Application of Foundational Knowledge

K. Kneas, J. A. MacKay, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 28. Comprehensive chemistry: An efficient approach. P. Schettler

8:55 CHED 29. Introductory investigation into the substituent effect on regio-selectivity of bromination across vinyl systems: A culmination of undergraduate chemical education. A.N. Schildkret, V. Fishback

9:15 CHED 30. Shippensburg University undergraduate research grant writing experience. R.L. McCann, A. Hurley Predecki

9:35 Intermission.

9:45 CHED 31. Senior capstone experiences at Stevenson University: Everybody's doing it. T.M. Mason

10:05 CHED 32. Ups and downs of a two-semester independent research project. J. MacNeil

10:25 CHED 33. Chemistry and biochemistry capstone course at Messiah College: A holistic interdisciplinary approach. R.W. Schaeffer

10:45 CHED 34. Electrifying the capstone chemistry experience. S. Chamberlin, N.C. Kallan

Section F

Sheraton Denver Downtown Hotel
Gold

NMR Spectroscopy in the Undergraduate Curriculum

Financially supported by Bruker; JEOL; Thermo Fisher Scientific; Anasazi Instruments

L. J. Anna, D. P. Soulsby, A. S. Wallner, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 35. Measurement of phosphates in soft drinks: A general chemistry experiment using NMR. L.J. Medhurst, F. Shahnaz, N. Ramnarine, G. Paniconi

8:55 CHED 36. Free-radical chlorination of alkanes in the undergraduate organic chemistry laboratory: Application of ¹H and TOCSY NMR experiments to the analysis of reaction products. D.P. Soulsby

9:15 CHED 37. Withdrawn.

9:35 Intermission.

9:45 CHED 38. Unequivocal assignment for all PMR and CMR signals of unknown butyl and pentyl acetate esters from Fischer esterification using 2D NMR experiments. F.J. Matthews

10:05 CHED 39. Real-time classroom comparison of structures and NMR spectra using Jmol/JSpeView and nmrd. R.M. Hanson, R.J. Lancashire, L. Patiny

10:25 CHED 40. Students using esters to construct for themselves the concepts of chemical shift correlation and spin-spin coupling. K.T. Smith, C.S. Hamann

10:45 Intermission.

10:55 CHED 41. Measuring structural and electronic effects on keto-enol equilibrium in 1,3-dicarbonyl compounds. S.C. Young, K.T. Smith, J.W. DeBlasio, C.S. Hamann

11:15 CHED 42. NMR-based activity assays to characterize enzymes in the biochemistry laboratory and in undergraduate research. B.J. Stockman

11:35 Concluding Remarks.

Undergraduate Symposium

Sponsored by AGFD, Cosponsored by CHED

SUNDAY AFTERNOON**Section A**

Sheraton Denver Downtown Hotel
Silver

High School Program

Cosponsored by SOCED

Financially supported by ACS Education Division
S. B. Mitchell, *Organizer, Presiding*

12:00 Luncheon.

1:00 CHED 43. Award Address (James Bryant Conant Award in High School Chemistry Teaching sponsored by Thermo Fisher Scientific). Through generations X, Y and Z, learning never ends. J.L. Ball

1:40 CHED 44. ChemSource, the NGSS, and the particle nature of matter: How to develop classroom-ready templates. P. Smith, M. Orna

2:00 CHED 45. Engaging chemistry resources from the Journal of Chemical Education and ChemEd X-. D. Cullen

3:00 Intermission.

3:20 CHED 46. Think safety = work safely. E.M. Howson

3:40 CHED 47. Using Popular Science Magazine articles to improve students' critical thinking and scientific literacy. M. Gmurczyk, P. Pages

4:00 CHED 48. How effective is lecturing in a high school chemistry class? D.M. Bunce

4:20 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research**K-12 and Professional Development**

J. Barbera, N. P. Grove, *Organizers*
D. G. Herrington, *Presiding*

1:30 Opening Remarks.

1:35 CHED 49. Using the ACAST to characterize high school chemistry teachers' data-driven inquiry practices. J. Hashman, E.J. Yezierski

1:55 CHED 50. Uncovering high school students' chemistry self-concept with cluster analysis. S.E. Nielsen, E.J. Yezierski

2:15 CHED 51. Tool trouble: Challenges with using self-report data to evaluate long-term chemistry teacher professional development. S.F. Bancroft, D.G. Herrington, E.J. Yezierski

2:35 CHED 52. Target Inquiry at Miami University (TIMU): Uncovering novel relationships among affective and cognitive measures of high school chemistry students. J.H. Carmel, J.T. Harshman, E.J. Yezierski

2:55 CHED 53. Efficacy of the connected chemistry curriculum. S. Ryan, M. Stief

3:15 Intermission.

3:30 CHED 54. STEM Modules: A multifaceted approach to enhancing science learning and perceptions in middle school classrooms. E.J. Andrews, T. Robinson, D. Banks, A.L. Curry, M.L. Curry

3:50 CHED 55. Technology integration in the undergraduate chemistry classroom. T.L. Vickrey, B. Riesen, M. Abebe, D. Golick, M.N. Stains

4:10 CHED 56. Building a teaching profile: Using a modified COPUS observation protocol to easily and reliably measure reformed instructional practice. M.N. Stains, T.J. Lund

4:30 CHED 57. Training faculty with the Teaching Dimensions Observation Protocol (TDOP): Process and pitfalls. M.L. Grunert, C. Henderson, A. Beach

4:50 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Spruce

Department, University, and National Models for Faculty Development to Support Adoption of Evidence-Based Teaching

Cosponsored by INOR, ORGN and PRES

R. Waterman, *Organizer, Presiding*

1:30 CHED 58. Creating a coherent STEM gateway for teaching and learning at Michigan State University: An AAU STEM initiative project. M. Cooper

1:50 CHED 59. Starting at the source: Foundational views about teaching influence adoption of learner-centered teaching practices. C. Renner

2:10 CHED 60. Inclusive excellence in the classroom. R. Hernandez

2:30 CHED 61. VIPER faculty development workshops: Cutting edge content development and sharing pedagogical best practices. H.J. Feig, A.R. Johnson, A.K. Bentley, E.R. Jamieson, C. Nataro, J.R. Raker, B.A. Reisner, S.R. Smith, J.L. Stewart, L.A. Watson, N. Williams

2:50 CHED 62. Cottrell Scholars Collaborative New Faculty Workshop program: Helping new faculty adopt effective approaches from day one. A.L. Feig, L.A. Baker, P. Beuning, L.M. Columbus, C.J. Douglas, R. Hernandez, M.N. Stains, R. Waterman, J.L. Wesemann

3:10 Intermission.

3:15 CHED 63. Steering the ship from the front – how can deans change the culture to support evidence-based learning. P.K. Dorhout

3:35 CHED 64. Responding to barriers to and drivers for faculty adoption of evidence-based instructional practices. S.E. Shadle, S. Ritter, P. Pyke, A. Marker, T. Roark, A. Moll

3:55 CHED 65. Development of a structured support fellowship for faculty innovation in teaching. R. Frey

4:15 CHED 66. Mentoring junior faculty: Pedagogy is only important if you keep the job where you use it. L. McElwee-White

4:35 CHED 67. Long-term impacts of the Cottrell Scholars Collaborative New Faculty Workshop. M.N. Stains, M. Pilarz, D. Chakraverty, R. Waterman, A.L. Feig, J.L. Wesemann

4:55 CHED 68. ISSUES: Investigating student success using evidence-based strategies. K.R. Cousins

Section D

Sheraton Denver Downtown Hotel
Denver

Undergraduate Research Papers**Analytical and Environmental Chemistry**

Cosponsored by SOCED

C. V. Gauthier, N. L. Snyder, *Organizers*
J. V. Ruppel, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 69. Green extraction of lycopene from tomato (*Lycopersicon esculentum*) using 2-methyltetrahydrofuran. M.C. Enright, J. Noseworthy

1:45 CHED 70. Improved protein digestion for the mass-spectrometric detection of cysteine palmitoylation. M. Torres-Caban, N. Gould, H. Ischiropoulos

1:55 CHED 71. Degradation of estrogen: An NMR study. K. Davis, K. Cossey

2:05 CHED 72. Analysis of application of interpolation techniques to ultraviolet-visible spectroscopy of critical vesicle concentration. G.P. Nguyen, S.E. Maurer

2:15 Intermission.

2:25 CHED 73. Determining the degradation of an antioxidant, lycopene. K. Forster, K. Cossey

2:35 CHED 74. Application of ionic liquids in forensic chemistry. M. Jones, R.E. Del Sesto

2:45 CHED 75. Analysis of sol-gel processing as a controlled release method for fragrance molecules of essential oils. **K. Ehret, C.H. Lisse**

2:55 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel
Columbine

From Cornerstone to Capstone: Culminating Experiences in the Undergraduate Chemistry Curriculum that Foster Integration and Application of Foundational Knowledge

K. Kneas, J. A. MacKay, Organizers, Presiding

1:30 Introductory Remarks.

1:35 CHED 76. Integration in upper-division instructional chemistry laboratories at Regis University. **S. Mahapatro**

1:55 CHED 78. Integrated lab: The first year of a laboratory course integrating the sub-disciplines of chemistry and open-ended research experiences. **J.G. Rowley, D.M. Hitt, D. Gretch, C. Pharr, C.A. Thomas**

2:15 CHED 79. Elizabethtown College Laboratory at Guilford College: A authentic research experience for chemistry majors. **G.H. Webster, R.M. Whitnell, A.G. Glenn**

2:35 Intermission.

2:45 CHED 79. Elizabethtown College chemistry and biochemistry capstone experience. **T.E. Hagan, K. Kneas, J.A. MacKay**

3:05 CHED 80. University curriculum meets departmental capstone: Integrating a novel seminar and research capstone into a liberal arts curriculum. **T.W. Johnson**

3:25 Discussion.

3:45 CHED 81. Transitioning students to four year schools via an introduction to scientific research course. **J. MacArthur**

4:05 CHED 82. Development of a pre-professional program at a rural community college. **J.L. Hayes, S. Burchett**

4:25 CHED 83. Advancing chemistry education in two-year college programs through self-assessment. **C.L. Velez, H. Sklenicka**

Section F

Sheraton Denver Downtown Hotel
Gold

NMR Spectroscopy in the Undergraduate Curriculum

Pedagogy

Financially supported by Bruker, JEOL; Thermo Fisher Scientific; Anasazi Instruments

L. J. Anna, D. P. Soulsby, A. S. Wallner, Organizers, Presiding

1:30 Introductory Remarks.

1:35 CHED 84. NMR in first year chemistry. **J. Alexander, J. Ashmore, A. Baker, S. Chadwick**

1:55 CHED 85. Implementation of NMR spectroscopy into the undergraduate experience at The College of New Jersey. **A.R. O'Connor, S.E. Sen**

2:15 CHED 86. New "spin" on integrating NMR spectroscopy into an undergraduate curriculum. **E.J. McIntee, K.J. Graham, C.P. Schaller, T.N. Jones**

2:35 Intermission.

2:45 CHED 87. More systematic approach to learning NMR spectroscopy.

C. Gabel, M.J. Magrini, S.S. Gordon, J. Salazar, A.N. Gamble, N. Kuehl, D. Rourke, S. Norris

3:05 CHED 88. Using spectra from undergraduate projects to improve higher order cognition. **S.M. Schellble, K. Elkins**

3:25 CHED 89. ¹³C should precede ¹H NMR in teaching organic chemistry. **D.D. Clarke, R. Orazi**

3:45 Intermission.

3:55 CHED 90. Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: An active-learning approach. **S.D. Riegel**

4:15 CHED 91. Providing access to a million NMR spectra via the web. **A.J. Williams, D. Lowe, C. Coba, P. Corbett, A. Pshenichnov, V. Tkachenko**

4:35 Concluding Remarks.

Graduate Student Symposium

Sponsored by AGFD, Cosponsored by CHED

SUNDAY EVENING

Section A

Colorado Convention Center
Hall D

General Posters

I. Black, Organizer

7:00 - 9:00

CHED 92. Impact of chemical demonstrations on student interest and learning in science. **H. Salazar, A. Moore, D.G. Watson**

CHED 93. Brewing alcoholic beverages as a means of incorporating writing instruction into an existing junior-level laboratory capstone course. **K.A. Brown, J.D. Mimbs, C.S. Seney, D.R. Goode, D.E. Moore, A.M. Kiefer**

CHED 94. Enhancing research for students and new faculty at undergraduate institutions. **M.E. Railing, J. Fuller, E. Sylvester, J. Coffield**

CHED 95. Scientific connections: Development of a chemistry of art course for non-majors. **S.E. Hubbard**

CHED 96. On the production of Chinese Purple in the art studio and chemistry laboratory. **J.D. Thoburn, M.M. Thoburn**

CHED 97. Under the Dome: Student-designed evidence-based inquiry to understand and predict climate change outcomes. **S.A. Stewart-James, J. Sutter**

CHED 98. The chemistry of Thomas Edison. **R.H. Wallace**

CHED 99. Application of mathematical concepts to teaching and learning of chemistry. **PK. Yuen, C.D. Lau**

CHED 100. FUTURE program: Ensuring that underserved populations become the scientific and civic leaders of tomorrow. **A.J. Reig, J. Pellegrino**

CHED 101. Expansion of the Science Resource Center. **S. Richards, P.J. Iles, L.D. Giddings, M. Alvarez, N.R. Bastian, R.V. Valcarce**

CHED 102. With the scientific research advantages in the discipline, the construction level of chemical characteristic specialty is enhanced. **Z. Jiang, Z. Yao, H. Yue, Z. Wang, C. Li, L. Zhao, M. An**

CHED 103. Cultivation of chemical engineering talents innovation ability based on the scientific research project trainin. **H. Yue, Z. Wang, J. Li, Y. Wang, Z. Yao, D. Liu, Z. Jiang**

CHED 104. The 2016 Biennial Conference on Chemical Education. **R.W. Schwenz, M.L. Miller, J.M. Smist**

CHED 105. "I want to be the inquiry guy!" How research experiences for teachers transform beliefs about teaching science as inquiry. **S.F. Bancroft, D.G. Herrington, M.M. Edwards, C.J. Schairer**

CHED 106. Using Special English as a tool to engage students in chemistry lecture. **D.J. Swartling**

CHED 107. Design, development, and delivery of the Nevada GEAR UP STEM Summer Institute. **S. Nealy, K. Carroll, H. Skaza, E. Marti, E. Gandhi, M. Dulger, D. Gerrity, T. Olson, P. Schrader, M. Orgill**

CHED 108. PROPEL Center at Colorado State University-Pueblo: The effect of a STEM tutoring center on academic excellence. **C. Barnett, T. Marshall**

CHED 109. Revision of chemical professional undergraduate training scheme guided by "Excellence engineers education program". **Z. Yao, Z. Wang, C. Li, L. Zhao, M. An, Z. Jiang, H. Yue**

CHED 110. High school students' perceptions and performances on predict-observe-explain tasks in chemistry laboratory. **P. Vadapally, J.P. Suits**

CHED 111. "Building Your Science Toolkit:" Encouraging young female undergraduates to pursue science through laboratory experiences and interactive, tiered mentoring. **C. Normand, D. Kumarjiguda, J. Canfield**

CHED 112. Leveraging REU programs to attract talents in STEM fields: A comparison of outcomes of a discipline-based education research and a molecular science REU program. **A.F. Kneideisen, D. Xue, M.N. Stains**

CHED 113. Balancing "wow" and "satisfying standards" with hands-on activities and critical thinking: Developing middle school science modules. **M.S. Reeves, C. Bradford, A. Bufford, D. Chappell, G. Griffin, B. Hart, L. Jackson**

CHED 114. Test-based learning with online vs. paper tests. **A. Priscari, T. Holme**

CHED 115. When teaching chemistry and text messaging do work together in a classroom. **J. Zhang**

CHED 116. Younger Chemistry Education Scholars (YCES) committee: Who we are and what we do. **M. Anzovino, T.J. Bussey, J.H. Carmel, K.R. Galloway, J. Harshman, K.J. Linenberger, E.B. Moore, J. Reed, S. Ryan**

CHED 117. Frequent assessment: Does it make a difference in student learning? **A. Wallace**

CHED 118. New chemistry advanced placement (AP) test: Hands-on inquiry based experiment workshops. **R. Grunglasse, C. Hamill, N.N. Pierre, S. Rolle, A. Riego, M. Exposito, M. Delgado**

CHED 119. Using missing data methods to address the problem of incomplete national normative datasets at the ACS Examinations Institute. **A. Brandriet, T. Holme**

CHED 120. Incorporation and evaluation of science practices in multiple-choice items. **J.J. Reed, T.A. Holme**

CHED 121. Importance of demo shows in the community. **J.T. Tomko, E.P. Kippenhan**

CHED 122. Fostering student success: Advanced topics and research at a community college. **T. Bledsoe, S. Hinote, M. Murphy, L.D. Burke**

CHED 123. Community outreach at Pima College East Campus: Summer research for high school teachers and high school students. **T. Bledsoe, G. Zreda, A. Frey, D. Donegan, M. Murphy, L.D. Burke**

CHED 124. Introduction of powder X-ray diffraction in K-12 education. **R. Boniak, C. Patel**

CHED 125. Investigating organic chemistry students' ideas about nucleophiles, electrophiles, and reaction mechanisms. **M.E. Anzovino, S. Bretz**

CHED 126. Developing an interdisciplinary medicinal plant research program that engages agriculture, biology, and chemistry undergraduate students across the curriculum. **W.E. Collier, M.A. Abdalla, C. Bradford, G. Griffin, D. Mortley, A. Russell**

CHED 127. Connecting organic chemistry and biochemistry. **W. Powell, K. Aghoram, K.A. Hinton**

CHED 128. Video instruction in organic chemistry: Student perceptions and preferences. **K.B. Fields**

CHED 129. Climate change outreach demonstrations. **P. Hills-Rieck, B. Chandler**

CHED 130. Using an online assessment tool to gain insight to students' usage of representations in chemistry. **J. Polifka, T. Holme**

CHED 131. Practical component to a biochemistry lab final exam. **K.R. Willian**

CHED 132. Investigating cellular steady state as a threshold concept in biochemistry. **T. Morgan, J.E. Lewis, J.A. Loertscher, V.M. Thorsell**

CHED 133. Water quality education. **B.R. Bricker, J.M. Weinkauf, M.W. Fultz**

CHED 134. Development of a self-efficacy survey instrument designed to gauge the relationship between completion of AP chemistry and comfort level in first-semester general chemistry. **M.A. Erdmann, L. Freeman, J. March**

CHED 135. Impact analysis of prerequisite incorporation toward student success in freshman-level college chemistry courses. **F.M. Yarberr, S. Cornish**

CHED 136. Manual dexterity: assessing its role in the chemistry laboratory. **I.L. Brown, S.D. Wiediger**

CHED 137. Analysis of meaningful learning in the General Chemistry laboratory. **K.R. Galloway, S. Bretz**

CHED 138. Teaching chemistry at a technical college through practical field work using performance based instruction: The Milwaukee River Project. **S.A. Schlipp**

CHED 139. Fearless investigators: Teaching science through experimental design. **R.E. Grote, P.J. Wendel**

CHED 140. Flipping general chemistry via a highly structured teaching pedagogy: Initial conclusions. **C. Uvarov, R. Gamage, G. Allen**

CHED 141. Using first-day assessments to determine math readiness for general chemistry. **C.M. Chant, D.S. Heroux**

CHED 142. Use of eye fixation sequence analysis to identify common cognitive processes among students solving conceptual stoichiometry problems. **J. Baluyut**

CHED 143. CLP: A collaborative learning program in chemistry with benefits for both students and facilitators. **B.A. Davis, M.A. Fisher, M. Raab**

CHED 144. Development of a service-learning introductory chemistry course for culinary arts students. **A. Wallace**

CHED 145. Transparency and electronic assessment. **E.M. Epp**

CHED 146. Constructing a consensus definition of conceptual understanding in chemistry from empirical data provided by instructors. **C.J. Luxford, T. Holme**

CHED 147. Water quality comparison of city facilities and residences in North Miami, Florida. **N.N. Pierre, S. Rolle, C. Harrill, K. Sanchez, A. Riego, L. Dean, J. Johnson, A. Laroche, Q. Lockhart, M. Exposito**

CHED 148. Lewis Misconstruction: An investigation into student's Lewis structure drawings. **N.L. Burrows**

CHED 149. Describing and characterizing the affective domain in middle and high school science students. **S.F. Bancroft, J.H. Carmel, J. Harshman, E.J. Yeziarski, D.G. Herrington**

CHED 150. Introducing computational chemistry: A hands-on spreadsheet approach. **PE. Hoerner, J. Beck**

CHED 151. Conformational analysis discovery activity using 3D potential energy surface models. **F.A. Carroll, D.N. Blauch**

CHED 152. Mathcad exploration of Fourier transforms found in physical and analytical chemistry courses. **T.C. Miller, J.N. Richardson, J. Kegerreis**

CHED 153. Mustard: Tiny seed – unlimited possibilities. **I.E. Popova, M.J. Morra**

CHED 154. Impact of supplemental video prelab material for a biochemistry lab practical on student overall preparedness. **T.M. Whealon, S.D. Wiediger**

CHED 155. Quantitative analysis of glucose and kinetic study of glucose oxidase for use in an introductory quantitative analysis laboratory. **T.C. Miller, E.E. Friebe, T. Frielle, J.N. Richardson**

CHED 156. Exploration of formaldehyde in apparel fabric using experimental and theoretical infrared and UV-visible spectroscopy. **K.A. Leets, K.B. Bramble, G.D. Gibbs, L. Tribe**

CHED 157. Measuring silver nanoparticle concentration by inductively coupled plasma optical emission spectroscopy: A laboratory experiment for chemistry and engineering students. **S.W. Brittle, J.D. Baker, K.M. Dorney, T. Ebrahimian, J.M. Dagher, I.E. Pavel Sizemore, S.R. Higgins**

CHED 158. Comparison of modes of delivery for safety information in an undergraduate laboratory. **A.M. Powe, A. Jamthrao, O. Ersin**

CHED 159. Microwave-assisted dye synthesis: A more efficient approach for an undergraduate laboratory. **A.B. Ormond**

CHED 160. Quantifying and recycling precious metals from printed circuit boards: An undergraduate laboratory. **S. Fields, C. Rector, K.J. Sorauf**

CHED 161. Use of the three levels of representation to introduce the concept of buffers. **Z. Medina Torres, E.L. Ortiz-Nieves, J. Padilla, J. Ortiz**

CHED 162. Periodic Table goes live. **E.J. Andrews, T. Robinson, A.L. Curry, M.L. Curry**

CHED 163. Concrete solar cells? An investigation into an alternative form of alternative energy. **B. Ackley, J. Bianchini, J.C. Warner**

CHED 164. Quantum dot sensitized solar cell for the undergraduate laboratory curriculum. **T.M. Tich, B.L. Oliva-Chatelain, A.R. Barron**

CHED 165. Integrated upper-division chemistry laboratory: synthesis and characterization of vandyli bis-acetylacetonate complex. **S. Mahapatro, C. Rector, G. Morgan, A.L. Stuckmeyer**

CHED 166. Separations of acetaminophen and caffeine by high temperature high-performance liquid chromatography. **A. Gizzi, J.V. Arena**

CHED 167. ¹H NMR Analysis of the Methylation of Oleic Acid Catalyzed by Tin (II) Bromide in the Presence of a Cosolvent. **N. Singh**

CHED 168. Determination of organic and inorganic priority pollutants in herbal teas and coffee. **R. Gray, R. Richter**

CHED 169. Organic chemistry laboratory sequence alternating experiments with guided inquiry exercises. **S.C. Young, K.L. Colabroy, M.R. Baar**

CHED 170. Using 3D printing to model steric interactions. **C. Diaz-Allen, P.A. Sibbald**

CHED 171. Simple technique for students to assign hydrogen atom resonances in heterocyclic ligand metal complexes. **D.P. Rillema, H. Nguyen**

CHED 172. Integration of green chemistry topics into the traditional organic chemistry experiments. **S.P. Lorimor**

CHED 173. Boiling point, azeotrope: A simple discovery-based experiment for organic laboratory course. **M.A. Rubin, M. Rubina**

CHED 174. How to PDB: a class exercise for professional Pharmacy Med Chem. **N.R. Natale, H.D. Beall**

CHED 175. Novel instructional undergraduate organic chemistry laboratory experiment exploring substitution patterns of various allylic halides. **T.M. Trygstad, N.W. Dykes, A. Radakovic, P.T. Chazovachii, E.W. Lake, M.M. Hite, J.C. Hicks**

CHED 176. Intermolecular forces: An organic laboratory experiment. **S. Candiello, R.B. Lettan II**

CHED 177. Isolation and identification of natural products in dried turmeric in undergraduate research. **G.R. Khalsa, A.J. Pohlod**

CHED 178. Multistep drug synthesis in the sophomore organic lab: Synthesizing *R*-rasagiline, a popular Parkinson's drug. **N. Aguilar, B.J. Garcia, S. David**

CHED 179. Education through an inquiry based environment in the physical chemistry laboratory: The thermodynamic of an electrochemical cell. **C.M. Torres Diaz, D.D. Alequin, R. Arce, A. Colom**

CHED 180. Synthesis and characterization of tricarboyanine dyes for use in physical chemistry laboratory. **G.R. VandeZande, A.L. Marsh**

CHED 181. Discovering pressure-volume-temperature phase relationships with 3D models. **D.R. Striplin, F.A. Carroll, D.N. Blauch**

CHED 182. Portable X-ray fluorescence spectrometry in the undergraduate chemistry curriculum at MWSU. **S.L. Hiley**

CHED 183. Preparation of samples for introducing undergraduate students to electron paramagnetic resonance. **A. Hanks, B.E. Sturgeon**

CHED 184. Quantitative determination of kidney cancer biomarkers in urine by liquid chromatography tandem mass spectrometry. **S. Gamagedara, L.M. Nguyen**

CHED 185. Research and practice of the mode of training research capacity through scientific innovation. **D. Lin, W. Qin, B. Pu**

CHED 186. Discussion on characteristic specialty construction and cultivating college students' technological innovation ability. **D. Lin, B. Pu, C. Li**

CHED 187. Development of a hybrid course in sustainable energy. **A. Kahl**

CHED 188. Using theoretical chemistry to explain S_N2, E2, S_N1 versus E1 mechanism for undergraduate organic chemistry. **A.S. Dutton, M.L. Dutton**

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Gold

ACS Award for Achievement in Research for the Teaching and Learning of Chemistry: Symposium in Honor of Vickie M. Williamson
Cosponsored by WCC

Financially supported by Pearson Publishing

M. R. Abraham, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **CHED 189.** Origins. **M.R. Abraham**

8:55 **CHED 190.** Visualization and the learning cycle: A great partnership. **J.J. Gelder**

9:15 **CHED 191.** Six years in: Surviving and thriving at a SLAC. **K.R. McCann**

9:35 **CHED 192.** Molecular visualizations through the lens of research and practice. **R.M. Kelly**

9:55 Intermission.

10:10 **CHED 193.** Visualizations in the chemistry classroom: A visual learner's perspective. **M.J. Sanger**

10:30 **CHED 194.** Developing and validating a measure of linked concepts for general chemistry. **S.E. Lewis**

10:50 **CHED 195.** Innovation diffusion in a single case: Adoption and re-invention of visualization research findings to improve applied research, instruction, and teacher professional development in chemistry. **E.J. Yezierski**

Section B

Sheraton Denver Downtown Hotel
Century

Experiments for Physical Chemistry Laboratory

Spectroscopy & Thermodynamics

A. Grushow, S. S. Hunnicutt, R. M. Whitnell, Organizers

F. J. Creegan, Presiding

8:30 Introductory Remarks.

8:35 **CHED 196.** Redesigning the hydrogen spectrum experiment for guided inquiry. **C. Salter, C.M. Teague**

8:55 **CHED 197.** Using the spectrum of HCl as a model building exercise. **A. Grushow**

9:15 **CHED 198.** Incorporation of single-molecule FRET measurements into an undergraduate Physical Biochemistry Laboratory course. **J. Knight, D. Giardina, A.J. Bonham, M.K. Maron**

9:35 Intermission.

9:45 **CHED 199.** Guided-inquiry approach for relating the fluorescence spectrum of the pyrene excimer to its thermodynamic properties. **A.R. Noble**

10:05 **CHED 200.** Constructing a binary phase diagram for aqueous salts. **R.R. Michelsen**

10:25 **CHED 201.** POGIL physical chemistry lab experiment: the vapor pressure of liquid. **B.D. Gilbert, M.A. Everest, D.E. Gardner**

10:45 Intermission.

10:55 **CHED 202.** Using food additives to enhance traditional bomb calorimetry experiments. **J.B. Dudek**

11:15 **CHED 203.** Are the molecules that make a solution red big or small? A POGIL-PCL recasting of the cyanine dye experiment. **S.S. Hunnicutt, R.M. Whitnell**

11:35 **CHED 204.** Guided inquiry solid-liquid phase diagram experiment. **S.S. Hunnicutt, R.M. Whitnell, A. Grushow**

11:55 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Spruce

Integrating Chemistry and Polymer Science Research into the Classroom

Cosponsored by PMSE and POLY

S. E. Morgan, Organizer

K. A. Cavicchi, Organizer, Presiding

K. Wingo, Presiding

8:30 **CHED 205.** Developing polymer and chemistry research lessons for the high school classroom – NSF GK-12 at The University of Southern Mississippi. **K. Wingo, S.S. Herron, S.E. Morgan**

8:50 **CHED 206.** Integration of polymer research into a lab-based polymer chemistry class at a small, primarily undergraduate institution. **B. McFarland**

9:10 **CHED 207.** Aerospace composites and the scientific method: Supporting high school classroom curriculum with real-world applications. **A.S. Frazee, B.F. Stringfellow, J.S. Wiggins**

9:30 **CHED 208.** Discovering chemicals through solid-phase microextraction gas chromatography/mass spectroscopy. **C. Rosu, C. David, R. Cueto, L. Veillon, R. Laine, E. Reichmanis, P.S. Russo**

9:50 **CHED 209.** Introducing the effect of additives on hydrogel properties. **D.N. Amato, K. Holmes, D.L. Patton**

10:10 **CHED 210.** Integrating polymer labs into the NGSS high school chemistry classroom. **M.T. Baker**

10:30 Intermission.

10:45 **CHED 211.** Using polymer properties to illustrate and explain concepts in introductory chemistry. **D.E. Bergbreiter**

11:05 **CHED 212.** Polymers in biomedicine and hydrophobic surfaces: Two RET experiences at the University of Akron. **D. Hess, D. Moore, G. Cheng, N. Zacharia, K.A. Cavicchi**

11:25 **CHED 213.** Research Experience for Teachers program at The University of Akron. **K.A. Cavicchi**

11:45 **CHED 214.** Transferring teacher research on wastewater wetlands into effective classroom activities. **A. Glimme**

12:05 **CHED 215.** Withdrawn.

12:25 **CHED 216.** Make it and break it: Employing a plant starch bio plastics experiment in the high school classroom for addressing engineering education standards. **J.E. Wissinger, A. Johnson, C. Ahrenstorff**

12:45 **CHED 217.** Activities in polymer optical physics for STEM education enrichment in the K-12 environment. **A. Fogel, J. Brownlow, S.E. Morgan**

1:05 **CHED 218.** Preparation and evaluation of antimicrobial films. **E.D. Matthews**

Section D

Sheraton Denver Downtown Hotel
Denver

Undergraduate Research Papers

Computational, Physical and Inorganic Chemistry

Cosponsored by SOCED

J. V. Ruppel, N. L. Snyder, Organizers

C. V. Gauthier, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **CHED 219.** Computational study of disubstituted ammonia borane derivatives for hydrogen storage. **T.E. West, A.S. Dutton**

8:45 **CHED 220.** Determining the activation energy of a series of spectroscopic imines. **C. Yeager, J.B. Dudek**

8:55 **CHED 221.** Why do Ala, Ala, Lys tripeptides preferentially rearrange to the Lys-Ala-Ala sequence in the gas phase? **E. Kowalczyk, J. Poutsma**

9:05 **CHED 222.** Tandem substitution-cyclization-elimination reaction that can account for the mutagenicity of arylamines without the need of nitrenium ions. **S. Shrestha, J. Bautista, A.G. Leach, A.S. Dutton**

9:15 Intermission.

9:25 **CHED 223.** Novel ligands for metal oxides colloid stabilization. **A.S. LaBeaud, C. Mitchell, R. Komati, G.Z. Goloverda, V.L. Kolesnichenko**

9:35 **CHED 224.** Development of a new method for graphene oxide thin-film growth. **M. Berens, B.J. Winters**

9:45 **CHED 225.** Iron-carbonyl clusters: Catalysts for hydrogen generation. **C.A. Mebi**

9:55 **CHED 226.** Withdrawn.

10:05 Intermission.

10:15 **CHED 227.** Shaped palladium nanoparticle synthesis on carbon substrates. **S.E. Sanders, P. Duffy, P.E. Colavita, K.M. Metz**

10:25 **CHED 228.** Silicate nanoparticles from spray flame synthesis for lithium ion batteries. **E. Maccato, J. Kovacevic, H. Wiggers, B. Mellis**

10:35 **CHED 229.** Morphological control of film structure in perovskite solar cells. **C. Jackson, C. Tassone**

10:45 **CHED 230.** Laminar-flow reactor study of the pyrolysis of 4-vinylguaicol. **J. Hoang, E. Ledesma**

10:55 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel
Columbine

Research at Community Colleges: Strategies for Enhancing Student Transfer & Success

Financially supported by 2YCS

D. M. Sarno, Organizer

P. D. Svoronos, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **CHED 231.** Using research as a tool to engage, retain and graduate STEM students at Queensborough Community College. **N. Gadura, P.D. Svoronos**

8:55 **CHED 232.** Goal, role, and soul of undergraduate research development at the Community College of Denver. **M. Haelele, H. Loshbaugh**

9:15 **CHED 233.** Black bear research: A case study in undergraduate research at a community college. **J.J. Van Niel**

9:35 **CHED 234.** Undergraduate research at Queensborough Community College: The first step for a successful transfer and eventual post-undergraduate career in STEM careers. **P.D. Svoronos**

10:15 Intermission.

9:55 **CHED 235.** Transporting an established undergraduate research program to a community college. **D.J. Schauer**

10:25 **CHED 236.** Strategies for funding undergraduate research at the community college. **R.H. Jarman**

10:45 **CHED 237.** Research-based and interdisciplinary curriculum design for general chemistry and beyond. **K.S. Owens, A.J. Murkowski, H. Price, A.M. Johansen**

11:05 Intermission.

11:15 **CHED 238.** Promoting undergraduate research at community colleges to increase STEM competency and transferability to 4 yr institutions within CUNY. **N.H. Phillip, T. Brennan, P. Meleties, J. Rachlin**

11:35 **CHED 239.** The STEPS Program – a pathway from Community College to Bachelor's degree and beyond. **R.D. Walker, T. Williams**

11:55 **CHED 240.** The Community College Undergraduate Research Initiative: A national collaborative. **P. Powers**

12:15 Discussion.

Section F

Sheraton Denver Downtown Hotel
Silver

Chemistry Education: International and Multi-cultural Perspectives

S. Raje, *Organizer*
S. Sandi-Urena, *Organizer, Presiding*
S. Hansen, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 241. Chemical education in India: Observations. L.H. Rickard

8:55 CHED 242. General Chemistry study habits and instructional practices across borders. J. Leiton Chacón, S. Sandi-Urena, A. Villalta-Cerdas, M. Sestillo, L. Pettygrove

9:15 CHED 243. Language challenges in teaching and learning General Chemistry. P.K. Yuen, C.D. Lau

9:35 CHED 244. Withdrawn.

MONDAY AFTERNOON

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Agricultural and Food Chemistry

Cosponsored by AGFD and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED 245. Improving quality control methods in the brewing industry through analytical characterization of hop alpha acids. K. Dahya, J. Moon, M. Brush, R.N. Dansby-Sparks

CHED 246. Analysis of metal ion absorption compared to pH and conductivity changes in hydroponic growing systems. T.E. Sheppard, M.E. Railing

CHED 247. Archaeochemical analysis: Using chemistry to inform history. D.A. Regan, A.A. Hill, D. Hill

CHED 248. Determination of chlorogenic acid and caffeic acid in fruits with evaluation of pesticide concentrations. J.C. Doverspike, C.A. Radford, J.E. Owens

CHED 249. Modifications of brewing parameters: Analysis of volatiles by SPME-GC-MS and hydrogen sulfide analysis in beer. L. Benedict, R. Byrnes, A.C. Ricardi, M.S. Qazi, P.J. Gregorich, D.A. Arris

CHED 250. Characterization of tissue browning products using attenuated total reflection: Fourier transform infrared spectroscopy. A. Steele, J. Walton, S. Chakraborty

CHED 251. Further defining acylsugar structural diversity within *Petunia axillaris*. M.C. Enright, X. Liu, A. Jones

CHED 252. Determining the effects of processing on antioxidant activity in cilantro, parsley, and rosemary. L.M. Patel, K. Daus

CHED 253. Mapping of oxidation products of tissue browning using 2,4-ditrophenylhydrazine and high performance liquid chromatography. J. Walton, A. Steele, S. Chakraborty

CHED 254. Using trace element signatures to determine cocoa liquor provenance. R. Khalsa, S.E. Stitzel, R.E. Sours

CHED 255. Analysis of e-cigarette flavors with gas chromatography. T. Massetti, K. Muller

CHED 256. Extraction and characterization of anthocyanins from organically grown grains. N. Strobel, G.L. Milligan

CHED 257. Comparison of eastern filbert blight resistance in two hazelnut cultivars. N. Lee, M. Hoang, A. Hoffman

CHED 258. Comparison between two extraction techniques used to isolate antioxidants from the pith and carpellary membrane of pomegranates. S. Ansari, K.A. Daus

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Analytical Chemistry

Cosponsored by ANYL and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED 259. Analysis of elements in nutritional beef bone broth. A. Poli, M.E. Piyasena

CHED 260. X-ray structure and variable-temperature photoluminescent properties of isostructural lanthanide cyanometallates containing DMSO. K. Xiang, J. Hendrich, F.D. White, J.D. Taylor, R. Sykora

CHED 261. Spectrophotometric determination of ethanol concentration in beer utilizing an enzyme activity assay. J.A. Schafer, E. Paine

CHED 262. Determination of cocaine concentrations in dried bloodstains. B. Gillease, G.P. Foy

CHED 263. Detection and extraction of date rape drugs from hair samples using liquid chromatography - mass spectrometry. L. Burns, G.P. Foy

CHED 264. Elemental analysis of CdSe/ZnS core/shell quantum dots by AA. K.M. Stallings, J.L. Dancler, B.E. Eichler, D.E. Weishaar

CHED 265. Analyzing thermal degradation of iso-alpha acids by high performance liquid chromatography (HPLC). J.M. Goff, K.M. O'Brien, T. D'Andrea

CHED 266. pH Dependent Zn(II) binding behavior of an analog methanobactin peptide. K.L. Cumpian, M. Deaconda, R. Ortiz, S.M. Wagoner, L.A. Angel

CHED 267. New method for improving solar energy conversion: Side selective modification of Photosystem I. L. Thal, E.A. Gizzie, G. LeBlanc, D.E. Cliffl, G. Jennings

CHED 268. Quantitative analysis of hydrogen peroxide using crude peroxidase extract from cucumber peel. L.E. Totten, S. Kradtap

CHED 269. Determination of bisphenol A in thermal receipt paper water samples and lake water samples using fluorescence spectrophotometry. B. Chitwood, S. Hubbard

CHED 270. Withdrawn.

CHED 271. Determination of bisphenol-A (BPA) in canned goods from Arkansas markets using fluorescence spectrophotometry. R. Pruetz, S. Hubbard

CHED 272. Rapid identification of designer drugs with NMR spectroscopy. F. Fowler, L. Huang

CHED 273. Optimization of silver shell and silica core nanoparticles as SERS active substrate. A.G. Telcy, S. Han, X. Li

CHED 274. Synthesis, characterization, and catalysis of halogen and nitro substituted Schiff-base organometallic complexes towards the copolymerization of CO₂ and epoxides. R.L. Ayscue, N.P. Deifel

CHED 275. Preparation of hydrophobic thermally polymerized sol-gel monolithic columns for reversed-phase liquid chromatography using "single-pot" approach. R. Hernandez, L. Narciso Meirelles, F. Svec, Z. Zajickova

CHED 276. Garnet classification and provenance using laser-induced breakdown spectroscopy (LIBS). P.A. Defnet, R.R. Hark, M. Wise, R.S. Harmon

CHED 277. HPLC method development for caffeine analysis with *Chlorella vulgaris* as a bioremediation agent for aquatic systems. A.L. Williamson, S.M. Etridge, C.A. Miderski

CHED 278. Laser-enhanced ionization-mass spectrometry for dried blood spot quantification of a biomedically important analyte. S. Sheffield, L. Miller, S. Shuttleworth, S. Faber, M. Pamuku, H. Kingston

CHED 279. Developing paper microfluidic devices to detect drugs of abuse. J. Bottoms, L. Wang, B. McCord

CHED 280. Characterization of patterned anti-fouling xerogel coatings. Z. Jones, J. Destino, F.V. Bright

CHED 281. Investigation of chemical interferences in vehicle arson accelerator identification. L. Humphrey, D.G. Klarup

CHED 282. Identifying more efficient methods for rare earth isobar separations. C. Meyer, L. Harvey

CHED 283. Using fast-scan cyclic voltammetry to quantify serotonin release in Huntington's disease model mice. S. Fantin, R. Gehringer, S. Kaplan, M.A. Johnson

CHED 284. Elemental analysis of enamel and dentin in healthy, carious, and periodontal diseased permanent human teeth using inductively coupled plasma mass spectrometry (ICP-MS). R. Reed, M.B. Jacobs

CHED 285. Extraction and concentration of caffeine from artificial saliva for GC/MS analysis. J. Mayhew, B. Zabka, B. Nespor, S. Cole-Harding, N. Winburn

CHED 286. Determination of fluoride levels in mouthwash and tap water samples. E.N. Henshaw, R. Fietkau

CHED 287. Quantitative determination of methionine sulfoximine by liquid chromatography tandem mass spectrometry. W. Gilbraith, S. Gamagedara

CHED 288. NMR Investigation of the effect of pH on aggregation, counterion binding, and amide proton exchange in amino-acid-based surfactants. C. Lewis, A. Wall, E. Billiot, F.H. Billiot, K.F. Morris

CHED 289. Effect of pH on isocyanate amino acid based surfactants. D. Georgiadis, F.H. Billiot, C. Lewis, E. Billiot, K.F. Morris

CHED 290. Surface immobilization of AMPs using click chemistry. M. Baria, Y. Li, Z. Chen

CHED 291. Analysis of nitrate content in vegetables using ion chromatography. C. Griffin, M.M. Ivey

CHED 292. Using regression analysis to determine the mechanism of solvent reactions. M. Durrant, M.J. D'Souza

CHED 293. Apparatus for ultratrace detection of arsenic in drinking water by hydride generation gas chromatography with photoionization detection. W.R. Borgesson, S.H. Fritsbe, J.N. Driscoll

CHED 294. Expanding and improving direct-analysis capabilities in mass spectrometry. S. Michalak, J.T. Shelley

CHED 295. Investigation of β -blocker association with a chiral molecular micelle by means of molecular dynamics simulations. C. Hoffman, E. Billiot, F.H. Billiot, Y. Fang, K. Morris

CHED 296. Investigation of the mechanism of chiral recognition by molecular micelles with molecular dynamics simulations. S. Zack, E. Billiot, F.H. Billiot, Y. Fang, K. Morris

CHED 297. Examination of silica sol-gels and aerogels containing silver nanoparticles and 4-mercaptobenzoic acid using surface-enhanced Raman spectroscopy. T. Corrado, E.J. O. Atkinson, B.D. Gilbert

CHED 298. Chromatographic analysis of bee propolis. K. Symczak, S.J. Pace, E.E. Mojica

CHED 299. Studies on the interactions of four nanoceramics (metal oxides) with serum albumin and hemoglobin proteins by spectroscopic techniques. E. Nguyen, P.M. Hanson, T.J. Batta, E.E. Mojica

CHED 300. Trace element analysis of commercially produced red wines and beers. M.J. Raub, N.S. Olson, N.J. Ronkainen

CHED 301. Comparing graphene oxide electrochemically reduced from aqueous and non-aqueous solutions for the purpose of serving as an electrocatalyst support material. I.B. Agbere, J.A. Bennett

CHED 302. Dependence of surface roughness on electropolish time on 316L stainless steel. E. Hammerstrom, K.E. Rohly

CHED 303. Mass spectrometry imaging of the *Torpedo californica* electric organ using MALDI-FT-ICR MS. A. McDonnell, E. Schenk, M. Harlow, F. Fernandez-Lima

CHED 304. Study towards the selective digestion of glyphosate in surface water. A.F. Bauer, A.K. Perry, A.R. Roerdink

CHED 305. Method development towards quantifying marijuana consumption using sewage based drug epidemiology: Preliminary results for Treatment Plant #2. M.C. Pellman, H. Fryhle, D.A. Burgard

CHED 306. C-arylation methods to a library of covalent modifiers. A. Diepenbrock, A. Cassidy, N. Asad, P.R. Hanson

CHED 307. Variance of caffeine in different brews of coffee. T.L. Self, K. Cossey

CHED 308. Method development towards quantifying marijuana consumption using sewage based drug epidemiology: Preliminary results for Treatment Plant #1. H. Fryhle, M.C. Pellman, D.A. Burgard

CHED 309. Study of the impact of ionization conditions on ion formation in electrospray mass spectrometry. T.J. Hulyk, S. Norris, K.H. Bennett

CHED 310. Optimization of the voltammetric analysis of heavy metals. J. Stapleton, A.F. Bange

CHED 311. Synthesis of variable size nanoprisms for application in signal enhancement using Raman spectroscopy. T.M. Keller, M.V. Schiza

CHED 312. Optical evaluation of fluorescent nanoparticles embedded into silica aerogel hosts. T. Lightner, J.N. Richardson

CHED 313. Direct and indirect detection of FMN and FAD released upon target binding. C.A. Dunlock, A.G. Gee, S. Sitaula, M.F. Ali

CHED 314. Preparation of FAD conjugates to signal target binding events. J. Grennell, S. Sitaula, A.G. Gee, M.F. Ali

CHED 315. Synthesis and photophysical and photochemical characterization of osmium complexes for luminescence-based sensing. A. Wagner, K. Kneas, J.A. Rood

CHED 316. Effects of cinnamon components on glycolysis by anion exchange-high performance liquid chromatography coupled to conductimetric detection. M. Jones, K.E. Garrison

CHED 317. Qualitative and quantitative analysis of fluorine containing synthetic cannabinoids. J. Davidson, D.P. Predecki, J.N. Richardson

CHED 318. Study of an alternative method for quantitative Ni(II) determination. O.N. Blackmore, K. Belt, R.V. Whiteley

CHED 319. Analysis of pharmaceuticals in water samples by gas chromatography-mass spectrometry (GC-MS). K. Altomose, Y. Mei-Ratiff

CHED 320. Comparison of solid phase extraction and solid phase microextraction for the quantitative analysis of *trans-resveratrol* in red wine samples by HPLC. J.J. Wukovits, Z.M. Colson, J.A. Bolani

CHED 321. Automated reaction monitoring using liquid chromatography-mass spectrometry. D.J. Alton, M.M. Smalley, S.A. Kurtovic, K.C. Lapworth, K.R. Evans

CHED 322. GC-MS characterization of cell culture media: Optimizing sample preparation using automation and design of experiments (DOE). L.M. Housel, C.M. Ingersoll

CHED 323. Evaluating graphene oxide electrochemically reduced on Pt-black as a support for H₂S detection. R. Custer, J.A. Bennett

CHED 324. Method of collection and detection for airborne organo-arsenic compounds. K.M. Clark, B.M. Hopkins

CHED 325. Selection of protein-binding DNA aptamers for bacterial detection. J.M. Clements, A.M. Bluhm, M. Blatz, J. Nava, S. Evans, A.G. Cavinato

CHED 326. Development of a DNA biosensor for rapid detection of *Renibacterium salmoninarum*. T.N. Keohakale-Loak, B.L. Mandella, A.M. Olivo, A.G. Cavinato

- CHED 327.** Analysis and quantification of D-aspartic acid in marine bivalve mollusks. **R. Gutierrez**, A. Delascagigas, T. Connick, E. Rodriguez, G. Fisher
- CHED 328.** Triarylmethane and xanthenes dye synthesis and characterization of their photophysical properties. **S.E. White**, A.B. Ormond
- CHED 329.** Analysis of analgesics in the Quittapahilla Creek watershed. **K. McCordle**, O.A. Moe
- CHED 330.** Cross-linker effect on metal ion detection using molecularly imprinted polymers. **D. Baumann**, V. Mai, C. Zanelotti, S.E. Stitzel
- CHED 331.** Analysis of trace metals in tattoo inks using Agilent ICP MP-AES. **S. Al-Khalifa**, H.S. Butman, M. Wieler, C.H. Jaworek-Lopes
- CHED 332.** Paper-based device for colorimetric detection of malondialdehyde in biological samples. **T.D. Steichen**, A. Fazzal
- CHED 333.** Optimization of solid phase extraction of petroleum residues implementing green chemistry principles. **R.B. Kamerman**, P.P. Vaughan, A.M. McKenna
- CHED 334.** Using solvent parameters for increased precision in chemical shifts. **E.E. Schiller**, W. Carroll
- CHED 335.** Lab curriculum development involving the synthesis and characterization of molecularly imprinted polymers in the detection of aspirin. **J.P. Cohen**, D.G. Sykes
- CHED 336.** Quantitative analysis of alcohol using nuclear magnetic resonance. **R. Hill**, C. Nicholson
- CHED 337.** Conformational kinetics study of microperoxidase-11 using TIMS-MS and molecular dynamics. **C. Harrial**, F. Fernandez-Lima
- CHED 338.** Surface modification of photopolymerized sol-gel monoliths using thiol-ene click chemistry. **T. Sabol**, Z. Rodriguez, G. Soto, D. Britsch, D.M. Gharbharan, F. Svec, Z. Zajickova
- CHED 339.** Solid phase extraction (SPE) of urine in postmortem toxicology testing. **V. Davidson**, D. Baker, R. DeRienz
- CHED 340.** Obtaining electricity from solar energy utilizing household products. **R. Senter**, E.D. Stemp, A. Calderon, D. Romero
- CHED 341.** Stabilities of mephedrone in biological and non-biological matrices. **H.L. Ciallella**, S.L. Oddi, K.S. Scott
- CHED 342.** Development of paper analytical devices for the detection of substandard azithromycin and erythromycin. **E.P. Aldrich**, T.L. Barstis
- CHED 343.** Raman probes as a rapid identification and detection tool for *E.coli* in fresh parsley. **A. Sotomayor-Albino**, A.N. Soler, C.R. Ruiz-Martinez, M.A. De Jesus
- CHED 344.** Withdrawn.
- CHED 345.** Studying the binding interactions of the chemokines CXCL12 and CXCL14 to heparin and heparan sulfate using affinity capillary electrophoresis. **A. Schrader**, A.K. Korir
- CHED 346.** Best spinach that Popeye ever ate. **K. Weishaar**, J. Potratz
- CHED 347.** Cyclic voltammetry of *tris*-dithiocarbamates in room temperature ionic liquids. **J. Becca**, A. Eisenhart, J. Coffield
- CHED 348.** Development of analytical methods for detection of pharmaceutical pollution of surface water in Georgia using purge-n-trap GC/MS. **K. Hachat**, N. Potter, C.H. Lisse
- CHED 349.** Withdrawn.
- CHED 350.** Investigation of toxic metals in over-the-counter eye shadow makeup. **J. Mendez**, R. Huschka
- CHED 351.** Assessing the reproducibility and applicability of a miniature gas chromatograph. **M. Akinlaja**, R.J. Noll
- CHED 352.** Synthesis of 1-butyl-3-methylimidazolium hexafluorophosphate: Investigation of its use as an electrochemical solvent for electroanalytical studies of metal dithiocarbamate complexes. **A. Eisenhart**, J. Coffield
- CHED 353.** Influence of the *cis/trans* ratio of hop iso-alpha-acids on beer bitterness. **M. Baginski**, B. Fleshman, D.L. Donohue
- CHED 354.** Separation of cations for waste reduction. **C. Cookenmaster**, M. Claus
- CHED 355.** Identification of volatile organic compounds present in cigarette smoke via purge-n-trap coupled with GC/MS. **P. Skersick**, E. Smith, C.H. Lisse

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Biochemistry

Cosponsored by BIOL and SOCED

N. Di Fabio, Organizer

12:00 - 2:00

- CHED 356.** In vivo expression of antimicrobial peptides in *Escherichia coli*. **S.A. White**, N.S. Muthunayake, C.S. Chow
- CHED 357.** Role of copper in the oxidative stress response of *Chlamydomonas reinhardtii* to heat shock. **M. Brann**, O. Marcu
- CHED 358.** Effect of anti-diabetic agents on the *in vitro* glycation of bovine serum albumin. **A.T. Shuck**, E.C. Daniels, R.L. Hein, A.M. Overman, M.E. Lee
- CHED 359.** Ion-pair reverse-phase liquid chromatography analysis for separating and quantifying RNA generated via *in vitro* transcription reactions. **M. Bestwick**, H. Wienkers
- CHED 360.** Inhibition of the bacterial fatty acid biosynthetic enzyme FabI by secondary metabolites isolated from *Artemisia californica*. **P.M. Joyner**, S. Bryant
- CHED 361.** Increased growth and mutagenesis in bacteria exposed to titanium dioxide nanoparticles. **V.F. Smith**, V. Mukherjee
- CHED 362.** Investigation of the effects of titanium dioxide nanoparticles on phospholipid bilayers using differential scanning calorimetry. **R. Gall**, V.F. Smith
- CHED 363.** Adsorption of snake venom by activated charcoal. **S. Sivakumar**, R.A. Kopper
- CHED 364.** Variation of protein components in successive regenerations of individual coralsnake venom. **P. Spradley**, R.A. Kopper
- CHED 365.** Metal ion cofactor requirements of phosphomonoesterase. **V. Ventrano**, R.A. Kopper
- CHED 366.** Inhibition of lecithin-cholesterol acyltransferase by reactive aldehydes in electronic cigarettes. **P. Hanna**, R.E. Rigsby
- CHED 367.** Phylogenetic analysis of the upstream region of the arcanolysin gene from smooth and rough biotypes of *Arcanobacterium haemolyticum*. **D.L. Ross**, H.S. Ruther, D. McGee
- CHED 368.** Identification and characterization of a membrane-associated esterase from *Propionibacterium acnes*. **R. Chapin**, B. Harville
- CHED 369.** Characterization of a *Tannerella forsythia* collagenase by SDS-PAGE and fluorescent spectroscopy. **B.J. Sanders**, B. Harville
- CHED 370.** Porphyrin derivatives and photodynamic therapy effects on triple negative breast cancer. **S. Rogers**, J.E. Bradshaw, T.E. Hayes
- CHED 371.** Expression of recombinant intimin and translocated intimin receptor proteins in *E.coli* cells. **K. Page**, C. Sobraske, L. OBrien
- CHED 372.** Influence of the second-sphere coordination on the nitrite reductase activity of globins. **A. Rodland**, J. Gowen, M.I. Galinato
- CHED 373.** Optimization of fragment inhibitors for the class D β -lactamase OXA-24. **R.C. Hoogmoed**, R.A. Powers
- CHED 374.** Fox-4 cephamycinase: Analysis of structure and function. **B. Biju**, M. Noel, E.C. Mundorff, R. Toro, V. Malashkevich, S. Almo, J. Aguilan, E. Nieves, K. Papp-Wallace, F. Prati, E. Caselli, J. Frere, G. Bou, R. Bonomo, S.T. Lefurgy
- CHED 375.** Denaturation resistance of polygalacturonase obtained from coffee mucilage. **J.M. Henning**, G.R. Oppenlander, A.F. Fillett, M.L. Zuteck, E.A. Gay, M. Caspers
- CHED 376.** Hydrogen deuterium exchange used to study the interface of *Plasmodium falciparum* glutathione reductase and the antimalarial drug methylene blue. **S. Lim**, H. Prieto
- CHED 377.** Role of cytochrome c and its effects on the programmed cell death pathway of *P. falciparum* using yeast as a model organism. **E. Orozco**, H. Prieto
- CHED 378.** Expression and purification of DPAP-1, a malaria protease, and its role in the putative apoptosis pathway of the parasite. **A. Bains**, H. Prieto
- CHED 379.** Yeast cell survival in different concentrations of canavanine. **P. Angkanaworakul**, J. Iverson, T.T. Saxowsky
- CHED 380.** Characterization of the non-native 1,2-naphthoquinone *in vivo* incorporation into the A, site in PS I complexes of *Synechocystis* sp PCC 6803. **E. Gosselin**, T.W. Johnson
- CHED 381.** Characterization of highly reducing anthraquinones in the A, site of PS I complexes of *Synechocystis* sp. PCC 6803. **P. Kerns**, T.W. Johnson
- CHED 382.** Effects of sphingosine 1-phosphate at the blood brain barrier. **A.C. Love**, S. Spampinato, A. Cotleur, R. Ranshoff
- CHED 383.** Characterization of a putative haloalkane dehalogenase from *Saccharomonospora azurea*. **E. Zhou**, E.C. Mundorff
- CHED 384.** Expression and purification of farnesyl diphosphate synthase from *Thermoplasma volcanium*. **C. Banos**, B. Horrigan, J. Himmelberger
- CHED 385.** Mutagenesis of a TfdA-like B. pertussis enzyme. **N. Pierce**
- CHED 386.** Quantifying *Escherichia coli* in recreational freshwater of the Saginaw Bay Watershed using Colilert and quantitative PCR. **A. Lukowski**, T. Sivy
- CHED 387.** Development of an LC-MS/MS-based assay for the quantification of trehalose. **P.M. Kretschmer**, A.J. Rouff, M.K. O'Brien, L.A. MacManus-Spencer, M.G. Paulick
- CHED 388.** Quantitative analysis of hydrocortisone levels in human saliva due to the effects of positive and negative stressors. **S. Riley**, H.S. Greenberg, M.B. Hargrove, R.L. McCann
- CHED 389.** Determination of the signaling pathway leading to tight junction disassembly in diabetic retinopathy. **S. Prettnner**, R.L. McCann
- CHED 390.** Modified ELISA to determine levels of TTX and its links to the life history of the eastern newt, *Notophthalmus viridescens*. **H. Winter**, P. Delis, R.L. McCann
- CHED 391.** Toxicity of imidazolium room temperature ionic liquids towards biofilms. **L. Sanders**, E.G. Ennis
- CHED 392.** Toward inhibitors of cystathionine β -synthase (CBS): Examination of both the transsulfuration and hydrogen sulfide evolution reactions. **L.M. Szczesniak**, M.L. Beio, C.D. McCune, W. Shen, D.B. Berkowitz
- CHED 393.** Conformational variability of MTHFR characterized by hydrogen-deuterium exchange and mass spectrometry. **S.S. Webster**, A. Stahly, E.E. Trimmer, E.M. Marzluff
- CHED 394.** Spectroscopic properties of the GFP chromophore containing substituted phenylalanine derivatives in place of tyrosine. **J.D. Stevens**, J. Tharp, A. Tuley, W. Liu
- CHED 395.** Investigation of IPTG and its products of oxidation in the induction of protein biosynthesis. **M.M. Schmauch**, M.Y. Kasmani, J.M. Chalker
- CHED 396.** Lipid dynamics of cardiolipin/DMPC and cardiolipin/DOPC in nanodiscs. **K. Stipe**, H. Steele
- CHED 397.** Biochemistry in the cosmetic industry: The effectiveness of synthetic and natural preservatives. **A.M. Wilburn**, J.T. Peace
- CHED 398.** Binding kinetics and transition of structural components of RNA polymerase. **M. Mecha**, M. Poulos, R. Sreenivasan, T. Record
- CHED 399.** Amyloid-perturbing dyes inhibit adhesion of *Cryptosporidium parvum* to the human ileocecal adenocarcinoma HCT-8 cell line. **D.R. Lee**, C.X. Chan
- CHED 400.** Relationship between redox potential and light production in the mucus of the marine tubeworm *Chaetopterus* sp. **FX. Migliolo**, D. Deheyn
- CHED 401.** Identification of acid/base residues important to the mechanism of Thil. **T. Brondhaver**, E.G. Mueller
- CHED 402.** General method for analysis of RNA structures by deoxyribozyme sensors. **R. Karadeema**, D. Kolpashchikov
- CHED 403.** Designing peptide-coated gold nanoparticles for the bottom-up assembly of amyloid nanocompartments. **A. Sementilli**, J. Smith-Carpenter, D.G. Lynn
- CHED 404.** Chemical characterization of novel bacterial LOV-domain photoreceptors. **K. El-Arab**, B.D. Zoltowski
- CHED 405.** Initial steps toward antimicrobial photodynamic textiles. **S.L. Stanley**, R. Ghiladi
- CHED 406.** Species differences in detoxification rates. **L. James**, L. Browning, C. Dadabay, J. Forbey
- CHED 407.** Effects of dia2 degradation on checkpoint recovery in *Saccharomyces cerevisiae*. **C.C. Torres Cabán**, D. Koepf
- CHED 408.** Computational and experimental approaches to investigate substrate binding of the enzyme OGA. **K.A. Brown**, K. Cotto, R. O'Keefe, G. Crawford
- CHED 409.** Characterization of xanthine dehydrogenase regulator protein of *Ralstonia solanacearum*, a tomato infecting bacterium. **D.T. Johnson**, S. Sivapragasam, A. Grove
- CHED 410.** Dissociation constant (pKa), pH and related thermodynamic functions of TRIS buffer from 5 to 55°C. **T.R. Wehmeyer**, R.N. Roy, L. Roy, L.S. Tebbe
- CHED 411.** Application of the Pitzer Formalism for the aqueous solution of HCl + KCl, HCl + NiCl₂, HCl + PrCl₃, and HCl + ThCl₄ at 25 °C. **K. Hundley**, L. Roy, R.N. Roy
- CHED 412.** Carbon nanotube separation beyond size-selective protein hydrogels. **J. Rowland**, K.C. Tvrdy
- CHED 413.** Combining metabolic inhibitors to preferentially target cancers with deregulated p27. **K.B. Chancellor**, A. Alarbi, N. Santa-Pinter, J. Sabo, R. Sheaff
- CHED 414.** Analogs of cisplatin: 4,4'-disubstituted-2,2'-bipyridine complexes of Pt(II) dichloride. **L. Cobani**, B.L. Bennett
- CHED 415.** Identifying biocompatible redox mediators for electrochemical imaging of *Dictyostelium discoideum*. **C. Chira**, A. Maselli, R.J. Lesuer
- CHED 416.** Detection and Identification of biochemical molecules secreted by *Entamoeba* varieties for taxa discrimination based on aggregative behavior. **S. McDonough**, J.A. Leitao, A. Espinosa

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

- CHED 417.** Effect of retinoid receptor agonists on K562 cellular adhesion, proliferation, and $\alpha 5 \beta 1$ integrin cell surface expression. **R. Phomakay, M.D. Kelley**
- CHED 418.** Thiophene N-substituted tetrahydro pyridinium salts as functionally selective muscarinic partial agonists. **J.F. Boulos, P.N. Nwokoye**
- CHED 419.** Lactate dehydrogenase: A study of kinetics and inhibition. **C. Chandler, N. Beres**
- CHED 420.** Effect of catalase overexpression on ethanol-induced hepatic mitochondrial DNA damage in mice. **S. Watkins, A.A. Caro**
- CHED 421.** Effect of oral chronic ethanol administration on hepatic mitochondrial biogenesis in mice. **T. Spradley, A.A. Caro**
- CHED 422.** Effect of ethanol and catalase overexpression on hepatic mitochondrial DNA content in mice. **S. Fobare, A.A. Caro**
- CHED 423.** Effect of catalase overexpression on ethanol-induced oxidative stress in mice. **C. Dunn, A.A. Caro**
- CHED 424.** N-acetylcysteine inhibits the upregulation of mitochondrial biogenesis genes in livers from rats fed ethanol chronically. **M. Bell, A.A. Caro**
- CHED 425.** Effect of chronic ethanol administration on hepatic genomic (nuclear and mitochondrial) DNA integrity in mice. **A. Stuppy, A.A. Caro**
- CHED 426.** Effect of polycystin-2 disruption on osmotic response of renal epithelial cells. **R. Comer, B.J. Siroky, B.P. Dixon**
- CHED 427.** Effect of transglutaminase on the deregulation of the p27 protein. **R. Patel, L. Zhang, A. Greene, W. Crawford, R. Sheaff**
- CHED 428.** Analysis of p53 protein in hepatocellular carcinomas using 2D and 3D culture models. **J.M. Pomo, R. Taylor, J. Wu, R.R. Gullapalli**
- CHED 429.** Turning off the lights: A novel luciferase inhibitor. **D. Stranford, J.C. Dicesare, R. Sheaff**
- CHED 430.** Isolation of bioactive compounds from novel actinomycetes strains. **W. Johnston, M. Fakhr, S. Marasini, R. Sheaff**
- CHED 431.** Molecular docking studies of novel flavonoid derivatives as dual binding site acetylcholinesterase inhibitors. **L. Gainey, B. Lor, O.M. Newman, C. Mills**
- CHED 432.** Standard buffer POPSO for use in the physiological pH range. **K. Hundley, R.N. Roy, L. Roy**
- CHED 433.** Mechanistic and kinetic studies of a new ROS-activated compound. **E.D. Pullen, E. Merino**
- CHED 434.** Dietary sodium suppresses digestive efficiency: Role of the renin-angiotensin system. **F. Morales-Santiago, J.L. Grobe**
- CHED 435.** Pattern analysis of abnormal blood producing low velocity spatter. **C.A. Weiss, G.P. Foy**
- CHED 436.** Alteration of the specificity of putrescine oxidase by mutations to the active site. **L. Woodcock, K. Colvert**
- CHED 437.** Identification of sulfopeptides as HIV entry inhibitors through phage display. **G.M. Roman, T. Ju, J. Guo, W. Niu**
- CHED 438.** Screening peptidomimetic ligands against patient-specific chronic lymphocytic leukemia monoclonal antibodies. **A.L. Hackler, S. Simanski, M. Sarkar, T.J. Kodadek**
- CHED 439.** Oxidation of cytochrome C by guanine radicals. **M. Safaeipour, M. Bekarian, M. Sanchez, J. Juaregui, S. Castillo**
- CHED 440.** Effect of glutathione on DNA-protein crosslinking caused by guanine oxidation. **M. Safaeipour, M. Bekarian, M. Sanchez, S. Castillo, J. Juaregui, E.D. Stemp**
- CHED 441.** Expression and purification of homocysteine methyltransferase *Sam4* recombinant in *Escherichia coli*. **L.J. Negron, W. Qu, Z.S. Zhou**
- CHED 442.** Analysis of the antibody binding of MUC1 peptides and substituted peptides by STD NMR. **A.R. Lynch, T. Yang**
- CHED 443.** Investigation of the aqueous chemistry in the elimination of glutathione from the glutathione-3-methyleneoxindole conjugate: A potential therapeutic agent. **K. Bukis, E.J. Brush**
- CHED 444.** Thermostabilization of water soluble variants of the human β_2 adrenergic receptor. **P. Kurtzweil, A. Kikonyogo, A.L. Parrill-Baker**
- CHED 445.** Evaluation of off-target effects through double-stranded RNA interference in *C.elegans*. **S.M. Litz, T.A. Sugrue, T. Dwyer**
- CHED 446.** Designing an undergraduate lab procedure for the synthesis of [R,S]-Boc-Phenylglycyltryptophan methyl ester. **T.J. Smith, D.A. Wing**
- CHED 447.** Arabidopsis MMD-like genes and their roles in chromosome biology during male reproduction. **M.M. Shroder, C.A. Makaroff**
- CHED 448.** Molecular recognition of diatomic gases in *Rhodospseudomonas Palustris* Cytochrome *c'*. **J.P. Bard, S.S. Safaie, Z. Nilsson, C.R. Andrew**
- CHED 449.** Natural antisense RNA plays a role in *Arabidopsis thaliana* growth and development. **A.A. Simoni, C.A. Makaroff**
- CHED 450.** Reaction of strained alkynes with cysteine proteases. **M.M. Tierney, G.H. Jones, J.M. Chalker**
- CHED 451.** Platinum(II) complexes with sulfur-containing peptide building blocks for use in RNA binding studies. **N. Hardin, C.S. Chow**
- CHED 452.** Role of H57 in synchronizing ammonia transfer within *E. coli* CTP synthetase. **M.R. Abbott, J.L. Johnson**
- CHED 453.** Kinetics of the reaction of 6-amino-hexanoic acid with chlorine(I): Evidence for a role for dichlorine monoxide. **Z.A. Cockrell, G.H. Purser**
- CHED 454.** Isolation of corticosterone and its effect on personality in convict cichlids (*Amatitlania nigrofasciata*). **C. Marshall, N. Ali, R. Fox**
- CHED 455.** Effect of brewed coffee from various sources on the formation of amyloid-beta fibrils in vitro. **R.J. Tokarski, M.A. Fisher**
- CHED 456.** Identification of bovine pregnancy markers in urine samples. **R. Lalmanasingh, A. Rafalowski, N.M. Wachter, M. DeCastro**
- CHED 457.** Interaction of anthrax toxin protective antigen protein with model cell membranes at the air-water interface. **J. Jarosz, N. Meyer, A. Serfis, J. Bann, S. Mamillapalli**
- CHED 458.** In silico studies of MMP-1. **D. Pusztai, E. Healy**
- CHED 459.** Investigation of the apoptotic biochemical mechanism of ajulemic acid in Ewing's sarcoma cell lines. **J. Ubeda, L. Hensley, M.D. Perry**
- CHED 460.** Enhancing the bioavailability of RAGE inhibitors: Toward new anti-Alzheimer's therapeutics. **T. Dwyer, M. Randolph, M. Ross, B.L. Miller**
- CHED 461.** Effects of apolipoprotein E on M2 microglia. **B. Bieger, H. Ferguson, S. Rose, R. Frye, S. Barger**
- CHED 462.** Use of enhanced chemically defined media to improve uptake of L-telluromethionine by *Escherichia coli* DL41(DE3). **V. Sublett, B. Cooper, J.O. Boles**
- CHED 463.** Role of apoptosis in modulating effects of 2-aminoanthracene in pancreatic tissue of Sprague Dawley rat dams. **J.W. Jay, E. Venable, E.W. Howerth, W.E. Gato**
- CHED 464.** Hepatic gene expression in pups exposed to 2-aminoanthracene in utero indicative of susceptibility to metabolic syndrome. **G.W. Barnett, W. Yau, E.W. Howerth, W.E. Gato**
- CHED 465.** Aliphatic protein side chain density correlates with phosphate crowding and helical curvature in protein/DNA crystal structures. **L.A. Isom, N. Hunter, B. Grant**
- CHED 466.** Protein purification and expression for glycetin complex with rat estrogen receptor beta. **A. Heldt, G.T. Marks**
- CHED 467.** 4T1 Murine breast cancer cell cytotoxins in *Rumex crispus* (Yellow Dock). **A.M. Rivera, S.C. Kelly, J.R. Kenneson, R.T. McCutcheon, T.E. McElwain, D.W. Capps, A.J. Reinhard, G.O. Gray**
- CHED 468.** Investigation of a HAD phosphatase from *Mycobacterium tuberculosis*. **C. Barner, A. Roberts**
- CHED 469.** Establishing RNAi in *Tribolium castaneum* at MSU Denver. **C.M. Lowrance, E. Ragan**
- CHED 470.** Measuring the stability of iso-1-cytochrome c variants using heme spectra. **S. Eikenberry, A. Wold, M. Cherney**
- CHED 471.** Effect of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) on estrogen receptor beta and aryl hydrocarbon receptor using RT-qPCR. **M. Kinney, G.T. Marks**
- CHED 472.** Investigating the mechanism of furfural inhibition in *E. coli*. **K.D. Hannie, S.D. Johnson, M. Holle, A. Sostarec, L. Moore**
- CHED 473.** Bacterial screening in search of novel pharmaceuticals. **A. Jorski, O. Oyewole, K. Lacey, M. Fakhr, R. Sheaff**
- CHED 474.** Fluorination of DNA aptamers through "Click Chemistry" synthesis. **J. Dotson, J.C. Eason**
- CHED 475.** Evaluating the expression levels of putative biomarkers in a panel of pancreatic cancer cell lines by qPCR. **A. Smith, N. Goonesekere, K. Dhanwada**
- CHED 476.** Probing the identity of the distal heme ligand in Cys80 variants of iso-1-cytochrome c. **A. Wold, S. Eikenberry, M. Cherney**
- CHED 477.** Investigation of macromolecular crowding on ferredoxin and ferredoxin-NADP⁺ reductase kinetics. **D. Bautista, S. Owen, D.W. Seybert**
- CHED 478.** RNA phosphoramidite monomer synthesis: An examination of phosphite selectivity improvement. **E.E. Yancey, K.F. Harvey, S.D. Holt, V.K. Durlap**
- CHED 479.** Detection of catecholamines using a paper-based microfluidic device. **C. Smith, M.A. Fisher**
- CHED 480.** Analysis for genetic polymorphism of eastern Pacific bluefin and yellowfin tuna with microsatellite sequence PCR primers developed for Atlantic and western Pacific bluefin and western Pacific yellowfin tuna. **S. Wagner, M.E. Pugh**
- CHED 481.** Purification and expression of modified calmodulin protein (N-Cam.Y). **D. Weiss, C. Chant, C. Ricciardi, M. Smith, D.E. Bourne**
- CHED 482.** Purification and characterization of *Bdellovibrio* derived α -glucosidase, malA. **A. Simpson, J.E. Hanson, M. Martin, J. Ginstead, P. Smith, C. Isabella**
- CHED 483.** Effects of floodplain silt on plant cell biochemistry. **A.N. Anderson, D.M. Anderson, A. Marry**
- CHED 484.** Potential effects of betulinic acid on the formation of the calmodulin/CaMKKII complex. **R. Woloshun, M.A. Fisher**
- CHED 485.** 2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD) induces cell death in human granulosa cells. **C.J. Venes, G.T. Marks**
- CHED 486.** Identification of genes involved in RQ₂ biosynthesis in *C. elegans* using RNAi knockdowns. **H. Xun, J. Shepherd**
- CHED 487.** Investigation of *Nocardioides* sp. metabolic, structural, biochemical properties, and its potential role in the sulfur cycle. **K. Lachmayr, E. Oduaran**
- CHED 488.** Investigation of the interference of extracted cinnamon components on the glucose oxidase-peroxidase test. **A. Diepenbrock, C. Breaux**
- CHED 489.** Screening an enaminone library for histone deacetylase inhibitors. **B. DeMier, N. Koduri, S.R. Hussaini, R. Sheaff**
- CHED 490.** Improved model to predict the free energy contribution of dinucleotide bulges to RNA duplex stability. **J.C. Tomcho, M. Tillman, B. Znosko**
- CHED 491.** Challenges in visualizing RecA-DNA interaction in chemiluminescent electrophoretic mobility shift assays. **J.R. Kenneson, R.L. Moore**
- CHED 492.** Analysis of rhodoquinone production in knockout strain candidates in *Rhodospirillum rubrum*. **B. Titus, J. Shepherd**
- CHED 493.** Rhodium(II) metallopeptides as a structural platform for selective Abl tyrosine kinase inhibition. **M.J. Wheadon, S. Knudsen, J. Ohata, F. Vohidov, Z.T. Ball**
- CHED 494.** Investigation of the change in expression of neuropeptides with gluten free based diets. **C.R. Fencil, B.A. Davis**
- CHED 495.** Role of aspartic acid 101 in *E. coli* alkaline phosphatase architectural activity and stability. **S. Chamberlin, A. Moaur, J.K. Brown, K. Wallerius**
- CHED 496.** Increasing the activity of *E. coli* alkaline phosphatase through a structurally destabilizing mutation. **S. Chamberlin, O. Kilbarger, B.J. Anderson, D.A. Than**
- CHED 497.** Why taking your vitamins is essential: The importance of architecture in metabolite sensing by the B_{12} riboswitch. **S. Chamberlin, L.D. Kramer, C. Hofmeister, D. Cutshall, O. Kilbarger, H. Kim, H. Benasutti**
- CHED 498.** Peptides designed to target G-quadruplexes for transcriptional and translational regulation. **S.K. Patel, A.L. Stewart**
- CHED 499.** Biobased composites produced from collagen and vegetable oil polymers. **R.L. Lewis, A.L. Stewart**
- CHED 500.** Peptides designed as mimics of NF- κ B for transcriptional regulation. **J. Page, A.L. Stewart**
- CHED 501.** Analyzing exonuclease-induced hyperchromicity by UV spectroscopy: An undergraduate biochemistry laboratory. **C. Ricciardi, D. Weiss, C. Chant**
- CHED 502.** Characterizing the aggregates of a mutant Alpha 1-Antitrypsin protein associated with Alpha 1-Antitrypsin Deficiency. **M. White, M.A. Fisher, O. Long**
- CHED 503.** Analysis of lipid membrane content in dynamic environments. **A. Chamberland, S.E. Maurer**
- CHED 504.** Investigation of bi-substrate enzyme kinetics for the introductory biochemistry lab. **K. Scinto, K. White, B.J. Alper**
- CHED 505.** Determining the function of Coq4 in *S. cerevisiae* coenzyme Q₂ biosynthesis via biochemical and genetic screening of Coq4 suppressors. **C.R. Colgan, N.R. Olivier, T.P. Nguyen**
- CHED 506.** Effects of deletion of the Rru₁A3004 gene on rhodoquinone biosynthesis in *Rhodospirillum rubrum*. **M.R. Kuenzi, J. Shepherd**
- CHED 507.** Characterization of a human orphan G-protein coupled receptor, GP133. **T.C. Miller, T. Frielle**
- CHED 508.** Prefractionation of natural product extracts provides a value added resource for high-throughput anticancer screening applications. **B. Beall, A. Musick, K. Gustafson**
- CHED 509.** Engineering of metalloenzymes with stacked metalloporphyrin dimers. **M. Getachew Zewde, J. Kleingardner**
- CHED 510.** Pedagogical innovation: Using 3D printer technology in an undergraduate biochemistry course. **K. Janousek, C. Mills**
- CHED 511.** Characterizing HIV-specific CD4 T cell targeting and proliferation among HIV controllers. **D. Walter, B. Walker, S. Ranasinghe**
- CHED 512.** Characterization of the haloalkane dehalogenase, DccA. **L.E. Carlucci, E.C. Mundorff**
- CHED 513.** Determination of aggregation equilibrium of fatty acid vesicles using gas chromatography with flame ionization detection. **L. Aakjar, S.E. Maurer**
- CHED 514.** Designing small molecule autoinducers for investigation into the binding pocket of LasR. **D.J. Kenney, E.S. Garcia Segal**

- CHED 515.** Acute and chronic effects of somatostatin on fast and slow calcium oscillations in the pancreatic β -cell. **K. Harms, B. Thompson, E. Glynn, L. Satin**
- CHED 516.** Effects of creatine supplementation on serum testosterone response in *Mus musculus*. **C. Gill, D. Martin**
- CHED 517.** Construction of a *Burkholderia cenocepacia*-specific gene replacement vector. **T.A. Demers, K.M. Specht**
- CHED 518.** Electron transfer reactions of cytochrome c oxidase: Isolation, characterization, and ligand binding studies. **S. Rodríguez, K.J. Farrell, S. Mahapatro**
- CHED 519.** Detection of melatonin and cortisol in hair. **M.R. Ferguson, A. Alarbi, W. Potter**
- CHED 520.** Purification of components from *Inula helenium* (elecampene) which are cytotoxic to the 4T1 murine breast cancer cell line. **S.C. Kelly, T.E. McElwain, A.M. Rivera, J.R. Kenneson, R.T. McCutcheon, G.O. Gray, A.J. Reinhart**
- CHED 521.** Discovery of a potential Middle East respiratory syndrome (MERS) PLpro inhibitor for the development of anti-MERS-CoV drugs. **S. Loperena-Medina, Y.M. Baez-Santos, A.D. Mesecar**
- CHED 522.** Inhibition of Y-family DNA polymerases. **E. Zilbut, N.M. Antczak, P. Beuning**
- CHED 523.** Purification and characterization of wild type nickel uptake regulator (NUR) from *Streptomyces coelicolor*. **D.J. Peppers, N.E. Grosseehme**
- CHED 524.** Inhibition of formation of blood clots by tetrapeptide inhibitors acet-LSPR-amide and acet-ISPRA-amide. **A. Lacerte, T.A. Trumbo Bell**
- CHED 525.** Probing the substrate specificity of lysine deacetylases using mutagenesis. **K.A. Nichols, T.B. Toro, D.S. Garrett, T.J. Watt**
- CHED 526.** Two systems for modulating back electron transfer between guanine radicals and 2-aminopurine in duplex DNA. **P. Garcia, D. Galindo, S. Cruz**
- CHED 527.** Conformational analysis of cyclic disulfides and selenenyl sulfides in peptide redox motifs. **D.B. Pollard, S. Rozovsky, C.A. Bayse**
- CHED 528.** DNA binding and selectivity of dapsone derivatives. **C. Blake, C.E. Stephens, K.L. Buchmueller**
- CHED 529.** Using acute promyelocytic leukemia cells to test for receptor binding of ajulemic acid. **B. Monk, A. Eubanks, L. Hensley**
- CHED 530.** Observing the folding behavior of b1 group II intron. **K.L. Weber, J. Potratz**
- CHED 531.** Development of small molecules as potential RNA-binding molecules. **J. Lewis, E.G. Segal**
- CHED 532.** Characterization of the disulfide crosslinking in lysyl oxidase. **M. Ali, K.M. Lopez**
- CHED 533.** Use of solubility tags to characterize lysyl oxidase. **A. Hussain, K.M. Lopez**
- CHED 534.** Cooperativity of TU100 and ascorbic acid in the production of reactive oxygen species. **P.C. Borden, J. Whelan, R. Sheaff**
- CHED 535.** Supramolecular guanine-rich quadruplexes and their transfection into mammalian cells. **E. Eklund, T.C. Marsh**
- CHED 536.** Detecting DNA-protein crosslinking in DNA with 2-aminopurine via fluorescence polarization. **H. Brueck, S. Cruz, M. Marquez**
- CHED 537.** Function of laforin in glycogen metabolism and lafora disease. **M.U. Raththagala, K. Brewer, K.D. Auger, B.D. Turner, C. Vander Kooi, M.S. Gentry**
- CHED 538.** Analysis of antibacterial components of honey. **L. White, J. Pruneski**
- Section A**
Colorado Convention Center
Halls C/D
- Undergraduate Research Posters**
Biotechnology
Cosponsored by BIOT and SOCED
N. Di Fabio, *Organizer*
12:00 - 2:00
- CHED 539.** Encapsulation of superparamagnetic nanoparticles in mPEG-PLGA micelles for targeted drug delivery. **H.M. Legaspi, M. Flores, Y. Ba**
- CHED 540.** Exploring simple pattern transfer using microcontact printing. **Y. Freeman, D. Shenault, V. Goss**
- CHED 541.** Identification of previously unsequenced viruses from wild-caught mosquitoes by metagenomic sequencing. **T.M. Biser, K.G. Frey, C.L. Redden, J.J. Anderson, J.C. Andersen, K.L. Schully, R.Z. Cer, V.P. Mokashi, K.A. Bishop-Lilly**
- CHED 542.** Modified coarse-grained DNA model and its application to surface density effects on decamer hybridization. **W.C. Scamman, J.M. Stubbs**
- CHED 543.** Proof-of-concept for rapid point-of-care LFCC detection of serum cancer biomarkers. **J. Mencke, C. Cox, K.J. Voorhees**
- CHED 544.** Sensor circuit for streamlining *E. coli* cell phase determination. **D. Stork, K.A. Haushalter**
- CHED 545.** Development of a cellular probe based on a synthetic receptor. **C. Young, B. Vinciguerra, L.D. Isaacs, A.R. Urbach**
- CHED 546.** Characterization of a cucurbit[7]uril-rhodamine conjugate as a chemical sensor. **S. Vivatson, B. Vinciguerra, L.D. Isaacs, A.R. Urbach**
- CHED 547.** D-Lactic acid biosynthesis from corn stover using engineered *Lactobacillus plantarum*. **E.L. Demel, Y. Zhang, P.V. Vadlani**
- CHED 548.** Engineering light-gated, transmembrane proteins for use in hybrid systems. **S.J. von Hoyningen-Huene, V. VanDelinder, G.D. Bachand**
- CHED 549.** Measuring amyloidogenic protein interaction with lipid membranes via colorimetric assay. **E. LaManna, E.A. Yates**
- Section A**
Colorado Convention Center
Halls C/D
- Undergraduate Research Posters**
Chemical Education
Cosponsored by SOCED
N. Di Fabio, *Organizer*
12:00 - 2:00
- CHED 550.** Gold(I) complexes of benzene-1,3,5-tricarboxamide ligands for Conia-Ene Catalysis. **J.B. Gordon, M. Raynal, L. Boutellier**
- CHED 551.** Greener synthesis of electroluminescent compounds. **N. Rosenfeld, J. Bennett**
- CHED 552.** Development of a simple, qualitative tyrosinase inhibition assay for organic chemistry laboratory. **E. Stopler, J. Bennett**
- CHED 553.** Greener synthesis of thiosemicarbazones. **D. Dragotta, K. Flessa, J. Bennett**
- CHED 554.** Synthesis of C-glycosides as potential antihyperglycemic agents. **C. Tucker, J.L. Chaytor**
- CHED 555.** Characterization of self-assembled monolayers on zinc selenide. **S. Zwart, A.R. Noble**
- CHED 556.** Reduction of infectious biofilms on the native oxide surface of titanium. **N. Bruneel**
- CHED 557.** Development in undergraduate organic chemistry laboratory curriculum. **E. Mueller, R. Starr, O. Michels**
- CHED 558.** Extraction and functional assay of cloned thymopentin 5. **R. Greenstein, K.S. George Parsons**
- CHED 559.** Modification of FTY720 for use as a prodrug for cancer therapy. **K.C. Cotto, B.E. Young, C.M. Watanabe**
- CHED 560.** Auto-oscillatory/excitability boundary and complex dynamics in the Belousov-Zhabotinsky reaction. **D. Prado, T. LongJohn, J.A. Wepey, E.R. Kast, D. Guralnik, S.G. Sobel, H.M. Hastings**
- CHED 561.** Ascorbic acid enhances cytotoxicity of a novel naphthoquinone containing a modified anthracycline Ring System. **R. Al-Refai, S. Shehata, J.C. Dicesare, R. Sheaff**
- CHED 562.** Site selective Pd-catalyzed intramolecular cyclization of oxygen nucleophiles. **D. Thach, S.J. Thompson**
- CHED 563.** Comparison of nutrient deprived cellular behavior in transformed and untransformed cells. **P.J. Gasser, R. Sheaff**
- CHED 564.** Photographic evidence of reactions in organic chemistry: The formation of *trans*-diols from cyclohexene and meta-chloroperbenzoic acid. **A.O. Diouf, D. Trana, J.M. Quirke**
- CHED 565.** Carbonic anhydrase as a model for matrix metalloproteinase inhibition. **D. DeGenova, R. Venna, R. Patel, A. Pionski, A. Forchione, W.A. Richert, S. Al-Abdul-Wahid, D.L. Tierney**
- CHED 566.** Completing a green chemistry laboratory manual for general chemistry. **K. Wood, S. Henrie**
- CHED 567.** Utilization of polymeric quaternary ammonium salts-clay composite in triphase catalysis. **A.P. Sneed, C. Chapple, N. Shabestary**
- CHED 568.** Efficiency of synthetic pyrazoline derivatives on inhibiting *Entamoeba histolytica* growth as novel treatment against amebiasis. **K. Schindlweg-Franca, J. Tashjian, H. Kumar, S. McDonough, A. Espinosa, L. Rossi**
- CHED 569.** Role of *GRK4* in bladder exstrophy-epispadias complex. **M. Ielmini, N. Wilken, D.J. Lamb, C. Jorgez**
- CHED 570.** Impact of nanoparticles on bacterial community. **J. Ha, A. Bally**
- CHED 571.** Hands-on activity incorporating the threefold representation on the limiting reactant concept. **A.M. Gonzalez-Sanchez, E.L. Ortiz-Nieves, Z. Medina**
- CHED 572.** Probing the question-order effect on chemistry concept inventories. **M. Undersander, T.J. Lund, M.N. Stains**
- CHED 573.** Impact of an intensive workshop on STEM faculty's fidelity of implementation of peer instruction. **K. Rosploch, M. Pilarz, M.N. Stains**
- CHED 574.** Elimination reaction of tropic acid as a simple example of an E1cb reaction. **D. Li, E.D. Helms, K. Best**
- CHED 575.** Chemistry teaching laboratories: What is the point? **A. Neybert, J. Barbera**
- CHED 576.** Effect of *Azadirachta indica* tree in the CYP450 system of chinese hamster ovarian cells. **N.I. Negrón, L. Santos**
- CHED 577.** Dioxygen activation by mononuclear non-heme iron oxygenases and the corresponding model complexes. **S. Kingston, L. Cunningham, J.P. Caradonna**
- CHED 578.** Developing and evaluating a collaborative learning environment in analytical chemistry. **A. Palmer, K.A. Pettigrew**
- CHED 579.** Holistic trace analysis: Development of an upper-level chemistry experience. **D. Hughes, C.D. Hatch**
- CHED 580.** Paper microfluidic method to quantify taurine in urine samples: A college-level introductory chemistry experiment. **L. Nguyen, O. Baawuah, S. Gamagedara**
- CHED 581.** Epoxyeicosatrienoic acid analog mitigates kidney injury in experimental radiation nephropathy. **B. Vo, A. Khan, J. Neckar, A. Sharma, K. Molter, J. Imig**
- CHED 582.** Toward a comprehensive integration of calorimetry across the curriculum. **O. Summers, B. Bruske, H. Sklenicka**
- CHED 583.** Documenting collective activity in a large scale introductory chemistry class. **J.D. Byers, C.L. Stanford, R.S. Cole**
- CHED 584.** Synthesis of highly functionalized nitrogen containing monoadducts via copper catalyzed atom transfer radical addition (ATRA). **J. Martin, G. Pros, T. Pintauer**
- CHED 585.** Targeting Glutaminolysis to selectively kill cancer cells with deregulated p27. **J.A. Sabo, M.R. Ferguson, P.J. Gasser, R. Sheaff**
- CHED 586.** Impact of cost on chemistry laboratory teaching practices. **R.A. Livermore, S.B. Boesdorfer**
- CHED 587.** Developing a redox themed assessment instrument using the three levels of representation. **S. Santos, A.M. Gonzalez-Sanchez, E.L. Ortiz-Nieves, Z. Medina**
- CHED 588.** Use of organic base to restore catalytic activity of [Cu(Me₆TREN)Cl][Cl] in Atom Transfer Radical Addition (ATRA) in the presence of ascorbic acid as a reducing agent. **M.C. Wasson, G. Pros, A. Kaur, T. Pintauer**
- CHED 589.** Investigation of HOBS methodology in nucleic acid NMR studies. **J.M. McKenna, J.A. Parkinson**
- CHED 590.** Enantiomeric interactions of aminoacids adsorbed in zeolites: An investigation, using solid-state NMR, thermogravimetry (TGA) and differential scanning calorimetry (DSC). **L. Topchyuan, S. Krishnan, S. Ira, M. Garcia, N. Sankari, M. Ramirez, A. Martinez, D. Cizmeciyan, R. Senter**
- CHED 591.** Synthesis of pyridone-based ligands for homogenous hydrogenation iron-based catalysts. **H.K. Caddes, S.L. Willis**
- CHED 592.** Adapting a set of organic chemistry experiments for delayed analysis time. **S.C. Kenea, N.J. Beyer**
- CHED 593.** Preparation of NiFe supported catalysts for hydrotreatment. **C. Peterson, E. Marceau, A. Lamic, G. Laugel**
- CHED 594.** Near infrared spectroscopy chemical imaging for the determination of component segregation. **T. Vélez-Burgos, E. Hernández, R.J. Romanach**
- CHED 595.** Preparing and screening brominated phenols: An organic laboratory experience. **J. Bietsch, T. McCoy, A.A. Yeagley**
- CHED 596.** Applying a greener approach to the Grignard reaction. **A.E. Burgos-Aviles, I. Montes Gonzalez**
- CHED 597.** Total synthesis of a calixarene cage. **A. Ferreri, E. Wade**
- CHED 598.** Human carbonyl reductase as target for alleviating anthracycline cardiotoxicity: Understanding small molecule binding by human carbonyl reductase. **L. Brown, H. Charlier**
- CHED 599.** Comparison of metacognitive abilities of introductory chemistry students. **J. Johnson, A.B. Mahoney, M. Nagel**
- CHED 600.** Biochemical analysis of G-quadruplex secondary structures in CDK5R2 mRNA and of their role in fragile X syndrome. **C.M. Gaetano, M. Mihailescu**
- CHED 601.** Theoretical description of chemical shift anisotropy. **K. Phillips, R. Iulucci**
- CHED 602.** Designing catalytic N-heterocyclic carbene complexes for enantioselective allylic oxidation. **R.J. Morrison, P.J. Lombardi**
- CHED 603.** Development of a selection marker for automated genome construction. **E. Aponte, J. Norville, G.M. Church**
- CHED 604.** Expression of major hominoid seminal proteins in a mammalian cell culture system. **M. Hockman, J. Vill, T. Pollock, A. Zielen, M. Jensen-Seaman**
- CHED 605.** Adsorption of thioethers on Au(111) using scanning tunneling microscopy. **R. Miller, A. Whitney, D. Del Sesto**
- CHED 606.** Heavy metal isotope analysis of historic skeletal remains using ICP-MS. **C. Klesner, N. Little, D. Owsley**

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

- CHED 607.** Detection of the *cp4 epsps* gene in maize line NK603 and comparison of related protein structures: An advanced undergraduate experiment. **N. Swope**, P.J. Fryogle, T. Sivy
- CHED 608.** Investigating the synthesis and role in molecule-based-magnets of bis(4-pyridyl) acetylene. **T. West**, A.C. McConnell
- CHED 609.** Laboratory course as journal house: An advanced organic chemistry course incorporating writing/reviewing scientific manuscripts and green chemistry. **R. Beltman**, T.M. Dierker, A.G. Fei, W.K. Fuchs, T.D. Gornall, A.M. Katsimpalis, M.J. Ponkowski, R. Wong, **M.J. Mio**
- CHED 610.** Electrocatalytic activity of metal-centered porphyrin thin films. **C. Myers**, W.M. Ames
- CHED 611.** Versatile lecture demonstration and laboratory exercise illustrating steric hindrance, electron induction, and catalyst nucleophilicity effects on catalyzed ester hydrolysis. **K.R. Smith**, D.J. Clague, D.J. Alexander, S.C. Butler, **R.N. Mason**
- CHED 612.** Lipid raft TNF- α pathway analysis of cytochrome C with methylparaben and UVB treatment. **R.S. Wood**, R. Stahl, K.S. George Parsons
- CHED 613.** Investigation of student understanding in spectroscopy labs. **D.P. Jacinto**, L.T. Tien, D. Rickey, M.A. Teichert
- CHED 614.** Novel regulation of p27 by transglutaminase. **A. Greene**, L. Zhang, R. Patel, W. Crawford, R. Sheaff
- CHED 615.** Development of histone deacetylase inhibitors. **R. Kidney**, L. Ma, T.D. Do, S. Szabolcs, S.F. Paula
- CHED 616.** Progress toward synthesis of a novel trifluoromethyl substituted aureone as a potential cyclooxygenase-2 inhibitor. **J. DePhillips**, M. Polk, C. Mills, A. Zuber
- CHED 617.** Modification of the p27 tumor suppressor by the transglutaminase enzyme. **W. Crawford**, L. Zhang, A. Greene, R. Patel, R. Sheaff
- CHED 618.** Analysis of organic compounds isolated from particulate matter produced by biodiesel and diesel fuel. **N. Brown**, M. Cavacas, N. Travis, J.R. Kraly
- CHED 619.** Synthetic studies toward *Corynanthe* indole alkaloid derivatives. **S. Petritis**, E.K. Leggans
- CHED 620.** Free radical effect on the quantum yield of silicon nanoparticles. **R. Ellison**, C. Radlinger, A. Goforth
- CHED 621.** Determining the rate of oxidation of promethazine to its sulfoxide and sulfone in atmospheric O₂ using HPLC-MS and UV-VIS spectrophotometric analysis. **C.M. Baker**, K.N. Beltridge, I. Webb, G. Guiterres, P. Chairsi, **A.L. Kesler**, S. Bedi, S. Christensen, K. Oakes, S. Bremer, R.V. Valcarce, P.J. Iles, M. Alvarez, L.D. Giddings, N.R. Bastian
- CHED 622.** Detection of organic pollutants using EVA with GC-MS and AFM analysis. **T. Schreyer**, C. Carr, A. Timmerman, C. Peak, K.N. Beltridge, I. Webb, M. Vanweerd, R.V. Valcarce, S.T. Lindsey, P.J. Iles, M. Alvarez, N.R. Bastian, L.D. Giddings
- CHED 623.** Analysis of University of Utah Fine Arts Museum Egyptian sarcophagus by scanning electron microscopy. **J. Van Wagoner**, R. Haynie, L. Kelly, S.T. Lindsey, S. Bremer, R.V. Valcarce, P.J. Iles, L.D. Giddings, N.R. Bastian, M. Alvarez
- CHED 624.** Determining source of discoloration in renaissance fresco using infrared spectrophotometry. **J. Van Wagoner**, R. Haynie, L. Kelly, S. Bremer, S.T. Lindsey, R.V. Valcarce, P.J. Iles, L.D. Giddings, N.R. Bastian, M. Alvarez
- CHED 625.** 1,3-Dipolar cycloaddition reaction. **M. Muni**, S.R. Hussaini
- CHED 626.** Solvation equilibria of proximally-substituted copper bis-phenanthroline derivatives. **N.A. Arnista**, S.P. Watton
- CHED 627.** Aromatization of fragrant monoterpenes via palladium-catalyzed dehydrogenation. **T.S. Hill**, A.M. Hartzel
- CHED 628.** Optimization of algae-derived biodiesel for use in undergraduate chemistry laboratories. **M.R. Barron**, C.S. Harper, K.L. Braun
- CHED 629.** Forensic analysis of commercial color and black inkjet printer inks by micellar electrokinetic chromatography. **C.S. Harper**, K.L. Braun
- CHED 630.** Enzymatic reduction of a ketone for a college-level organic chemistry course using alcohol dehydrogenase. **L. Zhao**, P.M. Joyner
- CHED 631.** Synthesis of the SRS and SSR isomers of lentiginosine from D-glucopyranoside and D-galactopyranoside. **D.C. Fager**, L.J. Liotta
- CHED 632.** Team-based assessment of introductory organic chemistry lecture. **R. Tieu**, J. Soria
- CHED 633.** Team-based assessment of a two-semester introductory organic chemistry laboratory course. **V.F. Vartabedian**, J. Soria
- CHED 634.** Initial investigation of pyrrolizidine alkaloids in *Pscidium decompositum*. **J. Burklund**, K. Hamann, D. Morales, R.B. Kelley
- CHED 635.** Cost effective ion selective electrodes from metal-azo complexes. **W.A. Nanney**, B.L. Belmont
- CHED 636.** Burning truth about sunscreens: Zinc oxide nanoparticle growth kinetics. **V. Smith**, P.A. Brietic
- CHED 637.** Small angle X-ray scattering (SAXS) of β_2 -glycoprotein 1 suggests an alternative mechanism for antibody interaction in antiphospholipid syndrome. **A. McLaughlin**, N. Pozzi, E. Di Cera
- CHED 638.** Dynamics study of the resorcin[4] arene supramolecular assembly. **P.B. Calio**, J. Harvey, W. Thompson
- CHED 639.** Synthesis and luminescence studies of rhenium(I) tricarbonyl complexes using LabQuest 2. **N.V. Vecchio**, M.O. Odago
- CHED 640.** Attachment inhibition of invasive species. **K. Marcus**, C. McKellar, R. Pearce, S. Beck, R. Del Sesto
- CHED 641.** Writing exam questions that elicit evidence of process skills. **H. Moon**, J.A. Schmidt, R.S. Cole
- CHED 642.** Understanding the cognitive load generated by constructing Lewis structures. **A. Coleman**, R. Balok, J.M. Tiettmeyer, T. Gamp, P. Duffy, K. Mazzarone, N.P. Grove
- CHED 643.** Synthesis of 2'-phenoxy-4-hydroxyacetophenone. **S. Ortiz-Piccard**, J. Peterson, T. Field, R.S. Givens
- CHED 644.** Longitudinal study of the effects of a professional development program on the content knowledge and teaching practices of middle and high school science teachers. **H.A. Hayes**, J.S. Corrales, R. Lewis, E.E. Gonzalez, B.D. McCormick, A.R. Chaudhuri
- CHED 645.** Southern Utah University general chemistry case study: Identification of curriculum obstacles. **K.B. Weaver**, R. Stewart, S. MacFarlane, A.C. McConnell
- CHED 646.** Research on surface modification of zinc oxide nanoparticles and incorporation into fibers. **T. DiPasquale**, J.E. Whitten, D.M. Steeves, J. Soares
- CHED 647.** Newly established documentation and imaging system detecting DNA hybridization serves as a potential point of care device to further distinguish genetic susceptibility to diseases. **D.W. Capps**, J.R. Kenneson, R.L. Moore
- CHED 648.** Analytical techniques in environmental chemistry: Detection and quantification of common herbicides in surface water. **T. McCall**, E.M. Marzluff
- CHED 649.** Determination of mercury levels in living and nonliving systems of southwest Arkansas. **D. Campbell**, J. Lowe, H. Wayland, D. Bateman
- CHED 650.** Physiological effects of massage therapy in college students and the elderly. **H.A. Wayland**, C. Dickson, D. Bateman
- CHED 651.** Continued study in Facebook™ as a collaborative learning platform for sophomore organic chemistry students. **S.F. Hornbuckle**, **J. Lawrence**
- CHED 652.** Isolation and characteristics of flavonoids from ash tree leaves. **A.M. Gallegos**, E.E. Wilson, M.P. Smith, S.T. Mirza, A.V. Daspat, B.A. Clement
- CHED 653.** Kinetics of the reduction of nitrobenzene using hydrazine hydrate and cobalt (II) sulfide. **D. Cedillo**, J. Garcia, T. Treviño, J.G. Parsons, J. Gutierrez-Gonzales
- CHED 654.** Biophysical analysis of *CDK5R2* DNA secondary structures. **K. Bandi**
- CHED 655.** Histone deacetylase (HDAC) inhibitors containing thioamide: Synthesis and biological evaluation. **A.J. Onate**, S. Szabolcs, E. Merino, S.F. Paula, L. Ma
- CHED 656.** Synthesis of (2R,3S,4S)-2-(hydroxymethyl)pyrrolidine-3,4-diol from α -methyl-D-galactopyranoside. **M.J. Smith**, L.J. Liotta
- CHED 657.** Withdrawn.
- CHED 658.** Synthesis and characterization of sol-gel monoliths as glucose biosensors. **S. Moore**, C.H. Lisse
- CHED 659.** Synthesis and characterization of potential TNF hairpin formation inhibitors. **S. Crowley**, M. Welch
- CHED 660.** Effect of pH in sulfactoperoxidase formation. **J. Feng Baez**, B. Rios-González, J. Lopez Garriga
- CHED 661.** Investigating the effects of steric bulk on γ -silyl bridging by variation of the γ -electron-donating and α -substituent. **L. Macary**, J. Hauck, L.J. Tilley
- CHED 662.** Synthesis of 9-fluoro-9H-fluorene-1-ol. **D. Memon**, R.E. Rosenberg, R. Ferrill, J. Johnson, J. Bier
- CHED 663.** Synthesis of polyhydroxylated pyrrolidine from a D-glucose derivative. **A. Hayney**, L.J. Liotta
- CHED 664.** Synthesis of lentiginosine form D-glucose. **K. McAndrews**, L.J. Liotta
- CHED 665.** Computational investigation of the surface tension of supercooled water. **T.R. Rogers**, K. Leong, F. Wang
- CHED 666.** DFT analysis of copper-based chemotherapeutics. **T.M. Kolb**, J.S. Anderson, L.A. Tyler
- CHED 667.** Peptide sequencing using gas-phase peptide carbocations. **A. Plaviak**, M.J. Van Stipdonk
- CHED 668.** Maximizing the extraction efficiency of arsenic in solid matrices followed by graphite furnace atomic absorption spectrometric analysis. **M. Wakeman**, C.D. King
- CHED 669.** Curriculum development for BSU's outreach program geared to spark interest in chemistry. **B. Morgan**, C.D. King
- CHED 670.** Microwave synthesized succinimides purified by flash chromatography. **T.F. Guetzloff**, **B. Dudding**, M. Fultz
- CHED 671.** Transesterification of hypophosphorous esters: Elucidating the synthetic scheme of phosphorous-based surfactants. **S. Deprele**, **A.L. Perez**, **N. Neris**, **C. Alvarez**
- CHED 672.** Accessing vinyl fluoroalkyl-substituted cyclopropanes from homoallyl mesylates via a destabilized cation-mediated electron cascade. **A.E. MacInnis**, L.J. Tilley, N.E. Leadbeater, E.R. Carnaghan, M. Doherty, D.C. Fager, J. Hauck, C.B. Kelly, M.A. Mercadante
- CHED 673.** Chemistry laboratory safety: Misconceptions among first- and second-semester general chemistry students. **J. Melvin**, W.E. Schatzberg
- CHED 674.** Chemical and biochemical stability of guanine lysine cross-links formed by guanine oxidation. **J. Mincitar**, **D. Esparza**, **N. Tran**, **A. Ramos**
- Section A**
Colorado Convention Center
Halls C/D
- Undergraduate Research Offices**
Computational Chemistry
Cosponsored by COMP and SOCED
N. Di Fabio, *Organizer*
12:00 - 2:00
- CHED 675.** Comparisons of Synaptotagmin 1 and Synaptotagmin 7 C2A domains in membrane associations by molecular dynamic simulations. **N.L. Chon**, J.A. Henderson, J.D. Knight, H. Lin
- CHED 676.** Computational modeling of STAT3 SH2 domain inhibition. **C.T. Williams**, P. Daka, E.E. Csatory, H. Wang, R.C. Page
- CHED 677.** Computational modeling of temporary anion states in the field of dipole or quadrupole moment. **E.M. Tharnish**, **L. Williams**, M.F. Falcetta
- CHED 678.** Computational modeling of resonant vibrational excitation of CO by electron impact. **L. Williams**, E.M. Tharnish, P.E. Linn, M.C. Fair, M.F. Falcetta
- CHED 679.** Cyclic voltammetric and computational structure-electrochemistry relationship studies of the reduction of a series of 9,10-antraquinone derivatives. **N. Fox**, T.W. Johnson
- CHED 680.** Effect of unequal strand length on DNA hybridization in a model microarray system via Monte Carlo simulation. **S. Cooper**, J.M. Stubbs
- CHED 681.** Journey of 4-HNE: How biochemistry became computational. **A.K. LaPidus**, C.M. Byron
- CHED 682.** Predicting the function of structural genomics proteins of unknown function in the cratonase superfamily. **S.R. Little**, C.L. Mills, P.J. Beuning, M.J. Ondrechen
- CHED 683.** Conformational sampling of glucose oxidase for bio-fuel cell applications. **E. Gomez**, T. Tran, N. Tran, D. Chakravorty
- CHED 684.** Role of glycosylation in protein structure: A bioinformatics-based computational study. **J. Rogers**, S. McHugh, Y. Lin
- CHED 685.** Effect of motor protein binding on microtubule depolymerization. **D.G. Witte**, N. Yu, R. Dima
- CHED 686.** Solid-state NMR chemical shift peak matching of geometry optimized organic crystals by computational methods. **S. Upadhyay**, M.N. Sreec, J.D. Madura, R. Iulucci
- CHED 687.** Theoretical study of the factors that contribute to the conformational energy of six-membered rings. **M. Abdulsalam**, R. Ballili, R. Baello, C. Brutofsky, S. Suresh, M.L. Kasner, R. Booth
- CHED 688.** Computational study of the contributions to the relative stability of the α and β conformers of D-glucopyranose. **R. Ballili**, M. Abdulsalam, R. Baello, R. Booth, S. Suresh, M.L. Kasner
- CHED 689.** Solid-phase heats of formation of energetic compounds using computational methods. **D. White**, M. Eloff
- CHED 690.** Computational studies of the hyperpolarizability of halogenated saccharins and their anions and salts. **M.B. McDaniel**, D.A. Clabo, Jr.
- CHED 691.** Electronic structure calculations of Li₂-II-IV-VI diamond-like semiconductors. **J. Worst**, A.J. Glaid, M.N. Sreec, J.D. Madura, J.A. Atken, J. MacNeil
- CHED 692.** Coarse-grained modeling of reverse micelles. **M. Rea**, A.T. Moser
- CHED 693.** Computational study of the visible spectrum of curcumin's protonation states. **P. Braegelmann**, J.D. Alia
- CHED 694.** In silico insight into mechanism for the formation of C8 products from the reactions of guanine with substituted aniline. **J. Bautista**, S. Shrestha, A.S. Dutton, A.G. Leach
- CHED 695.** Computationally simulating the metabolic enantiospecificity of CYP2C9 using molecular dynamics. **P. Onyuru**, G.P. Miller, M.D. Perry

- CHED 696.** Elbow room: How surfactant proportions modify interfacial properties. **J.A. Palumbo, K.E. Johnson**
- CHED 697.** Computational docking to analyze substrate metabolism in CYP2E1. **M. Rogers, G.P. Miller, M.D. Perry**
- CHED 698.** Computational investigations on ligand isomorph selectivity in the liver X receptors. **M. Ndukwe, B. Theard, K. Riley**
- CHED 699.** Studies of factors affecting the reaction mechanism of formation of the levoglucosan. **L. Aebersold, T. Daeschlein, J. Henry, B.N. Leja, D. Wang, A. Seitz, J. Song**
- CHED 700.** Mechanistic insights into the alkylation reactions of quinone methide precursors: Studies towards the realkylation of aged acetylcholinesterase. **R.J. Yoder, T. Blanton, K. Fitzpatrick, A.J. Franjesevic, S. Higgins, C. Callam, C.M. Hadad**
- CHED 701.** Unpaired electron density in retinal model compounds. **T. Vaid, E.D. Glendening**
- CHED 702.** Computational study on the formation of hexamethylene triperoxide diamine. **A. Sindt, J.N. Woodford**
- CHED 703.** ARGOS: A rigid geometry optimizer for supramolecular complexes. **R. Meyerson, S.E. Wheeler**
- CHED 704.** Group 13 chiral Lewis acid stereoselective control of enal Diels-Alder reactions. **A.N. Ahmed, B. Vernier, A. Kelly, J. Rohde, J.D. Evansack**
- CHED 705.** Solvation effects in bimolecular Diels Alder cycloaddition of cyclopentadiene: A tool for benchmarking expected errors in more sophisticated Diels Alder reactions. **A. Kelly, B. Vernier, A.N. Ahmed, J. Rohde, J.D. Evansack**
- CHED 706.** Computational modeling of fluorescent probes to understand how lithium treats manic depression. **S. Claridge, D.L. Nutbrown**
- CHED 707.** Using the relativistic particle in a box to model conjugated dyes. **B. Barrett, J.E. Lacy**
- CHED 708.** Using molecular dynamics to computationally simulate metabolic enantiospecificity of CYP2C9. **N.D. Hall, G.P. Miller, M.D. Perry**
- CHED 709.** Folding of meta-poly-phenylene ethynylene. **K. Hefel, A. Moser**
- CHED 710.** Further computational investigation on the conformationally-restricted allenyl cope rearrangement of *Syn-7*-allenylbornene. **M.A. Lyon, J.A. Duncan, C.S. Jamieson**
- CHED 711.** Possible explanation for the formation of trans-Whiskey lactone: A computational approach. **T. Le, E. Simanek, B.G. Janesko**
- CHED 712.** Investigation of biological anion effects on phospholipid structure and oxygen diffusion free energy. **T. Ricard, S.C. Pias**
- CHED 713.** First principle calculations of optical properties of platinum(II) diimine complexes. **L. Lystrom, S. Kilina, W. Sun**
- CHED 714.** Conformational distribution of cysteine and selenocysteine dyads in biological redox processes. **L.M. Froehle, S. Vyas**
- Section A**
Colorado Convention Center
Halls C/D
- Undergraduate Research Posters**
- Environmental Chemistry**
Cosponsored by ENVR and SOCED
- N. Di Fabio, Organizer**
12:00 - 2:00
- CHED 715.** Evaluating oil dispersant systems via emulsion stability and optical microscopy. **W. Fagan, W. Ervin, Y. Zhang, B. Gikonyo, M. Tsianou**
- CHED 716.** Core shell vs. alloy iron/nickel nanoparticles for water treatment. **M. Voecks, K. Estoque, L.F. Greenlee**
- CHED 717.** Orange G dye degradation using iron-nickel nanoparticles: Effect of iron to nickel ratio, concentration and pH. **K. Estoque, M. Voecks, L.F. Greenlee**
- CHED 718.** Electrochemical characterization of iron nanoparticle-clay interaction for groundwater remediation. **K. Roberts, B.A. Balko**
- CHED 719.** Analysis of mineral content in MWSU parking lot runoff water using PXRF, FAA, and EDTA titration. **J. Mitchell, S.L. Hiley**
- CHED 720.** Drugged wildlife: The potential impacts of environmental endocrine disruptors on reproductive development. **M.Y. Kramer, N.A. McNabb, L.J. Guillelte, S. Kohno**
- CHED 721.** Monitoring the long term effects of fracturing in Western Pennsylvania, Butler County: How long is long enough? **R.L. McLaughlin, C. Kiley, N. Rutter**
- CHED 722.** Development of 2-component surrogate mixtures for alcohol-to-jet fuel. **M.H. Jones, D.J. Luning Prak**
- CHED 723.** Analytical identification of polycyclic aromatic hydrocarbons: The bio-monitoring of Cyprus trees in Los Angeles. **A. Kerl, S. Castillo, Y. Torres, S. Depréle**
- CHED 724.** Potential heavy metal water remediation using 5-formylfuran-2-sulfonic acid thiosemicarbazone (DIFANEX) chelating resins. **A.L. Werlein, A.J. Crook, E.P. Hoy, D.D. Ensor, E.C. Lisic**
- CHED 725.** Novel method for the extraction of lead ions from bulk water supplies using chelation chemistry. **K.M. Sheetz, K.A. Mies**
- CHED 726.** Metal-sequestration from water using a polysulfide synthesized from sulfur and limonene. **A.M. Evans, M.P. Crockett, J.M. Chalker**
- CHED 727.** Determination of total mercury in the top three consumed seafood products of the United States. **A.L. Kramer, C.N. Hill, S. Aloisio**
- CHED 728.** Reactions of alcohol amines with atmospheric oxidants N_2O_5 , H_2O_2 and O_3 analyzed through a Particle-into-Liquid Sampler coupled to dual ion chromatographs. **R. Jauregui**
- CHED 729.** Analysis of the open limestone channel at the Swank 13 abandoned coal mine. **J. Krug, R.C. Krupa, D. Mosier, C.J. Weyant, E.P. Zovinka**
- CHED 730.** Degradation of the layer of calcium carbonate ($CaCO_3$) on the *Pyrodinium bahamense* (dinoflagellates) from bioluminescent lagoons in Puerto Rico. **A. Rodriguez-Velazquez, K.D. Ortiz, L. Delgado, S. Delgado**
- CHED 731.** Separation of oil contaminants from oil-in-water emulsions using nylon 6,6 non-woven fabric filters. **K.A. Murrell, E.S. Carter, F.D. Hileman, A.E. Orttega**
- CHED 732.** Synthesis of water filtration composites for use against microorganisms and heavy metal in water. **M.M. Samson, K.M. Metz**
- CHED 733.** Bioremediation of nickel and cobalt by *Bacopa monnieri*. **P.C. Vera-Santiago, Z. Serrano-Rivera, J. Arbelo-García, M. Ramos-Fontán**
- CHED 734.** Influence of cation charge density, ionic strength, and pH on NOM particle size distributions in aqueous solution. **H. Argersinger, G.M. Bowers**
- CHED 735.** Three years of full scale testing an enhanced bioswale. **N.P. Lesner, W. Kuzmishin, H. Yang, P. Edmiston**
- CHED 736.** Catalysis in chromic acid oxidations: A co-oxidation model for the detoxification of hexavalent chromium in water. **S. Mahapatro, A.I. Lujan**
- CHED 737.** Studying reactivity and leaving group effects in aryl chloroformate esters. **A. Bilbrough, D. Williams, M.J. D'Souza**
- CHED 738.** Correlation analyses of solvent reactions of 2-fluoroethyl chloroformate and 2-benzoyloxyethyl chloroformate. **V.M. DeBarros, M.J. D'Souza**
- CHED 739.** Confirming the use of phenyl chloroformate as an appropriate addition-elimination standard in LFER analyses. **J.K. Deol, M.J. D'Souza**
- CHED 740.** Integrins and multiple-antibiotic resistant bacteria in Minnesota surface waters. **K.H. Wammer, E.W. Beck, C. Haines, T. LaPara**
- CHED 741.** Viability of ozonation as a water treatment method for the elimination of the antibiotic roxithromycin. **C.H. Fuerste, D.C. Harnes, D.R. Stoll, K.H. Wammer**
- CHED 742.** Aqueous photochemistry of altrenogest. **K.C. Anderson, K.H. Wammer**
- CHED 743.** Analysis of San Antonio River water for metals using inductively coupled plasma-mass spectrometry. **H.A. Hayes, J.S. Corrales, P.P. Gonzalez, A.R. Chaudhuri, B.D. McCormick, E.E. Gonzalez**
- CHED 744.** pH profile determination of the cation exchange capacity of heavy metals from estuarine sediment and its correlation with outer shell content of benthic organism *Mercenaria mercenaria*. **J.M. West, S.K. O'Shea**
- CHED 745.** Characterization of metal cation binding to pyridine-based compounds in aqueous solution. **J. Moose, S. Tajc**
- CHED 746.** Analysis of heavy metal leaching from motor oil into water. **C.R. Stear, C.L. Fish**
- CHED 747.** Photochemical reactive oxygen species production by petroleum water accommodated fractions. **A.M. West, J. Haney, P.P. Vaughan**
- CHED 748.** Did the Bastrop wildfire affect the phosphorus content in the soil? **M. Abu-Esba, H.G. Altmeier**
- CHED 749.** Cd, Ni, Zn and Cu concentrations in fish muscles collected from sites along the Ashley River. **M. Mirano, B. Adair**
- CHED 750.** Algal toxin dynamics in a eutrophic lake and indicators of toxins in raw drinking water. **K. Rude, C. Weirich, S. Bartlett, M. Seaman, J. Platt, T. Miller**
- CHED 751.** Effects of woolly adelgid induced hemlock productivity decline on soil nutrient content. **B. Redder, J. Balnis, Z. Balogh-Brunstad**
- CHED 752.** Analysis of heavy metals in *Lutjanus griseus* and *Lutjanus campechanus* at the natural reserve "La Parguera", Puerto Rico. **N.M. Lopez Pena, R. Tremont**
- CHED 753.** Detection of precursors to methamphetamine in city sewers lines. **C. Craine, M.P. Butner, T.H. Boles**
- CHED 754.** Optimization of fly ash nanogeo-polymer and its application in pervious concrete for bioremediation of fecal coliform-containing water. **V. Hwang, E. Montalvo**
- CHED 755.** Extracting metal (II) cations from aqueous solution using dipicolinic acid. **M. Porter, A. Richardson, S.G. Tajc**
- CHED 756.** Pesticide analysis in Southeast Michigan waters by gas chromatography-mass spectrometry. **C.C. Conrad, P.M. Dine, D.M. Dreffs, B.H. Keith, S. Zoma, T.Y. Zurawski, R. Dutta, K.R. Evans, E.S. Roberts-Kirchoff**
- CHED 757.** Study of analyte recovery using headspace solid-phase microextraction. **J. Tillman, W. Weckel-Dahman, F.M. Durnivant**
- CHED 758.** Scanning electron microscope analysis of Columbia River, Chesapeake Bay, Lake Hartwell, and Mississippi River sediment suspensions. **X. Yi, J. Morgan, F.M. Durnivant**
- CHED 759.** Quantification of epoxides from their carbamate derivatives: Environmental applications. **G. Amon, W. McCue, C.M. Strollo**
- CHED 760.** Detection of amphetamine type substances in sewers using Polar Organic Chemical Integrative Samplers. **M.P. Butner, C. Craine, T.H. Boles**
- CHED 761.** *Mercenaria mercenaria* a potential bioindicator of heavy metal releases into Narragansett Bay, RI. **K.D. Audette, S.K. O'Shea**
- CHED 762.** Study of the effects of two PPCPs on algal growth. **T. Meece, T. Knight**
- CHED 763.** Exploring the interactions between citrate-saturated silver nanoparticles and humic acid via fluorescence quenching. **L.A. Warning, B.D. Anderson**
- CHED 764.** Investigating the formation of thioarsenic species under sulfidic conditions. **J. Loving, V. Stucker, J.F. Ranville**
- CHED 765.** Study on UV-Vis spectroscopic characteristics of soil humic substances. **J.L. Ragon, H. Zhang**
- CHED 766.** Rhodium catalyzed hydrodehalogenation of fluoroarenes in mild conditions. **A.M. Luke, A.A. Peterson**
- CHED 767.** Removal of phosphate from aqueous media by adsorption onto humic acid-coated magnetite. **N. Price, M. Rashid, K. OShea**
- CHED 768.** Use of CYCLAM and other tetraamines to probe the mechanism of influence of surfaces on ligand exchange. **S.J. Hinkle, N.E. Boland**
- CHED 769.** Studying the reactions of alcohol amines with atmospheric oxidants. **J. Dulla, R. Jauregui, D.J. Price, K. Purvis-Roberts, D. Cocker**
- CHED 770.** Effects of "real world" biodiesel and petroleum diesel combustion on PM composition and production of ROS in BEAS-2B cells. **N. Martin, A. Bosco, T. Pratt, N. Travis**
- CHED 771.** Impact of "real world" biodiesel and petroleum diesel combustion on particulate matter composition and oxidative potential. **P. Kelley, R. Klaski, N. Martin, N. Travis**
- CHED 772.** Enhancing the chemical mixture methodology: Revising the health code number assignments of hazardous chemicals to account for varying intensities of respiratory irritation. **J. Jablonski, J. Yao, X. Yu, C. Glantz**
- CHED 773.** Chemical analysis in the *Eryngium foetidum* L. **N.N. Olmeda, S.A. Maldonado, R. Tremont**
- CHED 774.** Static quenching of acridine yellow G and norfloxacin by humic acid. **R. Ferrie, B.D. Anderson**
- CHED 775.** Correlation of nitrogen dioxide and ozone gas concentrations between Milwaukee and Chicago. **T. Antoniewicz, T. Robers, M.D. Schuder**
- CHED 776.** Extraction of barium from aqueous solution using pyridine based small molecules. **J. Merchant, S.G. Tajc**
- CHED 777.** Design and characterization of a pulsed laser cavity ring-down spectrometer for use in the measurement of aerosol optical properties. **J.C. Castillo, J.M. Pittman, L.W. Bevil, K.S. Dooley**
- CHED 778.** Size characterization and metals analysis of particulate matter generated by candle burning. **L.W. Bevil, K.S. Dooley**
- CHED 779.** Quantitative determination of antidepressants in wastewater effluents and biosolids. **J. Brotman, C. Moffett, K. Shiovone, M.M. Schultz**
- CHED 780.** Closing the gap on secondary organic aerosol formation: Oligomerization of glyoxal. **L.E. Rusch, C.M. Strollo**

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.

- CHED 781.** Submarine groundwater discharge as a potential hidden pathway for eelgrass decline in San Juan county. **E.L. Johnson**, J. Beets, J. Dixon, R.A. Lyons, P. Swarzenski, S. Wyllie-Echeverria
- CHED 782.** Arsenic analysis and speciation of water samples from Chihuahua México, by HG-CT-AAS. **V. Medina**, Y. Rodriguez, D. Acosta, L. Ballinas-Casarrubias
- CHED 783.** Photodegradation of organic dyes using quantum dots of Cd(Se,S) in aqueous solutions. **G. Rivera Rodriguez**, O. Perales-Perez, F.R. Roman, S. Bailon-Ruiz, L. Alamo-Nole
- CHED 784.** Photodegradation of antibiotics in aqueous solutions using quantum dots of Cd(Se,S). **I.N. Leon Feliciano**, O. Perales-Perez, F.R. Roman, S. Bailon-Ruiz, L. Alamo-Nole
- CHED 785.** Cadmium phytoremediation of in vitro culture with micro-propagated clones of *Spermacoce assurgens*. **B.L. Vargas Perez**, L. Rodriguez
- CHED 786.** Profile of metal bioaccumulation in selected invertebrates from the eastern and western shores of the Susquehanna River near Hummels Wharf Pennsylvania. **A. Pritzlaff**, C.P. Hallen, C. Venn

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Geochemistry

Cosponsored by GEOC and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

- CHED 787.** Selective synthesis of ribose via the formose reaction under prebiotic conditions. **P.S. Donmoyer**, A.L. Marsh
- CHED 788.** Impact of methanotrophy on methane gas hydrate dissolution rates. **M. von der Lippe**, R.K. Larsen, L. Lapham
- CHED 789.** Formic acid uptake on montmorillonite clay: An FTIR study. **L.A. Hancock**, R.M. Weingold, C.D. Hatch
- CHED 790.** Exploring the mechanism for iron uptake by phytoplankton: A biomarker study. **M.J. Christie**, C.D. Hatch
- CHED 791.** Water adsorption on montmorillonite clays. **R. Meredith**, C.D. Hatch
- CHED 792.** Influence of a metal oxide surface on ligand exchange reactions between strong chelating agents. **J. Conrad**, N.E. Boland
- CHED 793.** Influence of pH on ligand exchange rate with phosphonate-containing chelating agents. **M.V. Harned**, T. Nelson, N.E. Boland
- CHED 794.** Sediment and water analysis of a glacially formed lake. **K.F. O'Connor**, Z. Balogh-Brunstad

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Green Chemistry & Sustainability

Cosponsored by SOCED

Financially supported by ACS Green Chemistry Institute; I&EC Green Chemistry

N. Di Fabio, *Organizer*

12:00 - 2:00

- CHED 795.** Southeastern Massachusetts student network for biodiesel research and education. **L. Sprague**, B. Ackley, K. Bukis, J. Hooper, I. Korslund, P. Kurriss, K. Roebuck, E.J. Brush
- CHED 796.** Series of meso-tetra-substituted porphyrins synthesized using mechanochemistry. **Q. Su**, T.D. Hamilton
- CHED 797.** Entrainment sublimation for purification of mechanochemically-synthesized porphyrins. **V.S. Hoelscher**, T.D. Hamilton
- CHED 798.** Effects of halide salt hydrates on isomerization of glucose to fructose. **M. Swannell**, C. Yoo, X. Pan
- CHED 799.** Plasticizing sulfur with limonene: A functional material synthesized entirely from industrial waste. **M.P. Crockett**, A.M. Evans, J.M. Chalker
- CHED 800.** Malonic acid as a green alternative to formaldehyde in cell fixation. **D. Szlosek**, R. Byrnes, P.M. Doherty, D. Finocchietti, D. Currie
- CHED 801.** Oxidation of anthracene catalyzed by a recyclable vanadium(IV) oxide complex using hydrogen peroxide in an aqueous biphasic medium. **S.L. Moran**, C.A. Mebi, A. Bhuiyan
- CHED 802.** Vacuum distillation via solar irradiation. **L. Nurmomade**, D.J. Swartling
- CHED 803.** Further progress with Claisen condensations via solar irradiation. **S.M. Amin**, D.J. Swartling
- CHED 804.** Further progress with Fisher esterification via solar irradiation. **C.R. Buckner**, D.J. Swartling
- CHED 805.** Preparation of tetraphenylporphyrins via solar irradiation. **T. Pinto**, D.J. Swartling
- CHED 806.** Research to develop a more efficient reflux process for methanol capture in biodiesel synthesis by applying green chemistry principles. **P. Kurriss**, E.J. Brush
- CHED 807.** 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 808.** Applying green chemistry principles in the synthesis of oxindole-3-acetic acid: The initial intermediate in the bromination of indole-3-acetic acid to 3-bromoxindole-3-acetic acid. **M. Steadman**, E.J. Brush
- CHED 809.** Synthesis of glucosamine-based single chain nonionic and cationic surfactants. **R. Gonzalez**, C. Coss, R. Palos Pacheco, J.E. Pemberton
- CHED 810.** Endo/exo thermal isomerization of a green Diels-Alder adduct. **S. MacColl-Garfinkel**, M.S. Erickson
- CHED 811.** Design of experiments approach to optimize the yield of 1-(4-vinylbenzyl) thymine. **R. Koellin**, H. Schalk, C. Horgan, K. Wickey, N. Chen, J. Pallozzi, K. McDonough, K. Dupuy, N.E. Lee, R.W. Gurney
- CHED 812.** Interactions of partially green double reduced gold nanoparticles with lead. **A. Cruz Torres**, R. Noriega Rivera, B. Mercado Toro, E. Medina, E.J. Ferrer Torres, C. Osorio Cantillo, J.I. Ramirez Domenech
- CHED 813.** Green synthesis of silver nanoparticles using extracts from *Leucaena leuccephala (Lam.) de Witt* leaflets. **J. Delgado Izarray**, J. Rodriguez Ortiz, R. Aleno, E. Medina, C. Osorio Cantillo, E. Ferrer Torres, J.I. Ramirez Domenech
- CHED 814.** Cross-linking and surface functionalization of polycarbonate films using thiol-ene click chemistry. **I. Blythe**, Y. Wang, D.J. Darenbourg
- CHED 815.** Chloride retention in biomass with the addition of lime and dolomite. **M.W. Smith**, G.P. Chea, T.A. Hoemberg, J.C. Barbour
- CHED 816.** Investigation of thiosemicarbazone ligands in "green" palladium catalyzed Suzuki cross-coupling reactions. **J.R. Hall**, B.J. Anderson
- CHED 817.** Discovery of a new copper bismuth oxide material for the conversion of sunlight into a solar fuel. **L.R. Sharpe**, J.S. Compton, C. Peterson, D. Dervishogullari
- CHED 818.** Mechanochemical synthesis of biologically relevant porphyrin targets. **D. Cordero**, T.D. Hamilton
- CHED 819.** Conversion of ethanol to gasoline over zeolite H-ZSM-5 catalyst. **A. Ali**, Z. Wang, S. Adhikari
- CHED 820.** Hydrolysis of fungal chitin utilizing ionic liquids as a solvent and catalyst. **J. Gayton**, C.D. Estefan, E.D. Anderson, M. Faralli, W. Reichert
- CHED 821.** Investigation of transesterification of canola oil using basic ion exchange resin. **R. Deal**, G.L. Milligan

- CHED 822.** Mechanochemical reactions for green chemical synthesis. **E. Hanna**, G.K. Kaufman
- CHED 823.** New metric to evaluate sustainability in the undergraduate organic laboratory course. **B. Saunders**, K. McMahon
- CHED 824.** Effects of cation structure on the acidity of Brønsted acid ionic liquids: A computational study. **C.D. Estefan**, J.N. Gayton, M. Faralli, E.D. Anderson, W.M. Reichert, E.A. Salter
- CHED 825.** Developing and applying new thin film combinatorial techniques for the discovery of new metal oxide semiconductors for the efficient photoelectrolysis of water. **V.A. Kong**, J.G. Rowley
- CHED 826.** Development of carbohydrate-based heterogeneous solid acid catalyst for biodiesel production. **M.L. Jordan**, B.S. Chilukuri, B. Jang

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Inorganic Chemistry

Cosponsored by INOR and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

- CHED 827.** Aminebis(phenolate) complexes of palladium as catalysts for the Suzuki-Miyaura coupling reaction. **A.K. Bowser**, B. Wile
- CHED 828.** Alternative to detection: Europium(III)-tetracycline species association with biological molecules. **B.G. Vo**, G. Muller
- CHED 829.** Triflimide activation of azaferrrocene-boranes for hydroboration of simple alkenes. **D.I. Szymanik**, T.J. Brunker
- CHED 830.** Liquid sorption studies of Co^{II}-4,4'-bipyridine 1D chains and 2D square grid MOFs. **K.C. Carlson**, C.L. Weeks
- CHED 831.** Synthesis and characterization of 1-D ladder crystals grown in methanol. **T.D. Petersen**, N.G. Weissenfluh, C.L. Weeks
- CHED 832.** Reaction of copper(II) chloride dihydrate with formamide. **A.G. Nicholson**, G.L. Seebach
- CHED 833.** Synthesis and investigation of novel thiosemicarbazone ligands and their metal complexes. **K.A. O'Rourke**, B.J. Anderson
- CHED 834.** Synthesis and characterization of a larger neutral macrocycle for transition and lanthanide(III) metal complexes. **A.J. Sprecher**, A.J. Jiricitano
- CHED 835.** Synthesis, characterization, and electrochemical properties of tris(3-isopropylpyrazolyl)borate nickel complexes. **V. Doll**, N. Piro, W.S. Kassel, W.G. Dougherty
- CHED 836.** Synthesis, characterization, and electrochemical properties of tris(3-tert-butylpyrazolyl)borate copper complexes. **O. Beale**, N. Piro, W.S. Kassel, W.G. Dougherty
- CHED 837.** Synthesis, characterization, and ion-binding studies of Ru(bpy)₃²⁺ macrocycle host complexes. **T. Carroll**, M. Harris
- CHED 838.** Complexation reactions of cerium (III) and cerium (IV) salts with amides. **T.L. Amburn**, G.L. Seebach
- CHED 839.** Synthesis and characterization of copper-thiosemicarbazone complexes: Interaction with DNA and anti-oxidant behavior. **K.R. Webb**, B.C. Helbert, F.A. Beckford
- CHED 840.** Curcuminoids as ligands in zinc and vanadium complexes: Synthesis and biophysical reactivity. **B. Helbert**, S. Smith, K.R. Webb, F.A. Beckford
- CHED 841.** New ethylene cross-bridged and side-bridged tetraaza macrocycles featuring acid and amide pendant arms and their transition metal complexes for oxidation catalysis. **M. Gorbet**, M.B. Allen, A.D. Shircliff, G. Yin, T.J. Hubin
- CHED 842.** 1,7-Dimethyl-1,4,7,10-tetraazacyclododecane complexes of Mn, Fe, Co, Ni, Cu, and Zn: Synthesis and characterization. **M.A. Ayala**, A. Walker, T.J. Hubin
- CHED 843.** Electrochemical stability of ruthenium-arene complexes. **M.T. Piedmonte**, S.M. Young, W.J. Vining
- CHED 844.** Ion selective redox chemistry of a rhenium (I) complex using cyclic voltammetry. **N. Rambhujun**, S.M. Young, W.J. Vining
- CHED 845.** Synthesis, NMR characterization, and x-ray crystal structure of quinoine-2-carboxaldehyde tert-butyl thiosemicarbazone: The [Pd(QCA-tBTSC)Cl] complex and MIC studies. **J. Chen**, J.D. Conner, N.P. Riggsbee, E.C. Liscic
- CHED 846.** Comparison of a series of 2-acetylpyridine-thiosemicarbazone Cu(II) and Pd(II) metal complexes. **B.C. McGill**, R.E. Scott, E.C. Liscic
- CHED 847.** Investigating bispyrrolidine based chiral C₂-symmetric tetradentate ligand. **J. Kaplan**, H. Reed, J.M. Keane
- CHED 848.** Quantitative determination of silver inhibition of halide accelerated aluminum corrosion. **K.D. Lopez**, H. Gill, S.G. Sobel
- CHED 849.** Metal-organic assemblies of meso-terrasubstituted porphyrins. **M. Basden**, M. Knol, T.D. Hamilton
- CHED 850.** Iodination and MWI cyanation of closo-dodecaborate(2-) and closo-1,2-dicarbododecaborate. **H.R. Midget**, M.A. Juhasz
- CHED 851.** Investigations of the halogenation, radiohalogenation, and functionalization of CB9 corborane clusters. **C.R. Vorauer**, M.A. Juhasz, D.S. Wilbur
- CHED 852.** Synthesis of new gold-isocyanide and acyclic diaminocarbene complexes for catalysis. **J. Coronado**, A.A. Ruch, V. Nesterov, L.M. Slaughter
- CHED 853.** Copper-catalyzed triazole synthesis in the presence of halides. **M.D. Womble**, R.M. Moorman, M.B. Collier, B.H. Frohock, J. Chalker
- CHED 854.** Mercury concentration in washed and unwashed leaves of differing plant species. **D.W. Lehmpuhl**, K.A. Wager, L.M. Bartolo
- CHED 855.** Designing novel electrodes of 3D porous V2O5/PANI films by colloidal particle lithography. **J.A. Zavala**, C.J. Chalker, A. Parija, H. An, J.L. Lutkenhaus, J.D. Batteas
- CHED 856.** Cobalt catalyzed cyclotrimerization of alkynes using a microwave reactor. **J. Legere**, E. Hawrelak
- CHED 857.** Modulating the electrochemical properties of iron-carbonyl clusters using thiolate ligands. **A.L. Haley**, L.S. McDaniel, L.N. Broadbent, C.H. Hinkle, S.T. Heckman, J.L. Randall, S.L. Moran, C.A. Mebi
- CHED 858.** Adsorption studies and immobilization of metal complexes on supports: Solid-state NMR and catalysis. **J. Benzie**, K.J. Cluff, J. Blumel
- CHED 859.** Chemical pressure effects on Ga_{2-x}Fe_xO₅ magnetoelectric ceramic structure. **E. Velasquez**, C. Lefevre, F. Roulland, A. Demchenko, N. Vart
- CHED 860.** Synthesis and characterization of a novel hydrozone thiophene ligand. **A. Angeleles**, W.A. Weigand
- CHED 861.** Synthesis and magnetic characterization of lanthanide 12-metalacrown-4 complexes. **C. Daly**, C.M. Zaleski
- CHED 862.** Corrosion testing of anti-corrosion coatings by Scanning Electrochemical Microscopy (SECM). **C. Lee**, M.C. Calhoun, R.L. Calhoun
- CHED 863.** DNA binding studies of [Rh(tacn)(dppz)(H₂O)]³⁺: A new metallointercalator with a modifiable coordination site. **I.M. Williams**, H.L. Hancock, S.C. Haefner
- CHED 864.** Speciation of europium(III)-tetracycline species. **A. Huy**, K. Deol, G. Muller
- CHED 865.** Toward the development of luminescent metal organic frameworks for use as sensors. **M. Peiffer**, K. Kneas, J.A. Rood
- CHED 866.** Interaction of DNA with [Cu(phen)(4-amino-pteridino(6,7-f)phenanthroline)](PF₆)₂, a potent DNA cleavage agent. **A. Lopez**, G.H. Rawji

- CHED 867.** Investigation of DNA binding and photocleavage properties of [Zn(4-amino-pteridino(6,7-f)phenanthroline)(triflate)]. P. Wong, G.H. Rawji
- CHED 868.** Ligand exchange of an enzyme-mimic Schiff-base copper(II) complex: A kinetic study. S. Colling, J.J. Stace
- CHED 869.** Synthesis of enzyme-mimic copper(II) Schiff-base complexes. S. Williams, J.J. Stace
- CHED 870.** Synthesis and reactivity of a enzyme-mimic nickel(II) complex. D.M. Beagan, J.J. Stace
- CHED 871.** Development of sulfhydryl-functionalized silica particles for use in diffusive gradient in thin-films passive samplers. D. Manley, A. Pham, H. Hsu-Kim
- CHED 872.** Capturing carbon dioxide with metal-organic frameworks. N. Oostendorp, E. Maslowski
- CHED 873.** Preparation of SnO₂ substrate for sensitized solar cells. Q. Yang, L.A. King, M. Kern, B.A. Parkinson
- CHED 874.** Synthesis of novel green inorganic catalysts. N. Wolford, E. Rajaseelan, S.A. Roberts
- CHED 875.** Studies of cytotoxicity and cellular internalization of small-molecule conjugates of metal oxide nanoparticles in tumor cells. A. Henry, P. Promdet, C. Blumenfeld, R.A. Moats, R.H. Grubbs, H.B. Gray, K. Sorasane
- CHED 876.** Investigating a hybrid organosilyl class of Dawson-Wells polyoxometalates through Langmuir-Blodgett. J. Perryman, E.J. Atkinson, R.C. Chambers
- CHED 877.** Synthesis of a novel green chemical catalyst. P. Bekere, E. Rajaseelan, S.A. Roberts
- CHED 878.** Synthesis and catalytic properties of a novel triazole based N-heterocyclic Iridium carbene complex. E. Dalbey, S.A. Roberts, E. Rajaseelan
- CHED 879.** Characterization of metal dithiocarbamate complexes derived from amino acids. G. Azzarello, E. Sylvester
- CHED 880.** Corrosion of aluminum by aqueous CuCl₂: An SEM-EDS study. A. Brodovskaya, S.G. Sobel, G.L. Polak, M. Akhtar
- CHED 881.** Microwave-promoted synthesis of heavily iodinated 10- and 12-vertex boron clusters. G.R. Matheson, M.A. Juhasz, P.S. Chang
- CHED 882.** Novel synthesis and catalytic properties of triazole-based N-heterocyclic carbene complexes of rhodium and iridium. W.J. Maximuck, E. Rajaseelan, S.A. Roberts
- CHED 883.** Heteroleptic salicylaldimine magnesium amides: Solid-state and solution characterization. S.M. Tretter, A.M. Landis, J.A. Road
- CHED 884.** Synthesis and characterization of ground and excited state properties of a new ruthenium(II) polypyridine complex. A.T. Vu, R.N. Garner
- CHED 885.** Time-based investigation of the vapochromic response of platinum(II) complexes. K.A. Mingle, M. Abdolmaleki, M. Riasi, W.B. Connick
- CHED 886.** Synthesis of Co-complexes with pentadentate ligands for catalytic hydrogen evolution. T. Tall, M. Vennampalli, M. Zhang, X. Zhao
- CHED 887.** Exploration of coordination chemistry with arsenazo III, DTPA and metal complexes using NMR and UV-VIS. C. Winking, C. Breaux
- CHED 888.** Coordination chemistry of divalent group 12 thiocyanate complexes containing phthalazine. T.J. Paca, P.M. Secondo, R. Baughman
- CHED 889.** Coordination chemistry of divalent group 12 thiocyanate complexes containing quinoxaline. C. Martello, P.M. Secondo, R. Baughman
- CHED 890.** Coordination chemistry of divalent group 12 thiocyanate complexes containing 2-amino-5-cyanopyridine. A. Shoroye, P.M. Secondo, R. Baughman
- CHED 891.** Imidazolium salts as reaction media for preparation of metal halide cluster networks. S.K. Gnewuch, D.H. Johnston
- CHED 892.** Catalytic oxidation of primary alcohols by transition-metal-TRIPHOX complexes. E. Lamping, C.M. Davis
- CHED 893.** NKU organometallic research: Examining new synthetic strategies that functionalize fullerene and coronene for organometallic supramolecular systems. C. Beneker, K.A. Walters
- CHED 894.** NKU Spectroscopic Research: Studies on polymers and their subunits that incorporate fullerenes and transition metal chromophores. S. Siemer, K.A. Walters
- CHED 895.** NKU Polymer Research: Synthesis of polymers and their subunits that incorporate fullerenes and transition metal chromophores. J. Callihan, K.A. Walters
- CHED 896.** NKU solar cell research: Fullerene-transition metal sensitized solar cells — construction and efficiency studies. H. Hearn, K.A. Walters
- CHED 897.** NKU organometallic research: Simplified synthetic strategies for fullerene-bipyridine ligands used in organometallic complexes for solar cell dyes. J. Horn, K.A. Walters
- CHED 898.** Dye inclusion on the {101} face of KDP crystals. L. Strange, J.R. Williams
- CHED 899.** New N-heterocyclic carbene (NHC) silver fluorides facilitate dihydrogen activation to form a silver hydride cluster where sterically demanding NHC ligands increase stability and rate of hydrogen activation. J. Nguyen, B. Tate, J.P. Sadighi
- CHED 900.** Synthesis and catalytic activity of tin (IV) halides functionalized with bidentate phosphine ligands. M. Leverich, R.W. Hartmann
- CHED 901.** Effect of ZnO morphology on the photodegradation of malachite green oxalate. S.C. Bryant, K.O. Laughlin, J.D. Harris
- CHED 902.** Synthesis, characterization, and reactivity of ruthenium(II) complexes involving p-cymene and hexamethylbenzene ligands. A.D. Riner, J.P. Lee
- CHED 903.** Synthesis and characterization of cyclopentadienyl- and pentamethylcyclopentadienyl-Co(III) mixed sandwich compounds containing either tridentate nitrogen, sulfur, or carbon donor ligands. T.P. Latendresse, J.P. Lee
- CHED 904.** Electronic properties and composition of GaAs_xP_{1-x} grown by close-spaced vapor transport. A. Davis, A. Greenaway, S.W. Boettcher
- CHED 905.** Synthesis and characterization of transition metal clusters/polymers supported by pyridylamide ligands. M. Pauly, L. Yang
- CHED 906.** Synthesis and bacterial activity studies of acetylacetonate metal complexes. N.P. Riggsbee, A.L. Koch, A.J. Crook
- CHED 907.** Stabilization of catalytic tin species with phosphine ligands. J.H. Murray, R.W. Hartmann
- CHED 908.** Towards the synthesis of a water-soluble β-brominated cobalt(II) porphyrin. J. Williams, K.C. McGill
- CHED 909.** Synthesis of a novel water soluble porphyrin-chalcone complex. R.E. Tucker, J.C. Bradshaw, J.E. Bradshaw
- CHED 910.** Electronic structure and electrochemical elucidation of human serum albumin-heme complex. G.O. Tomoiaga, E.M. Luteran, K.S. Kang, R.S. Fogle, M.I. Galinato, J.A. Bennett
- CHED 911.** Contrasting the biomimetic reactions of NO₂ with Fe (III) porphyrins and Fe (IV) corroles. S.M. Russo, S.K. O'Shea
- CHED 912.** Synthesis of a nickel(II) chloride chemosensor. M. Allegranza, J. Fautsch
- CHED 913.** Exchange between Fe(III) and Ni(II) dithiocarbamates in solution. N.M. Barker, J. Coffield, N.V. Duffy
- CHED 914.** Novel halometalates incorporating 2, 2'-biimidazole. E.L. Sears, J.G. Kelley, L. Peterson, Jr., M.D. Smith
- CHED 915.** Synthesis and high resolution powder diffraction pattern refinement of novel rare-earth substituted pyrochlores. J.D. Aldridge, D.A. Polvani
- CHED 916.** Synthesis and characterization of di-2-pyridyl ketone oxime complexes with transition and lanthanide metals. K. Knopf, B.L. Westcott
- CHED 917.** Synthesis and spectroscopic analysis of spin-crossover cobalt complexes. H. Zecca, H. Kim, A.C. Bowman
- CHED 918.** N-heterocyclic carbene ligands as supports for Cp*Co(I) fragments. J.M. Andjaba, C.A. Bradley
- CHED 919.** Developing a copper-catalyzed asymmetric reduction of 2H-azirines. D.K. Yi, T.J. Mathews, J. Unger
- CHED 920.** Investigation of the mechanism of arene perfluoroalkylation by iron perfluoroalkyl reagents. R.S. Thompson, J.D. Lawrence
- CHED 921.** SNC-Rh(I) pincer complexes bearing thioether and N-heterocyclic carbene donors: Catalytic activity in transfer hydrogenation. P.L. Osburn, T. Grimes
- CHED 922.** Utilization of pyrazole based copper complexes in atom transfer radical addition (ATRA) and atom transfer radical cyclization (ATRC). E. Perez, G. Pros, T. Pintauer
- CHED 923.** Iminophosphorane reagents for synthesis of electrically diverse diimine and N-heterocyclic carbene ligands. A.M. Hodge, C.A. Bradley
- CHED 924.** Comparative structural studies of A₂BTeO₆ (A = Ca, Sr, or Ba; B = Ca or Cd) double perovskites. A. Flores, H. Albert, A. Stiner, T. Mansur, P. Barnes, A. Fry
- CHED 925.** Design, synthesis, and characterization of zinc dithiolato/dithione (donor/acceptor) and vanadium dithione complexes. S.C. Ratvasky, M.J. Van Stipdonk, B. Mogesa, P. Basu
- CHED 926.** Bis(oxazolinyphenyl)amines complexes. A.J. Rupprecht, J.K. Vohs
- CHED 927.** Synthesis metal-organic frameworks containing Mn-SALEN active sites and their catalytic properties. B. Chicoine, M. Mathews, W. Schumacher, L.G. Beauvais
- CHED 928.** Formation of mixed monolayers on TiO₂ and Ti-6Al-4V using carboxylic and phosphonic acids. A. Dalal, N.A. Reger, E.S. Gawalt
- CHED 929.** Influence of annealing conditions on electrical properties in calcium cobalt oxide misfit layered compounds. D. Lofdahl, G. Whinery, C. Heidemann
- CHED 930.** Synthesis and characterization of symmetric and asymmetric bimetallic ruthenium(II) complexes. M.T. Mongelli, J. Pozo, P. Menta, L. Zierten
- CHED 931.** Modification of MOF-5 hydro-stability for peptide adsorption studies. M. Nivison, Z. Mensinger
- CHED 932.** Investigating aurophilic interactions: Synthesis, structural, and photoluminescent properties of lanthanide cyanometalates containing 1,10-phenanthroline. J.M. Hendrich, R. Sykora, J.D. Taylor, F.D. White, K. Xiang
- CHED 933.** Functionalization of the rho-ZMOF framework with fluorescent probes. A. Kalbach, J. Miksovska
- CHED 934.** Synthesis and reactions of a tris-(tributylamine)triborate cation. S. Bertrand, C. O'Keefe, G.M. Edvenson
- CHED 935.** Reaction of 1-[2-[diphenylboryl]benzyl]-2,2,6,6-tetramethylpiperidine with hydrogen. K. Gurung, T.K. Bader, G.M. Edvenson
- CHED 936.** Synthesis of mononuclear ruthenium complexes containing a tetradentate bipyridine dicarboxylic acid equatorial ligand and two N-heterocyclic carbene axial ligands. E.E. Kukura, J.K. Vohs
- CHED 937.** Characterizing novel Mg alkoxide compounds as potential precursor electrolytes for next-generation batteries. C. Nist-Lund, J. Herb, C.B. Arnold
- CHED 938.** Withdrawn.

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

International Research Experience for Undergraduates

N. Di Fabio, Organizer

12:00 - 2:00

CHED 939. Analysis of selective oligonucleotide release from photothermally active hollow gold nanospheres using surface enhanced Raman scattering. D.G. Mackanic, D. Graham, S. Mabbott

CHED 940. Examining bridged oligothiophenes as small-molecule semiconductors in organic photovoltaic devices. L.R. Savagian, N. Findlay, A. Kanibolotsky, P. Skabara

CHED 941. Synthesis and characterization of CdSe quantum dots via low temperature thermolysis of a single organometallic precursor. C.M. Gentle, S. Farniani, L. Tarpani, L. Latterini

CHED 942. Stabilization of light-harvesting complexes from *Rhodospseudomonas acidophila* in dipeptide gels. E.K. Reagan, N. Javid, S.K. Nalluri, R. Ulijn

CHED 943. S₂O₂ treated cuprous oxide electrochemical reactivity with carbon dioxide. G. Panetti, A.D. Handoko, B. Siang Yeo

CHED 944. Synthesis and characterization of divalent ligands with photoswitching capabilities. L. Hristov, A. Sent, S. Hecht

CHED 945. Optimization of ferroelectric behavior in lead-strontium-titanate (PST) ceramic thin films. G. Ruehl, M. Benkler, T. Hanemann

CHED 946. Synthesis and characterization of light-responsive hybrid polymer thin films. D. Brauer, N. Wagner, P. Theato

CHED 947. Synthesis and exploration of spiro-pyran-containing poly-(3-hexylthiophene) oligomers. A. Kim, M. Schulz, A. Staubitz

CHED 948. Growth of carboxylated UiO-66 metal-organic framework crystals for CO₂ capture. S.J. Faucher, D. Zhao, Z. Hu

CHED 949. Development of a sustainable and efficient protocol for palladium-catalyzed Sonogashira cross-coupling reactions. M. McLaughlin, G. Strappaveccia, M. Gruttadauria, L. Vaccaro

CHED 950. Investigation of temperature dependent electrochemical CO₂ reduction on copper by gas chromatography including formic acid detection via derivatization. B. Ferguson, J. Grote, K. Mayrhofer

CHED 951. Modification of ultrafiltration membranes for improved purification of nanoparticle dispersions. T.J. Myers, M. Ulbricht

CHED 952. Development in poly-thiophene and poly-benzotriazole block copolymer for use in polymer solar cell. T. Range, C. Ping Sen, S. Vallyaveetil

CHED 953. Experimental studies of shutdown procedures for water-gas shift catalysts in high temperature polymer electrolyte fuel cell systems. K. Fong, D. Krekel

CHED 954. Organoiridium catalyst as a functional mimic of both oxygen evolving complex and hydrogenase. S. Barnett

CHED 955. Threshold implementation and testing in local coupled cluster doubles theory (PNO-LCCD). J. Ford, M. Schwilk, H. Werner

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Medicinal Chemistry

Cosponsored by MEDY and SOCED

N. Di Fabio, Organizer

12:00 - 2:00

CHED 956. Identification and synthesis of novel cyclin-dependent kinase inhibitors. N.A. Pham, P. Tram, T.K. Nguyen, R.L. Schroeder, S. Jennings, T. Vu, H.E. McFerrin, J. Sridhar

- CHED 957.** Using isothermal titration calorimetry (ITC), circular dichroism (CD) and DNA unwinding studies to investigate the DNA binding properties of abietane diterpenes natural products. **G.S. Gullickson, B.S. Kasper, R.E. McKnight**
- CHED 958.** Study of antitumor effects of quercetin and amine or methoxy poly-substituted derivatives on metastatic and non-metastatic mouse cells. **J. Winkelbauer, D. Rzewnicki, A. Abel, C. Kriley, T. Homan, D. Ray**
- CHED 959.** Prevention and disruption of bacterial biofilms. **A. Newsham, D. Warner, R.E. Del Sesto**
- CHED 960.** Transition metal complex dual CXCR4/CCR5 antagonists. **D.J. Davilla, D. Schols, S.J. Archibald, T.J. Hubin**
- CHED 961.** New thiazolecarboxaldehyde thiosemicarbazone ligands: NMR structure studies and complexation with Cu(II) to form [Cu(TZCA-ETSC)Cl] and with Pd(II) to form [Pd(TZCA-ETSC)Cl]. **S.D. Simpson, J.D. Conner, N.P. Riggsbee, E.C. Lisic**
- CHED 962.** New 2-acetyl-6-bromopyridine thiosemicarbazone ligands: NMR and complexation with Cu(II) to form [Cu(ABRPy-TSC)Cl] compounds. **T.B. Milligan, B.C. McGill, L. Hatmaker, E.C. Lisic**
- CHED 963.** Comparison of a series of 2-acetyl-6-methoxypyridine (AMOPY) thiosemicarbazone metal complexes. **M.K. Monroe, A.M. Barnes, B.C. McGill, R.E. Scott, E.C. Lisic**
- CHED 964.** New terpenoids from the Caribbean gorgonian *Pseudopterogorgia acerosa*. **P.D. Scesa, L.M. West**
- CHED 965.** Antibacterial activity of 4-alkyl and 4-arylbutenolides. **W. Heartsill, J. Stevenson, A. Dameron, N. Estes II, J.M. Hutchison**
- CHED 966.** Insulin-specific inhibition of insulin-degrading enzyme using a synthetic receptor. **C. Young, L. Logsdon, A.R. Urbach**
- CHED 967.** Manganese-52: cyclotron production and PET/MR imaging. **R. Gross, A.L. Wooten, B. Lewis, P. Woodard, S. Lapi**
- CHED 968.** 4-methylimidazole effect on extrinsic tooth discoloration: A computational model of the Maillard reaction. **L. Tribe, M. Yacoub**
- CHED 969.** Computational model for tooth discoloration with sunset yellow treated with H₂O₂. **A. Naem, L. Tribe**
- CHED 970.** Synthesis of a highly fluorescent aminopyronin calcium sensor. **A.T. Bayasi, Z. Woydziak, N. Nayigihugu**
- CHED 971.** Evaluation of organogel nanoparticles as a means of drug delivery. **C.L. Spartz, F. Brouillet, J. Garrigues, S. Franceschi, E. Perez**
- CHED 972.** Progress toward synthesis of photomodulated SIRT1 activators. **T. Scheckelhoff, C.N. Streu**
- CHED 973.** Cytotoxicity and cell cycle studies of *trans*-diiodophosphate Pt (II) complexes. **S.M. Dennis, A. Medrano, A. Alvarez-Valdés, J. Perles, A. Quiroga, T. McGregor Mason**
- CHED 974.** Identification, synthesis, and biological activity of galloyl inhibitors of human low molecular weight protein tyrosine phosphatase. **S. Klinker, E.J. McIntee, H.V. Jakubowski**
- CHED 975.** Progress toward synthesizing transition metal complexes to mimic complex natural products. **N. Smith, S. Knecht, J.R. Oleka, C.N. Streu**
- CHED 976.** Selective nitration of Hsp90 by peroxytrinitrate in the presence of ALS-linked mutant SOD. **J. Titus, K. Thomas, C.N. Dennis, A.G. Estevez, M.C. Franco**
- CHED 977.** Antimicrobial effect of improved antibiotics combined with Ni and semi-green Ag nanoparticles in *Klebsiella pneumoniae*. **K. Rodriguez Graciani, R. Aleno, M.A. Miranda Belandria, J. Delgado Izariy, E. Medina, L. Diaz, E.J. Ferrer Torres, J.J. Ramirez Domenech**
- CHED 978.** Natural product discovery through bioassay methods on *Ilex decidua*. **O. Clem, M.J. Campbell**
- CHED 979.** Design and synthesis of a new mGluR₁ modulator. **L. Kalfayan, D. Kawamba, K.J. Friedrich**
- CHED 980.** Investigation of a synthetic approach to new substituted 1,2,3-triazoles. **A. Murdock, S. Alias, K.J. Friedrich**
- CHED 981.** Search for an ideal selective estrogen receptor modulator (SERM). **N. Till, R.G. Yahn, R. LaLonde**
- CHED 982.** Investigating pancreatic anticancer activity of spiroxin A derivatives. **H. Zhang, K. Kartub, R. Zhou, A.C. Webb, D. Carrico-Moniz**
- CHED 983.** Effect of cell culture components on the preferential cytotoxicity of isoprenylated coumarin derivatives. **H. Zhang, R. Zhou, M. Jun, A. Bacay, A.C. Webb, D. Carrico-Moniz**
- CHED 984.** Design of tautomatically ambiguous cytosine-based nucleosides as potential anti-HIV agents. **C.A. Elkin, Z.T. Ford, V.K. Dunlap**
- CHED 985.** Using rational drug design toward the synthesis of novel flavonoid derivatives as acetylcholinesterase inhibitors for the treatment of Alzheimer's disease. **J. Minnick, A. Kranzlein, O.M. Newman, C. Mills**
- CHED 986.** Molecular modeling and docking studies of peptide macrocycles as potent inhibitors of the 20S proteasome. **D.L. Wilson, M.G. Götz**
- CHED 987.** Design and synthesis of sphingolipid derivatives. **A. Chatters, M. Foroozesh, L. Lovings, J. Liu**
- CHED 988.** Design, synthesis, and evaluation of a novel hydroxamic acid series for treatment of human African trypanosomiasis. **J. Rutledge, K. Kim, G. Parfenov, A.B. Douay**
- CHED 989.** Synthesis of coumarin derivatives as potential inhibitors of human cytochrome P450 enzymes. **P. Pham, J. Liu, M. Foroozesh, L. Lovings**
- CHED 990.** Design and synthesis of coumarin propargyl ethers as potential cytochrome P450 inhibitors. **S. Bellow, J. Liu, L. Lovings, M. Foroozesh**
- CHED 991.** Design and synthesis of flavone propargyl ethers as potential inhibitors of human cytochrome P450 1A1 and 1A2 enzymes. **L. Mensah, L. Lovings, J. Liu, M. Foroozesh**
- CHED 992.** Synthesis of beta-lactam analogs of betalactosin A. **N.K. Dunlap, N. Shokur, J. Byrd, A.L. Pathirananage**
- CHED 993.** Synthesis of new toll-like receptors 2 (TLR2) ligands for pancreatic cancer imaging. **N.M. Haq, M. Doligalski, A.S. Huynh, J. Vagner, D.L. Morse, M.L. McLaughlin**
- CHED 994.** Synthesis of novel heterocyclic naphthoquinone imines and evaluation of their biological activity. **A. Delawder, D. Dopp, K. Liles, S. Elisha, M. Manpadi**
- CHED 995.** Ketoconazole activates CYP3A4-mediated metabolism of letrozole. **S. Black, J.M. Chan, J. Harrelson**
- CHED 996.** Determination of inhibitor specificity for low molecular weight protein tyrosine phosphatase isoforms A and B. **E. Sinner, H.V. Jakubowski, E.J. McIntee**
- CHED 997.** Potential antiviral effects of phenazine derivatives on the La Crosse virus. **Z. Carpenter, C.J. Monceaux**
- CHED 998.** Quantification of longevity of aminopyronin in *E. coli*. **N. Vita, A.T. Bayasi, N. Nayigihugu, Z. Woydziak**
- CHED 999.** Developing controlled-release chloroquine. **K. Davis, K.E. Rohly**
- CHED 1000.** Cyclic sulfonimidamides prospective use as non-GAT1 inhibitors. **S. Knudsen, C.J. Monceaux**
- CHED 1001.** Synthesis of 2-(2-sulfonamidophenyl)benzothiazole and 2-(2-sulfonamidophenyl)benzimidazole as potential inhibitors of anthrax lethal factor and other zinc metalloenzymes. **M.J. Roufflet, C. Kay**
- CHED 1002.** Triflic acid mediated thiophenyl sulfonylation of arenes and subsequent antimicrobial activity determination of thiophenyl aryl sulfones. **C. Foley, J.R. Mckee, B. Peethambaran**
- CHED 1003.** Oxadiazoles as biofilm and bacterial growth inhibitors. **K. Childers, A. Weber, A. Zanella, R.E. Grote**
- CHED 1004.** Synthesis of multitarget ligands for the treatment of Alzheimer's disease. **V. Anto, D. Fish**
- CHED 1005.** Withdrawn.
- CHED 1006.** Saccharin and its carbonyl-derivative-conjugate shows promise for isoform selective inhibition of carbonic anhydrase IX: A lead approach to anti-cancer drug development. **J.M. Driscoll, B.P. Mahon, G.M. Rankin, S. Poulsen, C.T. Supuran, R. McKenna**
- CHED 1007.** Using essential oils to combat the threat of multidrug resistant bacteria. **Z.T. Rahman, J. Mack**
- CHED 1008.** Optimization of thiazazole small molecule inhibitor of the hippo signaling pathway to reduce pro-EMT cancerous cell growth. **N.A. Werwie, S. Strellec, A. Rebbaa, R. Lettan**
- CHED 1009.** Targeting sphingosine kinase 2: Converting highly selective substrates into inhibitors. **R. Dyer, T.K. Dawson, Y. Kharel, K. Lynch, T.L. Macdonald**
- CHED 1010.** Novel anticancer drugs on the basis of diversely functionalized N-containing heterocycles. **K. Zingler, L. Frolova, S. Rogelj**
- CHED 1011.** Diastereoselectivity in an exhaustive bromination of anthracenyl-isoxazoles. **M.J. Campbell, M.J. Weaver, N.R. Natale**
- CHED 1012.** Preparation and photolysis of non-glucosinolates. **E.M. Voigt, E.H. Pauley, J.R. Mays**

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Nanochemistry

Cosponsored by SOCED

N. Di Fabio, Organizer

12:00 - 2:00

- CHED 1013.** Activity and selectivity of PVP-capped palladium nanocatalysts immobilized on silica microspheres for the hydrogenation of phenol. **J.E. Kauffman, N.D. Muench, A.L. Marsh**
- CHED 1014.** Luminescent gold nanoparticles-based fluorescence and dynamic light scattering dual-modality sensor for copper (II) detection. **A.J. Fatino, C. Zhou**
- CHED 1015.** Nanostructured metal oxides with tunable Lewis base sites for the conversion of L- α -phosphatidylcholine to biodiesel. **K.I. Tooke, D.S. Heroux**
- CHED 1016.** Characterizing the partitioning of hydrophobic solutes into the surfactant bilayer on gold nanorods. **I.M. DiMucci, L.B. Thompson**
- CHED 1017.** Investigating the interactions between gold nanoparticles and *L. catebeianus* and *L. sylvaticus*. **L.L. Lee, L.B. Thompson, P. Fong, K. Andresen**
- CHED 1018.** Low temperature, size-selective fluorescence spectroscopy of PbSe quantum dots. **I. Corcione, J. Peterson, W. Stephans, M. Ruggiero**
- CHED 1019.** Templated gold nanorod arrays for improved plasmonic biosensing. **S.L. Melnyk, I.R. Bruzas, L.B. Sagle**
- CHED 1020.** Developing a silica-coated nanovehicle for targeted cancer therapy. **Z. Liao, N.H. Kolodny, N.T. Flynn, A.C. Webb**
- CHED 1021.** Synthesis of activated palladium nanoparticles (PdNPs) on carbon microspheres (CMs) for use as a hydrogenation catalyst. **J.P. Pender, S.E. Sanders, M.R. Dix, P.E. Colavita, K.M. Metz**
- CHED 1022.** Self assembly and ordering at the nanometallic liquid crystal interface. **D. Hofmann, S. Crotty, A. Sharma, Y. Gao, T. Hegmann, E. Hegmann**
- CHED 1023.** Investigating the integrity of novel nanovehicles for targeting pancreatic cancer. **S.N. Musetti, A.W. Cheema, N.T. Flynn, A.C. Webb, N.H. Kolodny**
- CHED 1024.** UV spectrophotometric titration of graphene oxide with ascorbic acid to follow reduced graphene oxide formation. **E. Olson, G.J. Mancini-Samuelson**
- CHED 1025.** Nanosized organometallic building block synthesis for the formation of a poly-oxometalate-based framework. **M. Lund, W.A. Newirth**
- CHED 1026.** Organic dyes improving the efficiency of dye-sensitized solar cells. **J.L. Gesell, C. Kelley, S. Geiger, E.A. Nalley**
- CHED 1027.** Activation and stabilization of electrodeposited p-Cu₂O with underpotentially deposited Ni. **K. DeHority, G. Clause, A. Fillingner**
- CHED 1028.** Synthesis of silver gallium sulfide nanoparticles. **M. Kessler, S. Hughes**
- CHED 1029.** Tailoring cadmium selenide nanocrystals with mixed ligand systems. **C. Bloom, A.S. Tysoe, D. Jackson, J.D. Kehlbeck, M.E. Hagerman**
- CHED 1030.** Surfaced enhanced infrared absorption on optimized copper nanostructures. **W.A. Henry, D.A. Perry**
- CHED 1031.** Noble metal-TiO₂ and noble metal-ZnO nanocomposites for improved photocatalysis. **J.C. Franco, P.Z. Ray, R.M. Prevost, M.A. Tarr**
- CHED 1032.** Comparative interactions of gold and silver nanoparticles and lead in the rates of germination and root elongation of radish plants. **R. Noriega Rivera, B. Mercado Toro, A. Cruz Torres, E. Medina, C. Osorio Cantillo, E. Ferrer Torres, J.J. Ramirez Domenech**
- CHED 1033.** Functionalization of indole-3-acetic acid with gold nanoparticles synthesized through a double reduction reaction using leaflets' extracts of *Leucaena leucocephala* (Lam.) de Witt. **G. Maldonado Velez, E. Medina, C. Osorio Cantillo, E. Ferrer Torres, J.J. Ramirez Domenech**
- CHED 1034.** Synthesis of small, ligand-stabilized copper nanoparticles as building blocks for electroreduction catalysts. **A. DiAscro, S.L. Young, J.E. Hutchison**
- CHED 1035.** Probing nanosize-dependent oligomerization by using fluorescence dynamics of fluorescein amyloid beta 1-40 peptides. **C. Catalfamo, H. Chen, M. Spencer, E. D'Ambrosio, K. Yokoyama**
- CHED 1036.** Influence of pore size on cobalt loaded mesoporous materials for oxidation catalysis. **E. Murchie, D.S. Heroux**
- CHED 1037.** Comparative study of the application of nanostructured materials to fingerprints impressions. **M. Feliciano Sanchez, Y. Lugo, W.J. Rivera Martinez, E. Medina, J.J. Ramirez Domenech, C. Osorio Cantillo, E.J. Ferrer Torres**
- CHED 1038.** Comparative study and characterization of MgO, ZnO and CuO nanoparticles using amino acids as capping agents. **A. Lopez, R. Aleno, M.A. Miranda Belandria, E. Medina, C. Osorio Cantillo, J.J. Ramirez Domenech, E.J. Ferrer Torres**
- CHED 1039.** Functionalization and characterization of bimetallic silver-gold nanoparticles with antibiotics. **M.A. Miranda Belandria, M. Feliciano Sanchez, P. Rivera Pomales, E. Medina, J.J. Ramirez Domenech, C. Osorio Cantillo, E.J. Ferrer Torres**
- CHED 1040.** Preparation of metalloporphyrin nanoparticles. **J. Seidel, L.K. Lee**
- CHED 1041.** Synthetic methods of CTS and CZTS nanocrystals. **R.R. Bohling, B.J. Gerold, M.M. Davis, T.M. Pappenfus**
- CHED 1042.** Thin films of gold nanoparticles: Temporal stability and mechanisms of degradation. **J. Xu, N.T. Flynn**
- CHED 1043.** Synthesizing dendrimer-ligand conjugates for peptide mediated cellular delivery systems. **C.R. Pace III, J. Manono, S.C. Dimaggio**
- CHED 1044.** Diazonium-derived nitrobenzene layers on nanoporous gold. **C.L. Chevalier, E.C. Landis**
- CHED 1045.** Stability of alkane-thiol monolayers on nanoporous gold surfaces. **R.B. Chevalier, D. Patel, E.C. Landis**

- CHED 1046.** Zinc oxide and zinc sulfide nanoparticles for DNA detection: Synthesis, functionalization, characterization, and applications. **B. Etz, S. Oriley, S.M. Basu**
- CHED 1047.** Nano size, pH, and temperature dependence of interfacial self-assembly of α -synuclein peptide. **L. Morrow, M. Yuan, K. Chung, K. Yokoyama**
- CHED 1048.** Solvent interactions in vegetable oil solutions of C₆₀ fullerene. **L.D. Bienski, R.N. Callahan, J.A. Galvan, K.A. Morris, M. Wirianto**
- CHED 1049.** Ambient and UHV STM studies of metal surface restructuring by amino acids. **A.L. Lee, H.R. Morgan, J.A. Phillips, L.E. Jackson, E.V. Iski**
- CHED 1050.** Probing the interactions of polyethylene glycol-coated magnetic nanoparticles with human hemoglobin. **J.L. Bowers, Z. Liu, A. Fazal**
- CHED 1051.** Solution-processed templated organic semiconductor nanowires. **E. Avery, A. Haruk, J. Mativetsky**
- CHED 1052.** Toxic heavy metal removal via a recyclable gold nanoparticle complex. **O. Hull, R. Huschka**
- CHED 1053.** Nanostructured polymer lithography for photovoltaic applications. **A.J. Christy, N.L. McKibben, J.D. Harris, D. Estrada, J.S. McNatt**
- CHED 1054.** Impact of poly(ethylene glycol) molecular weight and degree of conjugation on the thermodynamics of DNA complexation and colloidal stability of poly(ethyleneimine-graft-poly(ethylene glycol)) copolymers. **R.J. Smith, R. Beck, L. Prevette**
- CHED 1055.** Deposition of gold nanoparticles on silicon via a galvanic displacement using a block copolymer technique. **R. Sronce, D. Dávila Pineda, C. Hierold**
- CHED 1056.** Double shell CdSe/ZnSe/ZnS nanoparticle spectral shifts before and after a manganese dopant is introduced. **A.N. Dobracki, S.J. Gravelle, J.K. Vohs**
- CHED 1057.** Structural and electronic properties of endohedral and exohedral derivatives of C₆₀ and C₂₄ fullerenes: TM@C₆₀, TM-C₆₀, TM@C₂₄, and TM-C₂₄ (TM = Group 11 & 12 metals): Density-functional theory investigations. **M. Gonzalez, K.A. Beran**
- CHED 1058.** Withdrawn.
- CHED 1059.** Inkjet-printed multisensor arrays on flexible substrates. **H. Mitchell, A. Wanekaya**
- CHED 1060.** Direct growth of alpha-Fe₂O₃ by vapor deposition on stainless steel as anode for Li-ion battery. **D. Phan, A. Dangerfield, A. Navulla, L. Meda**
- CHED 1061.** Chemical vapor deposition of cubic NiO nanoplates on stainless steel substrates as anode for lithium-ion battery. **C. Arnold, A. Navulla, L. Meda**
- CHED 1062.** Cyclic voltammetry study on the origin of excess capacity on ruthenium oxide. **L. Meda, A. Navulla, L. Douglas, J. Adkins**
- CHED 1063.** Synthesis of MnO nanoparticles and their electrochemical properties. **L. Leban III, M. Jones, A. Navulla, L. Meda**
- CHED 1064.** Vapor phase synthesis of cubic CoO nanocrystals as anode in lithium ion battery. **B. Tate, A. Navulla, L. Meda**
- CHED 1065.** Energetic effects of metal nanoparticle fuel additives on the combustion of ethanol. **C. Potter, P.W. Barnes**
- CHED 1066.** Fluorescence quenching in organic and inorganic solutions using gold nanoparticles. **A. King, H.G. Altmeier**
- CHED 1067.** Cheap and cost effective synthesis of metal (gold, silver)/reduced graphene oxide nanocomposites for antibacterial applications: A comparative study. **S.A. Alazzam, E.H. Alsharaeh**
- CHED 1068.** Enhanced visible light driven photocatalytic degradation of organic dyes and antibacterial properties of iron oxide/RGO nanocomposites. **M. Alturki, E.H. Alsharaeh**
- CHED 1069.** Synthesis, characterization, and antibacterial activity of reduced holey graphene. **A.S. Al Saud, S.A. Alazzam, E.H. Alsharaeh, Y. Aldawsari**
- CHED 1070.** Facile synthesis of reduced graphene oxide layer supported cobalt nanoparticles and their antibacterial activity against *E. coli*. **Y. Mussa, M. Alturki, E.H. Alsharaeh**
- CHED 1071.** Tuning the forces between conjugated nanoparticles. **G. Satishchandra, D. Venkataraman**
- Section A**
Colorado Convention Center
Halls C/D
- Undergraduate Research Posters**
Organic Chemistry
Cosponsored by SOCED
N. Di Fabio, Organizer
- 12:00 - 2:00**
- CHED 1072.** Investigation of the ability of dibenzyl sulfide and triphenylphosphine oxide to form cocrystals with carboxylic acids and phenols. **C. Kempainen, D. Adsmoed**
- CHED 1073.** Complete synthesis of analogs of a tuberculosis medication, ethambutol, with known intermediates, diethyl ethylmalonate and diethyl phenylmalonate. **K.C. Haney, D.S. Masterson, D. Rosado**
- CHED 1074.** Investigation of the ability of sulfonamide to form cocrystals with carboxylic acids. **S.H. Douglas, D. Adsmoed**
- CHED 1075.** Synthesis of novel bactericidal aminoglycosides. **A. Elleman, A. Felten, J. Weibel, P. Pale**
- CHED 1076.** Palladium-catalyzed coupling of O-benzylbenzimidoyl iodides and boronic acids. **B. Sharma Poudel, S.K. Ayer, Z. Li, K.H. Shaughnessy, T.S. Snowden, D.D. Dolliver**
- CHED 1077.** Palladium-catalyzed Songashira coupling reaction between diaryl telluride and alkyes. **J. Diaz, J. Jin, S. Zhang, C. Ailneri**
- CHED 1078.** Investigation of the non-covalent binding between benzo-crown ethers and bis(trifluoromethyl)dibenzylammonium ion. **K.A. Carter, S.L. Blosser, L. Webber, D. Nguyen, P.A. Bonvallet**
- CHED 1079.** Tethered quionolide ligands for stereoselective lactide polymerization. **E. Draper, M. Haaf, Z. Jones**
- CHED 1080.** Diversifying covalent organic framework designs through nonreversible linkages and non-planar aromatic monomers. **R.L. Snyder, A. Alsbaiie, X. Zhang, M. Haaf, W. Dichtel**
- CHED 1081.** Studies on Suzuki and Hiyama coupling of halopyridines with bromoacetates. **A.M. Walls, C. Linne, R.W. Fitch**
- CHED 1082.** Design and synthesis of multifunctional peptid-NSAID conjugates. **B. Auvil, K.L. Molchany, C. Young, A. Schell, S.C. Young**
- CHED 1083.** Desilylation and deuterium enrichment of ethynyl substituted pyridines. **B.S. Gelinas, J.A. Jaye, E.H. Fort**
- CHED 1084.** Synthesis of 3,4-bis(2-ace-toxybenzoyl)-1,2,5-oxadiazole-2-oxide. **S. Aggarwal, N.M. Wachter**
- CHED 1085.** Investigating the stereochemistry of 2-pyridinecarboxaldehyde in aldol reactions. **S. Morich, N.M. Wachter**
- CHED 1086.** Impact of cyclopentadienone substitution on the activity of (cyclopentadienone)iron tricarbonyl catalysts. **D.J. Ruff, K.P. Fodale, T.W. Funk**
- CHED 1087.** Towards the synthesis of a photo-cleavable linker for GlcNAc-ligated protein purification. **K.R. Mrugalski, R.I. Meador, T.W. Funk**
- CHED 1088.** Synthesis of diepoxy- and triepoxy c-ring analogs of triptolide: An antileukemic, male contraceptive and an anti-inflammatory diterpenoid triepoxide. **C. Fussell, S. Jiva, G.E. Rudd**
- CHED 1089.** Synthesis of HIV-1 capsid protein inhibitors based on SAR analysis. **Z. Whitescarver, J. Brown, T. Jarvis, A.K. Schrock, M.T. Huggins, M.F. Summers**
- CHED 1090.** Factors affecting the product distribution of substitution and elimination reactions: An experiment for an undergraduate organic lab. **K.N. Hipp, R.V. Macri**
- CHED 1091.** Synthesis of phthalocyanine photosensitizers for potential use in photo-dynamic therapy. **E. Baker, K.P. Schultz**
- CHED 1092.** Potassium detection using crown ethers. **M. McConville, K.P. Schultz**
- CHED 1093.** New methyl-imidazolecarboxaldehyde thiosemicarbazones ligands: NMR structural studies and complexation with Pd²⁺ to form [Pd(MIZCA-TSC)Cl] compounds. **R.E. Scott, B.C. McGill, N.P. Riggsbee, W.F. Carroll, E.C. Liscic**
- CHED 1094.** Utility of C2 substituted imidazolium room temperature ionic liquids in basic reaction media. **M.K. Gard, E.G. Ennis**
- CHED 1095.** Synthesis of dicalix[4]arenes with methylene-bridge flexible linkers. **R.S. Rabb, J.L. Fantini**
- CHED 1096.** Synthesis and reactions of a 2-oxocalix[4]arene. **I.M. Delahunty, J.L. Fantini**
- CHED 1097.** Synthesis of calix[4]arenes with a triaryl- or tetraaryllalkene group at the 2-position. **N.J. Tran, J.L. Fantini**
- CHED 1098.** Synthesis of rhodium(III) azulopyrins. **L.M. Steteman, T.D. Lash**
- CHED 1099.** Study of the substituent effects on the anti-oxidant potential of anthocyanidins: A computational investigation. **T.L. Seto, B.W. Gung**
- CHED 1100.** Mechanistic aspects of the photocatalytic peroxidation of squalene on TiO₂. **M.E. Byrd, M.L. Kaak, J.A. Ganske**
- CHED 1101.** Separation of alpha and beta sodium glucoheptonate. **E.M. Lewoczko**
- CHED 1102.** Progress toward the synthesis of (S)-curvularin. **M.W. Fultz, T. Slater**
- CHED 1103.** Synthesis of capsaicin analogs. **T. Slater, E. Higginbotham, M.W. Fultz**
- CHED 1104.** Energies and conformational preferences of perfluorinated β -furanoses. **A.A. Hunt, J.S. Rhoad**
- CHED 1105.** Synthesis and purification of aspernigrin A analogs. **L.M. Martin, P.G. Roth, A.M. Reeve**
- CHED 1106.** Efforts toward synthesis of isoindolinone core of muiranolide A. **C.A. Olson, B.L. Thompson, C. Shaner, T.A. Mitchell**
- CHED 1107.** Sequence-specific, nanomolar peptide recognition via the folding and inclusion of neighboring sidechains in cucurbit[8]uril. **D. Leach, B. Blaylock, L. Smith, O. Ali, A.R. Urbach**
- CHED 1108.** On the reaction of strained alkynes with cysteine thiolates. **G.H. Jones, M.M. Tierney, J. Chalker**
- CHED 1109.** Synthesis of dimethoxyindole-based eumelanin and indigo analogs. **W. Ryu, J.C. Quirke, J.M. Belitsky**
- CHED 1110.** Investigation of [5+2] oxidopyrylium cycloadditions. **C.R. Zwick, J.A. Simanis, T.A. Mitchell, J.R. Goodell, C.M. Law**
- CHED 1111.** Halide inhibition of the copper-catalyzed azide-alkyne cycloaddition: An NMR analysis. **B.H. Frohock, R.M. Moorman, M.B. Collier, M.D. Womble, J.M. Chalker**
- CHED 1112.** Exploring the rearrangement of complex benzylic trichloroacetimidates to benzylic trichloroacetamides. **R.J. Gilbert, A. Adhikari, J.D. Chisholm**
- CHED 1113.** Quantitative assessment of the effect of reaction variables on racemization of alpha-amino acids during amide bond formation. **A. Ott, D. Castagna, C. Jamieson, A.J. Watson**
- CHED 1114.** Preliminary assessment of volatile organic compounds (VOCs) in indoor parking facilities in the greater Houston area. **R.B. Reed, S. Tarver, B. Wilson**
- CHED 1115.** Progress toward the total synthesis of hemerocallisamines. **D. Bruce, B. Maki**
- CHED 1116.** Synthesis of antioxidants: Modified arginine derivatives. **M. Ouhoue, M. Perea, K. Molinar, B. Maki**
- CHED 1117.** Continued efforts toward the total synthesis of solomonamide B. **L. Calvo, J. Hazlerig, S.C. Butler**
- CHED 1118.** Utilization of monohalogenated alkyl halides in copper-catalyzed atom transfer radical addition (ATRA) at elevated temperature. **A.B. Jansto, T. Pintauer**
- CHED 1119.** Determination of products formed by the photolysis of 2,4,6-trinitrotoluene in seawater. **E.A. Rios, D.W. OSullivan, D.J. Luning Prak**
- CHED 1120.** Oximes derivatives from ferrocenyl chalcone as potential antibacterial agents. **N.E. Caldero-Rodriguez, I. Montes Gonzalez**
- CHED 1121.** Improving the efficiency of fluorescein diether cytochrome P450 substrates. **A.J. Milto, J. Norley, R.A. Cloyd, L. Wysocki**
- CHED 1122.** Designing an efficient and practical polarity assay for xanthene dyes. **J.S. Santana, J.C. Miller, L. Wysocki**
- CHED 1123.** New frontiers in organizing crystals by molecular shape. **M. Schutzbach, K.A. Wheeler**
- CHED 1124.** Nucleophilic [4+4] cyclodimerization of cyclopropenylmethanol derivatives to 4,9-disubstituted-2,7-dioxatricyclodecane. **T. Benin, A. Edwards, M.A. Rubin**
- CHED 1125.** Synthesis of precursors of aromatic diamidines: Bisnitriles and hydroxylamine with ether and amide as linkers. **R. Luciano, S. Colón, A. Batista**
- CHED 1126.** Synthesis, characterization, and kinetic application of tris-(2-aminoethyl) amine (TREN) ligand derivatives. **J. Connell, K.D. Oshin**
- CHED 1127.** Library synthesis of novel Xanthogluo fluorophores. **J.I. Garcia, Z. Woydziak**
- CHED 1128.** S_NAr reactions utilizing iterative decomposition of formamides. **J. Sorrentino, Z. Woydziak, J.I. Garcia**
- CHED 1129.** Study of the photodimerization of 4-vinylbenzylthymine and 4-vinylbenzyl trialkyl ammonium chloride using UV-Vis spectrophotometry and gel permeation chromatography. **N. Chen, N.E. Lee**
- CHED 1130.** Polymer bound Wittig reaction under solvent free ball milling conditions. **K. Benson, K. Leahy, J. Mack**
- CHED 1131.** Investigations of the conjugate hydrocyanation of α,β -unsaturated aldehydes in organic synthesis. **M.A. Hubbuck, W.P. Serrano, T. Black, N.C. Kallan**
- CHED 1132.** Synthesis of nonsymmetric ferrocene derivatives from 1,1'-diacetylferrocene. **S. Ramos-de Dios, I. Montes-Gonzalez, M.R. Otaño**
- CHED 1133.** Determining the benefits of alternative haircare conditioning practice. **D. Miller, H. Sklenicka**
- CHED 1134.** Microwave-enhanced synthesis involving aliphatic alcohols & other compounds. **L. Farber, K. Hess, J.M. Wetherell, K. Konieczny**
- CHED 1135.** Progress toward the synthesis of N-methyl impropag. **M.M. Siepsiak, M.A. Vanalstine-Paris**
- CHED 1136.** Synthesis and investigation of silyl-alkyl anions. **C. Duke, W.R. Winchester**
- CHED 1137.** Trends observed in solvent studies of 2-ethylhexyl chloroformate. **A. Wilson, K. Null, M.J. D'Souza**
- CHED 1138.** Kinetics and mechanism of cyclohexyl chloroformate. **L.C. Malinowski, C.E. Gross, M.J. D'Souza**
- CHED 1139.** Polyphenolic compounds from an acetone extract of *Hypericum pyramidatum*. **E. Fortier, D.K. Ngo, J. Heneks, R. Force, S. Chen, G.E. Henry**
- CHED 1140.** Xanthenes and a caffeic acid ester from an acetone extract of *Hypericum stragulum*. **S. Chen, J. Heneks, R. Force, B. Rhodes, G.E. Henry**

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

- CHED 1141.** Flavonoids and stilbenes from an acetone extract of *Hypericum stragulum*. **R. Force**, J. Heneks, S. Chen, B. Rhodes, G.E. Henry
- CHED 1142.** Chemical constituents of *Scirpus atrovirens* leaves. **M. Bruer**, J. Kizina, S. Chen, G.E. Henry
- CHED 1143.** Synthesis of indole derived fluorine-containing amino acids. **H. Cade**, M.A. Lnu, M.H. Blocker
- CHED 1144.** Lewis acid-catalyzed decarboxylative addition of keto acid to trifluoromethyl imines. **M.A. Lnu**, D. Van Leuven
- CHED 1145.** Use of Langlois' reagent in the synthesis of CF₃-containing bicyclic aromatic compounds. **L.R. Miner**, A.M. Wilson
- CHED 1146.** Selective oxazole and thiazole formation from a common intermediate. **B. Sciarra**, A.M. Wilson
- CHED 1147.** Methodology for trifluoromethylation. **T. Crandall**, A.M. Wilson
- CHED 1148.** Ozonolysis of silyl enol ethers: Synthesis of 3-silyloxy-1,2- and 3-alkyl-3-silyloxy-1,2-dioxolanes. **K. Wilson**, D.P. Soulsby
- CHED 1149.** Organic synthesis of novel SSRI analogs. **E.L. Kantor**, B. Jean, R. Lettan, J. Madura
- CHED 1150.** Quorum sensing in *P. aeruginosa*: Synthesis of natural derivatives. **M.W. Coon**, E.G. Segal
- CHED 1151.** Synthesis and evaluation of symmetrical biphenyltetrols as aggregation inhibitors for Alzheimer's amyloid- β peptide. **S.L. Wicks**, J.K. Logan, J.M. Hanna, R.K. Lammi
- CHED 1152.** In search of objective measures of molecular structural similarity. **L. Smith**, M.S. Erickson
- CHED 1153.** Survey of bracket and crust fungi for the presence of monacolin K and citrinin. **B.A. Clement**, E. Jeong, A. Teh, T. Sitorus, K.A. Morris
- CHED 1154.** Survey of pesticide presence in local honey compared with migratory bee keepers. **W.L. Nason**, S.A. Waratuke
- CHED 1155.** Evaluating the leaching of phthalates and bisphenol A from children's drinking cups. **S.A. Waratuke**, N. Monteiro
- CHED 1156.** Comparison of BPA migration levels from polycarbonate food storage containers subjected to detergents, dishwasher, and microwave use. **E.D. Umali**, S.A. Waratuke
- CHED 1157.** Antibiotic compounds isolated from fungal endophytes. **K.L. Bair**, S.J. Coval
- CHED 1158.** Synthesis of flavanones from 2-hydroxychalcones using 1*H*-1-hydroxy-5-methyl-1,2,3-benzodioxathiole 3,3-dioxide. **J. Rhoads-Lorigan**, M.W. Justik
- CHED 1159.** Derivatives of ferulic acid. **A. Feigley**, K.M. Halligan, J.J. Beck
- CHED 1160.** Synthetic modifications of hyper-valent iodine reagents. **A. Brkic**, M.W. Justik
- CHED 1161.** Oxidative-substitution reactions of polyaromatic hydrocarbons with BF₃-activated iodonium ylides of 1*H*-1-hydroxy-5-methyl-1,2,3-benzodioxathiole 3,3-dioxide. **Z. Ekstrom**, M.W. Justik
- CHED 1162.** Computational analysis of monomethylated and dimethylated Hückel and Möbius [12]-, [14]-, and [16]annulenes. **S. Luo**, G. Vinnacombe, C. Castro, W.L. Karney
- CHED 1163.** Electronic characterization of organic materials. **R. Sechrist**, J.J. Rezek
- CHED 1164.** Synthesis of small molecule inhibitors of LOX using BAPN and its derivatives. **N. Oragwam**, H. Hashim, D.M. Solano
- CHED 1165.** Progress towards *N*-alkylbenzamides as potential antimalarials. **Z. Beggs**, M.J. Campbell
- CHED 1166.** Preparation of trifluoromethylated vanillins for preparation of new curcumin. **J. Brown**, M.J. Campbell
- CHED 1167.** Environmentally conscious one pot synthesis of isoxazolines in aqueous media. **S.E. Lewis**, T.K. Carcamo, A. Avina, D.M. Solano
- CHED 1168.** Reduction of nitrobenzene derivatives using crystalline polymorphs of cobalt(II) sulfide and sodium borohydride. **L. Ramirez**, J. Gutierrez-Gonzales, J.G. Parsons, N. Izquierdo
- CHED 1169.** Preparation and NMR studies of 2-benzoyl-1-naphthols. **M. Miffin**, D.J. Crouse, T. Mathis
- CHED 1170.** General route to C-nucleosides. **J. Sheena**, A. Washington, K.J. Friedrich
- CHED 1171.** Synthesis and purification of cyclohexylphosphoserine for application as a potential phosphatidylserine analog. **T.A. Scott**, J.C. Amburgey-Peters
- CHED 1172.** Formation of a protected carbobenzyloxy-L-serine-benzyl ester cyclohexyl H-phosphonate diester towards the synthesis of cyclohexylphosphoserine as a potential phosphatidylserine analog. **J.W. Polster**, J.C. Amburgey-Peters
- CHED 1173.** Synthesis of a potential phosphatidylserine analog: Cyclohexyldiphosphoserine. **K.W. Murray**, J.C. Amburgey-Peters
- CHED 1174.** Extraction of *N*-methylcytosine from *Caulophyllum thalictroides* (blue cohosh). **L. Sluis**, M.P. Maddox
- CHED 1175.** Synthesis of homoleptic bismuth(III) sulfurylimide complexes. **D. Gingerich**, R. LaLonde
- CHED 1176.** Rapid synthesis of *N*-(4-chlorobenzyl)-*N*-methylformamide. **K. O'Keefe**, M. Bobylev
- CHED 1177.** TPEN and TPEN⁺ ligands and ATRA in polar aprotic solvent system. **E. Gorse**, A. Kaur, G. Pros, T. Pintauer
- CHED 1178.** Microwave promoted synthesis of diethyl phenylmalonate. **H. Meer**, K.A. Moon, C.C. Marvin
- CHED 1179.** Synthesis of tetrabenazine via visible light photoredox catalysis. **L.R. Orgren**, E.E. Matherick, C.C. Marvin
- CHED 1180.** Withdrawn.
- CHED 1181.** Microwave promoted malonate arylation: Regioselectivity. **J.B. Pierce**, C.C. Marvin
- CHED 1182.** "Click" synthesis of triazole-based cefotamide derivatives. **N. Swope**, S.A. Brouet
- CHED 1183.** Acetamide as a solvent in the rapid synthesis of *N*-(2,4-dichlorobenzyl) formamide. **M.A. Falkenberg**, J.A. Collins, L.I. Bobyleva, M.M. Bobylev
- CHED 1184.** Rapid synthesis of *N,N*-dipiperonylformamide. **M.A. Bell**, N.L. Gillis, L.I. Bobyleva, M.M. Bobylev
- CHED 1185.** Rapid synthesis of *N,N,N*-tri-(4-*t*-butylbenzyl)amine. **S. Park**, L.I. Bobyleva, M.M. Bobylev
- CHED 1186.** Rapid synthesis of *N,N,N*-tri-(1-naphthylmethyl)amine. **H. Lee**, L.I. Bobyleva, M.M. Bobylev
- CHED 1187.** Rapid synthesis of *N,N'*-(4-chlorobenzylidene)-bis-formamide. **S.W. Olson**, M.M. Bobylev
- CHED 1188.** Synthesis of 1,1'-ferrocenyl chalcones derivatives as potential biological active compounds. **I. Lehman-Andino**, I. Montes Gonzalez
- CHED 1189.** Synthetic approach toward attaching a pyridine based cation receptor to solid support. **M. Mills**, S.G. Tajc
- CHED 1190.** Diastereoselective dipolar cycloadditions for the synthesis of pyrazoline and pyrazolidine pharmacophores. **E.F. Dohmeier**, A. Beebe, D.C. Seaman, C.A. Castro, G. Moura-Letts
- CHED 1191.** Blue copper protein models: Characterization of copper (I/II) complexes of the N₃S₂ macrocycle 1,8-dithia-4,11-diazacyclotetradecane and derivatives. **J. Ziebiec**, I. Taschner, T.L. Walker
- CHED 1192.** Mass scale-up of pyrazolidinones and *N*-alkylation tests. **K.M. Jensen**, C.P. Jasperse
- CHED 1193.** Palladium cross-coupling reactions enhanced with aromatic co-catalysts. **A. Sterdjovich**, J.J. Rezek
- CHED 1194.** Hydrodehalogenation of aryl halides using sodium borohydride. **A. Mayhugh**, D.B. Cordes
- CHED 1195.** Preparation of a simple acetylenic poly(aryl ether). **B. Montz**, T.W. Nalli
- CHED 1196.** Synthesis and characterization of novel boron cluster carboxylic acids. **G.E. Dwulet**, M.A. Jusasz
- CHED 1197.** Liquid-liquid extraction and analysis of the antioxidant, resveratrol, from various red and white wines. **F.C. Mayville**, N.E. Brandstetter, D.L. Mandracchia
- CHED 1198.** Soxhlet extraction and analysis of capsaicin from various pepper flesh. **F.C. Mayville**, L.N. Amiano, C.P. Sulpizio
- CHED 1199.** Electrophilic aromatic substitution reactions with naphthalene and guaiazulene using ionic liquids. **F.C. Mayville**, J. Park, C.P. Saboe
- CHED 1200.** Synthesis of four putrescine analogs using 95% and 100% ethanol. **F.C. Mayville**, A.L. Cosentino, R.J. Fischer, C.J. McCarthy, H.C. Santos
- CHED 1201.** Synthesis of five spermidine analogs using 95% and 100% ethanol. **F.C. Mayville**, N.S. Carvis, D.J. McGouldrick
- CHED 1202.** 4,4'-Bis(bromomethyl) diphenyl ether as a monomer for a new poly(arylene) ether. **J. Schultz**, T.W. Nalli
- CHED 1203.** Hydrogenation using palladium nanoparticle catalysts: Functional group survey. **P.L. Ankney**, C.L. Hathaway, C.E. Harris
- CHED 1204.** Synthesis of symmetrical biphenyls using phenylboronic acids and manganese(III) acetylacetonate. **N.J. Webster**, A.M. Lelle, C. Ybarra Garcia, C.E. Harris
- CHED 1205.** Drug delivery systems utilizing modified nucleobase hydrogelators and polyamines: Synthesis of polyamines. **D. Benson**, D. Johnson, C.M. Lawrence
- CHED 1206.** Utilization of nucleobase interactions to develop supramolecular polymer hybrids. **M. Porter**, G. Glyot, C.M. Lawrence
- CHED 1207.** Drug delivery systems utilizing modified nucleobase hydrogelators and polyamines: Synthesis of modified nucleobases. **D. Johnson**, D. Benson, C.M. Lawrence
- CHED 1208.** Multiple methods for analysis of organic materials using the GC/MS. **T.L. Beck**, B.J. Karels, T.M. Pappenus
- CHED 1209.** Diastereoselective dipolar cycloadditions for the synthesis of imidazole and imidazolidine pharmacophores. **A. Beebe**, E.F. Dohmeier, D.C. Seaman, C.A. Castro, G. Moura-Letts
- CHED 1210.** Synthesis of hydrazone heterocycle for development as an organocatalyst. **S.A. Brouet**, A. Warhausen, T.F. McMillan
- CHED 1211.** Investigating the stereoselectivity of magnesium Oppenauer oxidations. **C.M. Webb**, K.J. Brown
- CHED 1212.** Natural fiber welded chitin composites. **E. Brown**, M. Brusoski, E. Fox, C. Sweet, H.C. De Long, P.C. Trulove
- CHED 1213.** Production of methyl-ester (biodiesel) using oleic acid and methanol and lipase *B. Candida antarctica*. **J. Sekhon**, R.W. Hartmann
- CHED 1214.** Stereoselective synthesis of fluorinated β -lactams. **A. Knulty**, J.C. Easdon
- CHED 1215.** Synthesis, characterization, and phototoxicity studies of paraben derivatives. **K. Becker**, S. Merrill, C. Janson, A. Schaeffer, I. Hildebrandt, K. Pate, K.S. George Parsons
- CHED 1216.** Progress toward the synthesis of fluorinated antimalarial analogs. **J. Roos**, H.E. Vaghoo
- CHED 1217.** Synthesis of the benzotropine derivative as a precursor of fluorescence labeled analogs to be used in dopamine transporter binding affinity assays. **W. Liang**, S. Xie
- CHED 1218.** Synthesis of molecular electronic components for self-assembly onto metal electrodes. **K.S. Williams**, J.E. Meany, S. Woski
- CHED 1219.** Thiosemicarbazone-derivatives from ferrocenyl chalcones as potential antibacterial and antimalarial agents. **A. Molina-Villarino**, I. Montes
- CHED 1220.** Synthesis of (2-fluorophenyl) methanol followed by an investigation of hydrogen bonding via ¹H-NMR. **Y.V. Tsai**, L. Johnson, R.N. Ferrill, R.E. Rosenberg
- CHED 1221.** Synthesis of novel GLP-1 stimulants. **O. Zamulko**, A.M. Heuer, D. Hincley, J.D. Goodwin, J.T. Ippoliti
- CHED 1222.** Synthetic investigation of Diels Alder reactions with α - β unsaturated ketones. **L. Soong**, K. Catto Bales
- CHED 1223.** Synthesis and characterization of new oxadiazole-containing compounds. **M. Packard**, J.L. Crane
- CHED 1224.** Synthesis of a novel blue light-emitter for use in organic light emitting diodes (OLED's). **M. Benda**, C. Pharr
- CHED 1225.** Synthesis of fluorescent bisimidazole sensors for heavy metals. **S. Anstatt**, B.N. Norris
- CHED 1226.** Synthesis of an alkyne-containing isoprenoid mimic for the investigation of the role of substrate length on prenyl transferase activity. **K. Caron**, J. Wollack
- CHED 1227.** Formylation of substituted phenols using microwave irradiation. **E. Young**, V.P. McCaffrey
- CHED 1228.** Progress towards the synthesis of a norbornene containing substrate for the enzyme protein farnesyltransferase. **L. Crepeau**, K. Caron, J. Wollack
- CHED 1229.** DNA binding affinity and cleavage of aryl sulfoxides. **H. Rensch**, A. Hurley Predecki
- CHED 1230.** Transesterification of hypophosphorous esters: The tales of secondary alcohols. **A.V. Carmona**, A.C. De La Cruz, S. Deprele
- CHED 1231.** Polymeric melamine-metal catalysts in Suzuki-Miyaura couplings and azide-alkyne cycloadditions. **M.A. Trafford**, G.A. Edwards, J.M. Chaker
- CHED 1232.** 1H NMR analysis of the methylation of acetic acid catalyzed by tin (II) bromide: A kinetic study. **N.L. Bayona**, R.W. Hartmann
- CHED 1233.** Synthesis of biphenyl urea derivatives related to 3-iodothyronamine. **A.S. Nijibizi**, A. Snyder, M.E. Hart
- CHED 1234.** Asymmetric design and synthetic studies of monoterpene indole alkaloid analogs. **S.L. Pilicer**, E.K. Leggans
- CHED 1235.** Reaction of *O*-silylated cyanohydrins with epoxides as an alternative for the enantio- and diastereoselective preparation of aldols. **D.R. Melendez**, A.M. Hartel
- CHED 1236.** Synthesis of enamines using copper as a catalyst. **E. Lopez Quiroz**, S.R. Hussaini
- CHED 1237.** Diversity oriented synthesis of an alkaloid-like library via cyclotrimerization of easily accessible aminonitriles. **N.M. Chang**, A. Bates, J.A. Santos, C.W. Livesey, G.J. Haun, C.B. Stein, N.A. Lopez, G. Moura-Letts
- CHED 1238.** Cross-coupling reactions of fluorinated aryl chlorides and aryl chloride acetals with 1-hexylmagnesium bromide. **G. Camassi**, K.J. Brown
- CHED 1239.** Synthesis of highly substituted anthraquinone derivatives via microwave assisted self-condensation of benzoic acids. **L. Holokai**, J.J. Rezek
- CHED 1240.** GC-MS analysis of phytosterol content of dried mushrooms. **A.M. Overgard**, T.W. Nalli
- CHED 1241.** Preparation of functionalized dendrimers and their effectiveness in organocatalytic reactions. **A.R. Flynn**, A. Kopp, N. Brown, T.N. Jones, M. Cloninger
- CHED 1242.** Direct esterification of H₃PO₄: A Dean Stark methodology. **J.N. Sanchez**, A.M. Castillo, S. Deprele
- CHED 1243.** Synthesis of α -chalcones and derivatives via a microwave Knoevenagel condensation. **A.A. Bayly**, M.J. Pesch, A. Gogos, B.C. Weideman, S.R. Sieck
- CHED 1244.** Diversification of thiol phosphonamides. **J.L. Fulton**, K.R. Sittig, M.A. Hardy, S.R. Sieck
- CHED 1245.** Characterization of α -substituted chalcones. **B.C. Weideman**, P. Leger, S.R. Sieck

- CHED **1246**. Purposeful biofilm disassembly with unnatural alkyl and aromatic D-amino acids. **K. March**, M.A. Bertucci
- CHED **1247**. Manipulation of n to π^* orbital interactions in the hydrolysis of *para*-substituted *N*-acyl homoserine lactones. **S.R. Dunbar**, M.A. Bertucci
- CHED **1248**. Intramolecular oxazolium salt/azomethine ylide cycloaddition reactions with varying dipolarophile tether position. **S.L. Wolfe**, D.L. Warner
- CHED **1249**. Microwave accelerated deprotections of aryl silyl ethers. **A. Boyington**, R.D. Crouch
- CHED **1250**. Look at biodiesel produced using *Chlorella vulgaris* microalgae. **M. Centore**, D. Fish
- CHED **1251**. Structural elucidation of pyrrolizidine alkaloids from *Arnoglossum plantagineum*. **E.L. Feldkamp**, K. Chattin, R.R. Christensen, R.B. Kelley
- CHED **1252**. Studies on "under air" direct arylation. **L. Armstrong**, J. Fritz, T. Murray
- CHED **1254**. Reactions of the highly pyramidalized alkene pentacyclo[4.3.0.0^{2,4}.0^{3,6}.0^{5,7}]non-4-ene. **M.A. Forman**, C. Adams, A. Savarese
- CHED **1255**. Studies toward the synthesis of altersolanol P. **M. Hensinger**, A. Smaligo, S.M. Kennedy
- CHED **1256**. Studies toward the synthesis of Hunanamyacin A and its derivatives. **S.M. Kennedy**, J. Dreier
- CHED **1257**. Microwave synthesis and cytotoxicity studies of novel amino-substituted chalcones. **J.C. Bradshaw**, R.E. Tucker, J.E. Bradshaw
- CHED **1258**. Synthesis and characterization of a reversible carceplex. **K. Nogales**, D. Nogales
- CHED **1259**. Construction of the Choi framework. **S. Wytovich**, J. Tropp, M.S. Leonard
- CHED **1260**. Progress towards the synthesis of 2-amino-1,3-dihydroxyphosphonates via oxazolidinone phosphonates. **B.A. Gibson**, S.M. Hurlle, K.J. Graham, T.N. Jones
- CHED **1261**. Progress on the synthesis of a fluorescent lead(II)-trapping coumarocryptand. **J. Wilson**, M.R. Baar
- CHED **1262**. Antiaromatic dications containing sulfur: Dications of sulfur analogues of tetrabenz[5.5]fulvalene. **W. Mobley**, N.S. Mills, V. Romano
- CHED **1263**. Relationship between delocalization and antiaromaticity in 5,5'-bisindenylidene dications. **P. Poliak**, C. McKay, N.S. Mills
- CHED **1264**. Exploring and optimizing new palladium-catalyzed reactions. **R.T. Dove**, W.E. Brenzovich
- CHED **1265**. Optimizing the purification of diarylacetic acid derivatives. **A. Denton**, W.E. Brenzovich
- CHED **1266**. Synthesis and characterization of curcumin ferrocenyl analogs. **J. Rivera Hernandez**, M.R. Otaño, I. Montes, R. Gutiérrez, Y. Rivera-Torres, D.J. Sanabria Rios, E.E. Colón Lorenzo, A.E. Serrano Brizuela, M.D. García Maldonado, A.R. Guadalupe Quinones
- CHED **1267**. Factors affecting aggregation of beta-sheets. **B.R. Linton**, E.R. Kuhn
- CHED **1268**. Hydrogen bonding principles and synthetic beta-sheet mimics. **E.J. Schneider**, B. Linton
- CHED **1269**. Benzylideneanilines and benzonitrile oxides: Solid-state structure and reactivity studies. **K. Kassekert**, W.H. Ojala
- CHED **1270**. Effects of molecular structure on crystal structure and solid-state reactivity of some nitrogenous organic compounds. **K. Van Auken**, W.H. Ojala
- CHED **1271**. Solid-state structures and reactivity of some nitrogen-containing organic compounds. **B. Vickerman**, W.H. Ojala
- CHED **1272**. Structures and reactivity of some nitrogenous organic solids. **J. Dhami**, W.H. Ojala
- CHED **1273**. Synthesis of aziridinomitosene anticancer analogs that vary at the C6/C7 positions. **S. Irving**, R. Olsen, R. Reeves, D.L. Warner
- CHED **1274**. Developing a synthesis of α -diazoamides. **L. Terrab**, S. Moss, J. Unger
- CHED **1275**. Transition metal-catalyzed coupling of organic sulfonates and metal azides. **F. Xu**, R. Rowlands, J. Unger
- CHED **1276**. Studies toward total synthesis of axinellolide A and its analogs. **Z.A. Rumlow**, L. Wiles, M. Walczak
- CHED **1277**. Synthesis of core-substituted naphthalene diimide derivatives. **L. Abocad**, J.J. Reczek
- CHED **1278**. Surface orientation analysis of naphthalene diimides using infrared spectroscopy. **R. Antonio**, J. Reczek
- CHED **1279**. Investigations of green and microscale methods in the synthesis of several flavones. **P. Martinez**, M. Davis, N. Gammons, P. Powers
- CHED **1280**. Computational study on the high temperature isomerization of phenanthrene. **B. Fregoso**, C. Castro, W.L. Karney
- CHED **1281**. Antibacterial activity of cefotaxime and terpenes. **E. Haiderer**, E. Campau
- CHED **1282**. Analysis of porphyrin doped thiophene nanoparticles as potential water oxidizing catalysts. **R. Bogdan**, W.M. Ames
- CHED **1283**. Stabilized copper(I) N,S containing cryptands. **V. Keehn**, I. Taschner, T.L. Walker
- CHED **1284**. Adapting a conventional synthesis of dihydrotetrazines to microwave conditions. **C. Bethae**, M. Druelinger, D.L. Dillon
- CHED **1285**. Energy decomposition analysis to predict the explicit solvent shell in the keto-enol tautomerism of acetylacetone in water, acetone, and chloroform. **V. Deturi**, C.C. Jenkins, T. Reeves
- CHED **1286**. Synthesis, characterization, and analysis of diarylylidene-piperidone analogs of curcumin. **Z. Ligus**, D. Fish
- CHED **1287**. Effect of aromaticity on the stability of isonitriles prepared from the deprotonation/metalation of oxazolic species. **W. Howitz**, R.S. Majerle
- CHED **1288**. Synthesis of β -fluoroamines from alkenes. **J.M. Mutz**, M.L. Druelinger
- CHED **1289**. Synthesis and characterization of potential polyol antifreeze coatings on glass substrates. **D. Vandemark**, E. McGurk, J. Hall, P.W. Baures
- CHED **1290**. Analogs for blue copper protein: Thio-pendant arm derivative of 9[ane]S₃N. **K. Tomczak**, I. Taschner, T.L. Walker
- CHED **1291**. Role of acetic acid in kinetic isotope effects observed in Pd(IiPr)(OAc)₂(H₂O) catalyzed oxidation of alcohols. **B. Lampkin**, J.A. Mueller
- CHED **1292**. Investigation of the role of Hagemann's ester as a catalyst for natural product synthesis. **M. Samoriski**, D. Fish
- CHED **1293**. Synthesis of symmetric and asymmetric porphyrins. **C.L. Carter**, E.M. Mitchell
- CHED **1294**. Synthesis and properties of donor- π -acceptor polyene dyes with azacycloalkane donors. **G.R. Ashley**, D.J. Keith, C.O. Adereti, H.O. Bradley, A.C. Friedli
- CHED **1295**. Synthesis of secondary amines. **A. Westlie**, J.T. Ippoliti
- CHED **1296**. Template-catalyzed polymerization of modified DNA nucleosides. **A. Cragoe**, M.P. Maddox
- CHED **1297**. Synthesis and experimental and computational analysis of curcumin derivatives and their difluoroboron complexes. **K. Paavola**, R. Ciochina, K.E. Johnson
- CHED **1298**. Concerted nature of isocyanate reactions with alkenes. **K. Alexander**, C.J. Licata, R.D. Robinson, D.F. Shellhauer
- CHED **1299**. Cu(I)-complexes as photoredox catalysts: An alternative to Ru(bpy)₃²⁺. **M.S. Maple**, D. Hockersmith, T. Peelen
- CHED **1300**. Synthesis and analysis of a series of *N*-acetyl D-glucosamine derivatives as organogelators. **K. Mays**, A. Chen, G. Wang
- CHED **1301**. Synthesis and characterization of glucose triazole derivatives as organogelators. **H. Mangunuru**, D. Liu, A. Espiritu, G. Wang
- CHED **1302**. Self-healing polymers: Studies of the Diels-Alder reaction between furan and *N*-4-fluorophenylmaleimide. **T.A. Wells**, W.G. Hollis, P.A. Deck, J.B. Stegall
- CHED **1303**. Self-healing polymers: Synthesis of highly-fluorinated dienes and their model Diels-Alder reactions. **D.E. Layo**, W.G. Hollis, P.A. Deck, J.B. Stegall
- CHED **1304**. Synthesis of resveratrol. **B.L. Bradley**, G.L. Milligan
- CHED **1305**. Synthesis of 5- and 6-(4-fluorophenyl)-*N*-acetylglucosylamides. **N. Ngo**, A. Umhire-Juru, S. Hernandez, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin
- CHED **1306**. Synthesis of 5- and 6-(4-methoxyphenyl)-*N*-acetylglucosylamides. **A. Umuhire-Juru**, S. Hernandez, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin
- CHED **1307**. Synthesis of aspartame *N*-acetylglucosylamides: A sweet reaction. **S. Hernandez**, A. Umhire-Juru, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin
- CHED **1308**. Green synthesis of spiropyrrolidines from isatin, proline, and *E*-4-phenylbut-3-en-2-ones. **J. Murdock**, L. Desrochers, T.E. Goodwin
- CHED **1309**. Enantioselective synthesis and characterization of phase 1 warfarin metabolites. **R. Nshimiyimana**, L. Desrochers, G.P. Miller, T.E. Goodwin
- CHED **1310**. Synthesis of 5- and 6-(4-trifluoromethylphenyl)-*N*-acetylglucosylamides. **F. Musariri**, A. Umhire-Juru, S. Hernandez, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin
- CHED **1311**. Salt formation of potential acetylcholine esterase inhibitors. **S. Hickmann**, L.P. Dennis, T.L. Greiman, T.K. Nguyen, D.M. Sikazwe, B.F. Wood, J.M. Davis
- CHED **1312**. Design and synthesis of potential acetylcholine esterase inhibitors. **L.P. Dennis**, K.N. Gorena, S. Hickmann, T.K. Nguyen, G.L. Tristyn, D. Hernandez, D.M. Sikazwe, B.F. Wood, J.M. Davis
- CHED **1313**. Preliminary testing of *N*-benzyl isonipicotate derivatives as a potential acetylcholine esterase inhibitors. **T.K. Nguyen**, L.P. Dennis, T.L. Greiman, B.F. Wood, J.M. Davis
- CHED **1314**. Molecular docking of isoform-selective histone deacetylase 2 (HDAC2) inhibitors. **N. Brusman**, E.M. Hogle, R. Kline, E.J. Merino, S.F. Paula, L. Ma
- CHED **1315**. Kinetic control mechanism: 1,2 vs. 1,4 addition in conjugated dienes. **J. Painter**, D.J. Oostendorp
- CHED **1316**. Use of dimethoxymethane in place of chloromethyl methyl ether to prepare methoxymethyl (MOM) esters. **N. Meckes**, G.L. Milligan
- CHED **1317**. Isonitrile ligands in iron-catalyzed Kumada couplings of *N*-aryl chloride. **K.C. Dornhofer**, M.C. Perry
- CHED **1318**. Role of dialkylmagnesium species in the cobalt-catalyzed Kumada coupling of aryl bromides. **J.M. Myles**, M.C. Perry
- CHED **1319**. Synthesis of NHC ligands for use in iron- and cobalt-catalyzed cross-coupling reactions. **J.A. Montemurro**, M.C. Perry
- CHED **1320**. Synthesis of (-)-durynie and homologues. **M. Keener**, D.B. Ball
- CHED **1321**. Microwave synthesis of *N*-phenyl succinimides and malenamides in undergraduate organic chemistry laboratory. **T.F. Guetzloff**, B. Dudding, M. Guetzloff, M.W. Fultz
- CHED **1322**. Synthesis and characterization of furan-based ligands for use in lactide polymerization. **B. Kasting**, A. Anderson-Wile
- CHED **1323**. Withdrawn.
- CHED **1324**. Caged phosphates in organic molecules. **A. Dame**, B.R. Sculimbrene
- CHED **1325**. Catalytic asymmetric monophosphorylation of diols. **M. Lougee**, B.R. Sculimbrene
- CHED **1326**. Synthesis of an amine-containing cyclooctyne via an intramolecular Nicholas reaction and subsequent dipolar cycloaddition with benzyl azide. **S. Huang**, G. Ortiz, K.M. Shea
- CHED **1327**. Evaluation of copper photocatalysts in the enantioselective α -alkylation of aldehydes. **M.R. Hurst**, C.L. Kotelman, K.H. Jensen
- CHED **1328**. γ -Cyclodextrin mediated photoheterodimerization between cinnamic acids and coumarins. **A. Clements**, M. Pattabiraman
- CHED **1329**. Probing the effects of conformation on concerted proton-electron transfer. **M. Vettleson**, I. Rhile
- CHED **1330**. Characterizing the excited states of multiple carbene and nitrene reactive intermediate precursors: A computational study. **V.E. Pane**, S. Vyas
- CHED **1331**. Complex decalin formation through the use of an asymmetric Rauhut-Currier reaction. **A. Friant**, W.P. Malachowski
- CHED **1332**. Development of π -stacking compounds for stationary phase modification. **T.G. Trimble**, G. Lohani, B.A. Logue, K.H. Jensen
- CHED **1333**. Synthesis of polymers for organic light emitting diodes. **A. Place**, J. Birmer, A. Ephron, A. Schroeder, D. Speed, J. Mimmis, N. Jackson, A.K. Schrock, M.T. Huggins
- CHED **1334**. Synthesis and recrystallization of diapocynin and its derivatives. **C.R. DeClerck**, B.L. Coffaro, D.K. Johnson
- CHED **1335**. Gold catalyzed cross-coupling using arenediazonium salt as the oxidant. **E.Y. Aguilera**, X. Shi
- CHED **1336**. Exploration of long chain dialdehydes for use as linkers in catalytic metalloporphyrins. **C.E. Gehman**, W.M. Ames
- CHED **1337**. Structural changes induced by 8-Oxo-7,8-dihydroadenosine in RNA oligonucleotides may result in loss of function of RNA aptamers. **A. Chauca-Diaz**, Y.J. Choi, M. Resendiz
- CHED **1338**. Biological degradation of acetaldehyde in marine waters. **M.K. Senstad**, W.J. De Bruyn, C.D. Clark, S. Hok, O. Barashy
- CHED **1339**. Reverse anomeric effect-mediated synthesis of carbohydrate 1,2-orthoesters. **M.J. Obrinske**, W. Du
- CHED **1340**. Solvent-free synthesis of biologically active stilbene derivatives. **J.L. Dickson**, S.A. Angel
- CHED **1341**. Synthesis of 2,5-disubstituted 3-fluorothiophenes from 2-thienyl carbamates via a directed fluorination/cross-coupling approach. **N. Onuska**, J. Zhang, A.J. Sead, P. Sampson
- CHED **1342**. Au(I) catalyzed imine formation from α -diazoesters and azide. **E.J. McClain**, X. Shi
- CHED **1343**. Expansion of electrophile scope in the transition metal-catalyzed coupling of Corey-Seebach *umpolung* reagents. **E. McKinsty**, J.R. Schminck
- CHED **1344**. Intramolecular halogen bonding of fluorinated haloarenes in solution. **R.A. Thorson**, G.R. Woller, Z.L. Driscoll, B.E. Geiger, C.A. Moss, A.L. Schlapper, E.D. Speetzen, E. Bosch, M. Erdelyi, N.P. Bowling
- CHED **1345**. Manipulating the electronic properties of aryleneethynyls with halogen bonding. **G.R. Woller**, N.P. Bowling

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

CHED 1346. Intramolecular halogen bonding of non-activated aryl halides in solution. **E.R. Robinson, D.L. Widner, N.P. Bowling**

CHED 1347. Metal binding and electronic properties of aryleneethynylene trapezoids. **Z. Driscoll, E. Bosch, N.P. Bowling**

CHED 1348. Novel method of stereochemical management of Morita-Baylis-Hillman chemistry: Controlled acrylate ester synthesis. **R. Vaclav, J.A. Struss**

CHED 1349. Total synthesis of the cyclic depsipeptide natural product Aspergillicin A, and investigation of its cell permeability, pharmacokinetic property, and bioactivity. **C.L. Etienne**

CHED 1350. Multicomponent reaction to produce diversely substituted 2-imidazolines. **A. Ellsworth, R.A. Mosey**

CHED 1351. Click, click, cyclize: Amino wester-derived β -ketosultams via Dieckmann cyclization of the corresponding methylsulfonamides. **T.R. Atkinson, M.Y. Hur, J.H. Jun, P.R. Hanson**

CHED 1352. Synthesis of functionalized biscavitands. **M. Escamilla, J. Buenafior, L.M. Tunstad**

CHED 1353. Structural studies of oligonucleotides of RNA containing 7,8-dihydro-8-hydroxyadenosine. **Y. Choi, A. Chauca-Diaz, M. Resendiz**

CHED 1354. Investigating the use of copper photoredox catalysts in an enantioselective reaction. **S.A. Souder, K.H. Jensen**

CHED 1355. Synthesis of conformationally constrained diarylether cyclophanes. **H.I. Caldera**

CHED 1356. Anion-responsive liquid crystals. **K. Grabias, L. Lam, P. Cohn, H. Martinez**

CHED 1357. Synthesis and characterization of novel polyester polyols. **B. Thompson, K.D. Ulrich, W.D. Coggio**

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Physical Chemistry

Cosponsored by SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED 1358. Asymptotic behavior of travelling wave solutions to reaction-diffusion equations. **M.M. Nason, S. Bricher**

CHED 1359. Interfacial interactions and adhesion properties of selected monomer and polymers probed by SFG spectroscopy and atomic force microscopy. **K.A. Gimatu, K. Hafer, S. Chan, C.A. Ng**

CHED 1360. Why is there order in the purple membrane? A biological application of ultrafast Raman imaging. **K. Wilhelm, W.R. Silva, R.R. Frontiera**

CHED 1361. Structures and CH...O interactions of fluorinated ethylene...carbon dioxide complexes as determined by microwave spectroscopy. **R.E. Dorris, C.L. Christenholz, A.M. Anderton, R.A. Peebles, S.A. Peebles**

CHED 1362. Electronic spectroscopy of gold sulfide (AuS). **B. Pearlman, I. Wyse, T.D. Varberg, D. Kokkin, T. Steimle**

CHED 1363. Investigation of the spectroscopic properties of newly synthesized pyrimidines. **L. Streacker, N.M. Karn**

CHED 1364. Gas-phase reactions of Cu⁺ (^S, ^D) with CF₃CH₂Cl, CF₂CH₂CH₂Cl, and CF₂CH₂CH₂Br: Proximity effects in substrates with competitive reactive sites. **B.A. Scheuter, X.S. Redmon, W.S. Taylor**

CHED 1365. Photodecomposition of phenylalanine on the surface of titanium dioxide. **C. Arp, B. Molnar, H.M. Bevesek**

CHED 1366. State-specific reactions of Cu⁺ (^S, ^D) with SF₆ and SF₅Cl: Thermochemical control over product formation. **X.S. Redmon, B.A. Scheuter, W.S. Taylor**

CHED 1367. Thiol based adsorbate detection using Surface Enhanced Raman Spectroscopy. **M. Gray, E. Bean, A. Deckert**

CHED 1368. Electron stimulated desorption and post-irradiation analysis in a single ultrahigh vacuum chamber. **C. Belvin, J. Zhu, C. Arumainayagam**

CHED 1369. Metastable fragmentation and photofragmentation of photoionized thiophene clusters. **M.W. Krone, D.A. Hales**

CHED 1370. Computational study of nitrogen oxide decomposition by copper exchange ZSM-5 zeolites. **J. Rumley, H.K. Hernandez**

CHED 1371. Determination and prediction of infinite dilution equivalent conductivities for ions in water at high temperatures and pressures. **S.J. Davis, G.H. Zimmerman**

CHED 1372. Characterization of novel cyano-based room temperature ionic liquid electrolyte for lithium-ion batteries. **A. deKeraty, T. Bergholz, C. Korte**

CHED 1373. Revisiting water radiolysis. **J. Lukens, M. Marković, S. Abdullahi, C. Arumainayagam**

CHED 1374. Silica sol-gels containing calcein blue as surface-enhanced Raman spectroscopy (SERS) sensors for metal ions. **E.R. Carlson, E.J. Atkinson, B.D. Gilbert**

CHED 1375. Xenon-129 NMR and surface tension of aqueous micelle solutions. **J. Wetmore, T. Endreo, S. Grant, A. Calhoun**

CHED 1376. Ammonia radiolysis of astrochemical interest. **H. Cumberbatch, Z. Peeler, K. Tran, C. Arumainayagam**

CHED 1377. Kinetic modeling of catalytically active aerogels. **Y. Cao, M.K. Carroll, A.M. Anderson**

CHED 1378. Kinetics of aminopropyl-triethoxy silane on porous silicon and subsequent reaction with 4-(methylthio) benzoyl chloride studied using FTIR. **S. Kennemuth, B. McCauley, A. Deckert**

CHED 1379. Colloid particle motion and aggregation in silica aerogels: Experiment and simulation. **K.A. Mengle, J.N. Richardson, J. Kegerreis**

CHED 1380. Determination of the hydrogen bond effect on nitrile vibrational frequency through solvatochromic models. **H. Sun, R.S. Moog**

CHED 1381. Computational analysis of conformational tunneling of glyoxylic acid. **V.T. Lim, K. He, W.D. Allen**

CHED 1382. Surface IR spectroscopy and computational study of MhDA on GaAs(100) surface. **H.M. Barroso, H.K. Hernandez**

CHED 1383. Diffusion of alkylbenzenes in *n*-alkanes. **P.M. Register, B.A. Kowert**

CHED 1384. Characterization of an ethanol-benzene complex using matrix isolation infrared spectroscopy. **M. Silbaugh, J.C. Amicangelo**

CHED 1385. Conformational elucidation of diphenylureas in varying solvent environments. **D.L. Ali, J.F. Galan, M.I. Galinato**

CHED 1386. Synthesis and extraction of metal-carbohydrides. **C. Shelmire, B. May**

CHED 1387. Reaction mechanism for the conversion of creatine to N-formyl-N-methylglycine by hypochlorous acid in aqueous solution. **M.C. Williamson, C.A. Lareau, L.A. Clough, A.J. Becker, G.H. Purser**

CHED 1388. Energetic, structural, and spectral data for noble gas hydride cations in the interstellar medium. **R.A. Theis, W. Morgan, R.C. Fortenberry**

CHED 1389. Spectroscopic and microscopic analysis of aggregation effects in N-alkylated perylene diimides. **A. Austin, J.M. Szarko**

CHED 1390. Role of low-energy (< 20 eV) electrons in astrochemistry. **K.D. Tran, S.M. Abdullahi, C. Arumainayagam**

CHED 1391. Calculating the J=0 vibrational states of noble gas trimers using an energy selected basis. **J. Yudichak, J. Montgomery**

CHED 1392. Analysis of the metal sulfate-sodium silicate "reverse chemical garden" reaction. **S. Partovi, H. Basinger, C. Jensen, G. Miter, S. Ogden, M.A. Horn**

CHED 1393. Matrix isolation studies of tetrakis(dimethylamino)titanium IV & ozone. **H. Mosley, B.S. Ault**

CHED 1394. Investigating the influence of lithium intercalation on dispersive electron mobility kinetics in dye-sensitized solar cells. **M.A. McFarland, I.J. McNeil**

CHED 1395. Thermodynamics contribution to the stability of PrP^C in model plasma membranes. **P. Soto, R. Gonzales**

CHED 1396. Computational and crossed molecular beam study in the synthesis of boronyllene. **B. Ganoie, S. Maity, R. Kaiser, R.J. Bartlett**

CHED 1397. Characterization and the effect of pH and temperature on the degradation of creatine ascorbate, di-creatine ascorbate and creatine di-ascorbate. **M.A. Henneberry, A.S. Wallner**

CHED 1398. Investigating the neutron inelastic scattering crossSections for ¹⁶Fe through γ -ray spectroscopy. **A.J. French, S.F. Hicks, B.P. Crider, T.J. Howard, S.H. Liu, M.T. McEllistrem, R.L. Pecha, E.E. Peters, F.M. Prados-Estévez, T.J. Ross, Z.C. Santonil, J.R. Vanhoy, S.W. Yates**

CHED 1399. Compositional characterization of cobalt lithium phosphate thin films using atomic absorption spectroscopy. **A.M. Bluhm, J.M. Clements, C. Heideman**

CHED 1400. Driving forces of the stability of Alzheimer's A β aggregates in model membranes. **C.R. Bertsch, B. Aoki, P. Soto**

CHED 1401. Vacuum ultraviolet photolysis matrix isolation infrared spectroscopy of GeH₄ in argon and nitrogen matrices. **P. Mott, J.C. Amicangelo**

CHED 1402. Sum frequency generation at the DMSO/air interface: Theory meets experiment. **T. Ueltschi, A.L. Milfin, P.Z. El-Khoury, H. Wang**

CHED 1403. Determination of the limiting equivalent conductivity and thermodynamic equilibrium constant for the formation of LaC²⁺ ion-pairs in water. **E. Thompson, G.H. Zimmerman**

CHED 1404. Accurate quantum models of methylphosphonate adsorption onto a stable rutile surface. **S.W. Clifford, M.N. Smeck, E.S. Gawalt, J.D. Evansack**

CHED 1405. Synthesis and characterization of indium phosphide quantum dots for use in laser diodes. **J. Charlonis**

CHED 1406. Rovibrational analysis of SiOH⁺, HSiO⁺, and other third row atom hydroxides. **M. Kitchens, R.C. Fortenberry**

CHED 1407. Impact of tetrazine location in benzobisaxozole possessing cruciforms. **J. Ellett, A.L. Tomlinson**

CHED 1408. Proposal for a more efficient acoustic array design to determine flow through a cylindrical conduit. **K.J. Ham, A. Shue, K. McGill**

CHED 1409. Kinetics and dynamics of the photorearrangement reactions of aryl-substituted thiophenes. **D.J. Morrow, J.M. Wasylenko, C.G. Elles**

CHED 1410. Characterization of a methanol-hexafluorobenzene complex using matrix isolation infrared spectroscopy. **C.M. Kindle, J.C. Amicangelo**

CHED 1411. Microparticle transport across ionic liquid based interfaces. **M. Ngan, D. Frost, L. Dai**

CHED 1412. Location of deuterated ammonia in Sagittarius B2. **A. Clements, E. Mills**

CHED 1413. Synthesis of chloromethylsilyl isocyanate. **S. Askarian, G. Guirgis, T. Barker**

CHED 1414. Sustained photocurrent in CdS/ α -Fe₂O₃ stacked thin films on titania-coated transparent conductive substrates. **T.C. Douglas, C. Harris**

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Polymer Chemistry

Cosponsored by PMSE, POLY and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED 1415. Gel properties of polyisoprene and stearic acid shape memory composite. **B.J. Hukill, N. Brostowitz, K.A. Cavicchi, R.A. Weiss**

CHED 1416. Smart hydrogel thin films for organophosphorus nerve agent detection. **C. Whitaker, N.R. Kaufmann, J.J. Snyder**

CHED 1417. Synthesis and characterization of polyaniline-TiO₂ nanocomposites. **J. Dickens, A. Stimmell, A.O. Sezer**

CHED 1418. Ring-opening metathesis polymers (ROMP) with organic radical groups for treatment of traumatic brain injuries (TBI). **K.A. Orr, H.J. Schanz**

CHED 1419. Synthesis and characterization of 3-trifluoromethylstyrene copolymers. **K.M. Dubiak, R.W. Kopitzke**

CHED 1420. Novel polymeric redox mediator for use in biofuel cells. **A.J. Halmes, M. Retherford, D.T. Glazhoffer**

CHED 1421. Phase-selective studies of polyisobutylene-bound dyes using anti-leaching agents. **C. Torres-Lopez, M.L. Harrell, D.E. Bergbreiter**

CHED 1422. Synthesis of hierarchically porous polymer network for carbon dioxide capture. **A. Siwinski, H. Gao, D. Lee**

CHED 1423. Synthesis of four-armed calixarene-core polylactide/polyethylene glycol star block copolymers using click chemistry. **K.A. Bogner, A.C. Falls, P.S. Corbin**

CHED 1424. Investigating the polymerization mechanism of cyanoacrylate with fingerprint constituents. **K. McCarthy, E.M. Persson, A.S. Dutton**

CHED 1425. Synthesis of a macroinitiator and its use in the preparation of poly(styrene-*b*-methacrylonitrile): An advanced undergraduate laboratory project in polymer chemistry. **B.A. Arce, L. Calvo, H.N. Gray, S.C. Butler**

CHED 1426. Synthesis of aloelectin-containing latexes by emulsion polymerization. **A. Johns, M. Channell, M. Ming, R. Quirino**

CHED 1427. Synthesis and applications of ionic liquid monomers in free radical polymerizations. **M. Sea, B. McFarland**

CHED 1428. Synthesis of high molecular weight poly(ϵ -caprolactone) star polymers and their degradation properties. **R.L. Collette, K.A. Boduch-Lee**

CHED 1429. Synthesis and polymerization of (*E,E*)-[6,2]-(2,5)furanophane-1,5-diene. **N. Doppler, J. Glans**

CHED 1430. Biocompatible material used for drug delivery. **A. Gomez, G. Craft, J. Harmon**

CHED 1431. Poly(ionic) liquids: Imidazoles with ester linkages. **M.A. Andrews, M.J. Campbell**

CHED 1432. Synthesis of metal-organic frameworks for adsorption of disease-relevant peptides. **B.J. Karels, Z. Mensinger, M.W. Smith**

CHED 1433. CdSe quantum dot band edge tuning through photooxidation on nanopatterned polymers for applications in hybrid cell photovoltaics. **J. Custer, J.D. Batteas, N. Stinglein**

CHED 1434. Synthesis of sustainable monomers for a polyurethane. **C. Johnston, E. Black, L. Salzi, C.P. Schaller**

CHED 1435. NMR study of the active form of the polymerization catalyst formed between T²Rh(cod) and 4-ethynyltoluene. **H.K. Blakely, R.M. Tarkka**

CHED 1436. Titanium and tantalum complexes bearing optically active tartrates as catalysts for the polymerization of D,L-lactide. **T. Bumpus, M. Holcomb, B.M. Chamberlain**

- CHED **1503**. Expanding our community involvement. **T. Ebener**, M.E. Jöhl, P.K. Yong, T.L. Thacker, J. Damron, M. Allen, R. Marlett, L. Tomaszewski, A. Schalk, A. Molin
- CHED **1504**. Student chapter events and activities done at Tennessee Tech University. **K. Richards**, M.P. Butner, S.B. Reynolds, S.M. Amin, B.C. McGill, V. Sublett, A. Renodemic, A.J. Ferry, A.J. Crook, D.J. Swartling
- CHED **1505**. Non-Newtonian fluids as a student affiliates chapter event: Chemistry, logistics, and outreach. **A.M. McCollum**, A.M. Longo, K.J. Goosherst, L.M. Jablonski, M.L. Kaak, A. Li, D.G. Sacenti, D.B. Green, J.M. Fritsch
- CHED **1506**. ACS student affiliates chapter of Seattle Pacific University. **S. Eng**, R. Hawkins, R. Kenyon, K.M. Pierce
- CHED **1507**. American Chemical Society Student Chapter at The University of Texas at Tyler. **P. Martin**, B. Western, J.J. Smee, L.E. Boyd
- CHED **1508**. Activities of Ferris State University student affiliate chapter. **E.K. Utke**, L. Bass, K.J. Robb
- CHED **1509**. Discover gold with the Alchemist Club at Missouri Western State University. **A.J. Luke**, S. Warren, S.P. Lorimor
- CHED **1510**. NSF Community College Innovation challenge: A proposal. **A.J. Sanders**, J. Weber, S. Comshaw-Arnold
- CHED **1511**. Saint Francis University Chemistry Club: Safe but fun. **S. Ciraula**, C. Fry, D. Mosier, E.P. Zovinka
- CHED **1512**. Discerning student interest in science activities. **M. Love**, A. Bilbrough, A. Wilson, M.J. D'Souza
- CHED **1513**. Wayne State University ACS Student Affiliates. **K. Mullan**, S.A. White, R. Dixon, Y.K. Elghoul, A.R. Breckenridge, M. Farhat, R. Donovan, H. Ahmed, J.A. Degg, J.L. Fischer
- CHED **1514**. Belmont SMACS: Engaging in awesome science. **A.B. Moore**, V.T. Lim, L. Patel
- CHED **1515**. Molloy Chemical Society. **A. Stockhausen**, M. Pogash
- CHED **1516**. SIUE Chemistry Club: Promoting science education on campus and beyond. **A. Fox**, D. Wright, M. Ontl, A. Cox, S.B. Luesse
- CHED **1517**. American Chemical Society Student Chapter at Peninsula College. **B. Weintraub**
- CHED **1518**. Gruen Chemistry Society: Student affiliate activities at Olivet College. **M. Piper**, A. George, Z. Kitzmiller, T. Thorn, S.M. Lewis
- CHED **1519**. Millersville University ACS Student Chapter 2014-2015. **D. Hofmann**, J. Charlonis, J. Dreer, H. Ashberry
- CHED **1520**. Improving leadership and programming: Finding the balance between quality and ability. **K.B. Bramble**, L. Saint-Fort, K.A. Leets, G.D. Gibbs
- CHED **1521**. Online fundraising activities to support student travel and research at Illinois State University. **E. Jugovic**, L.M. Stateman, E.C. Sullivan, J. Kim
- CHED **1522**. Student Affiliates of the American Chemical Society San José State University Chapter. **A. Hui**, N. Nguyen, M. Lim, Q. Lam, D. Lee, C. Lionel, G. Muller
- CHED **1523**. Aquinas Chemistry Society: 2015 successful chapter poster. **N. Pierce**
- CHED **1524**. ACS Student Chapter of the University of St. Thomas: At the center of the energy and medical capital of the world. **A. Rivera**, K. Foss, C. Chidi, P. Zaibaq, J. Hoang, C. Anderson, B. Mellis, E. Ledesma
- CHED **1525**. Florida Southern College student chapter growth 2014-2015. **S. Wilson**, K. Fussell, J.C. Sessums, W. Teh, J. Yudichak, G. Beggs, B. Crosby, J.M. Montgomery
- CHED **1526**. Small but mighty Centenary College Chemistry Club. **B.M. Bourgoyne**, P.R. Pritchett, R.S. Thompson, T.R. Johnson, T.M. Tichich
- CHED **1527**. NCW 2013 at UPR Humacao: A sweet celebration. **C. Algarin**, S. Luquis, J. Suarez
- CHED **1528**. Speaker series at Northeastern: Inspiring the next generation of chemists. **M. Nianong**, W. Timson, R. Timson, J. Conway, J. Conway
- CHED **1529**. American Chemical Society University of New Mexico Chapter. **D. Martin**, A.C. Segura, E. Milarch, A. Fernandez, D.A. Garcia
- CHED **1530**. ACS Wilkes Student Chapter applying green chemistry principles. **B.S. Clem**, A. Fadel, T. Weaver, K.M. Rehrig, A. Dinescu, C. Henkels
- CHED **1531**. SMACS attacks chemistry. **T.A. Knippenberg**, S. Ansteatt, B.N. Norris
- CHED **1532**. Events and outreach of the University of Colorado Denver SAACS Chemistry Club. **J. Henderson**, M.K. Maron, R. Rodriguez
- CHED **1533**. Restarting the student affiliate in the oldest town in Texas. **D.A. Fry**, C. Huckaby, J. Moreland
- CHED **1534**. University of Central Arkansas ACS chemistry chapter: Using an inter-chapter relations grant to increase chemical outreach. **A.D. Rolland**, J. Castillo, H.H. Agrama, J.D. Henderson, J.G. Schmidt, K.S. Dooley, K.L. Steelman, F.M. Yarberry
- CHED **1535**. Leading a successful ACS Student Chapter. **J. Ewing**, A.J. Garrett, J.R. Ligas, M.P. Snyder, A.J. Sanders
- CHED **1536**. Cultivating and communicating chemistry on campus and in the community. **D. Walter**, T. Meece, M.D. Perry, S.E. Hubbard
- CHED **1537**. New Mexico Highlands University Chemistry Club: Starting a student chapter. **B. Maki**, P. Dimas
- CHED **1538**. Successful student chapter, Suffolk University 2014. **S. Shrestha**, J. Bautista, E.M. Persson, T.E. West, K. McCarthy, T. Nguyen, A.S. Dutton
- CHED **1539**. Eastern Oregon University ACS Student Member Chapter: Promoting community outreach and professional networking. **T. Winegar**, M.L. Gathright, D.A. Ladendorff, S.A. Sorensen, A.G. Cavinato
- CHED **1540**. Saint Louis University brings the wonder of chemistry to local Saint Louis students. **N. Schlarman**, L. Green, B. Znosko
- CHED **1541**. Surface modification to impact our community. **A.G. Colon**, P.N. Gonzalez Colon, M.A. Miranda Blandria, C. Pellier Rodriguez, J.I. Ramirez Domenech, E.J. Ferrer Torres
- CHED **1542**. Ecofriendly chapter: Education and implementation for a sustainable world. **L. Ramirez Santiago**, A.D. Almodovar Ortiz, P.N. Gonzalez Colon, J.I. Ramirez Domenech, E.J. Ferrer Torres
- CHED **1543**. PCUPR student affiliate chapter celebrates a summer festival. **N. Rivera**, J.K. Vale, N.I. Negrón, L. Santos
- CHED **1544**. Metamorphosis: Our chapter evolution. **A. Zapata Feliciano**, J. Vélez, G. Lopez-Perez, E. Francheschini, S. Ramirez de Arellano, S. Vargas-Padilla, N. Caraballo, A.M. Gonzalez
- CHED **1545**. ChEmory: Emory University's undergraduate chapter of the American Chemical Society. **K.E. Leon**, J. Elinburg, Y. Lin, K. Woolard
- CHED **1546**. Exploring chemistry through candy at Carroll University. **A. Ott**, K. Rude, J. Rountree, S. Marton, G.T. Marks
- CHED **1547**. Successful student chapters abstract: Hofstra University student members of the American Chemical Society. **E. Zhou**, B. Biju, L.E. Carlucci, E.K. Reagan, P. Fernandes, D. Prado, B. Xuan, S.T. Lefurgy, E.C. Mundorff
- CHED **1548**. Student Affiliate Chapter of the American Chemical Society: Minot State University. **K.T. O'Keefe**, S.W. Olson, K.A. Dockter, M.A. Bell, J.M. Miller, S. Park, H. Lee, J.A. Collins, M.M. Bobylev
- CHED **1549**. Georgia College's outstanding student chapter: "Sweeter" than Georgia peaches. **J.L. Minnick**, K. Taylor, H.E. Pekarek, J. Minnick, P. Skersick, K. Ehret, C.H. Lisse
- CHED **1550**. Miami Chemical Society from Miami University (Ohio). **M.M. Shroder**, B.D. Center, R. Comer, A.A. Simoni
- CHED **1551**. SMSU Chemistry Club: Activities of an outstanding student chapter of the ACS. **S.C. Kenea**, M.M. Bruns, N.J. Beyer
- CHED **1552**. First Loras College chemistry carnival: The chemistry of candy. **M. Rea**, D.J. Oostendorp
- CHED **1553**. Stimulating interest and enthusiasm for chemistry. **R.J. Wood**, T. Glasgow, V. Linero, J. Castro, J. Allen, U. Swamy
- CHED **1554**. Successful chapter activities of the Monmouth University Chemistry Club. **S.J. Ebner**, K. Flynn, N. Famularo, K. Muratore, D. Szwajkajzer, G.A. Moehring
- CHED **1555**. University of Puerto Rico- Rio Piedras ACS Student Chapter: A role model to our society. **R.E. Martinez-Quinones**, W.M. Pedreira-Garcia, E. Santiago-Aponte, I. Lehman-Andino, I. Montes
- CHED **1556**. Reactions to increase the yield of involvement. **Z. Hicks**, B.H. Cameron, M. Simmons, U. Phan
- CHED **1557**. Tethering community and academic pursuit: A story of success. **D. Fager**, R. Morrison, A. MacInnis, K. McAndrews, C. Schnitzer
- CHED **1558**. Arkansas Tech University Chemistry Club: Encouraging and broadening participation through outreach and on campus activities. **S. Zuller**, T. Schultz, E.W. Turner, B.D. Curry, S.L. Moran, M. Fuller, C.A. Mebi
- CHED **1559**. Promoting science with the "Chemistry CirCus". **C. Garcia**, J.D. Guerra, V.M. Gonzalez Vazquez, L. Griego, J.S. Enriquez, J.E. Becvar
- CHED **1560**. Outreach, teaching, and university connection programs for two-year college students. **T. Bledsoe**, J.S. Bloodsworth, C.M. Marshall, P.E. Flores Gallardo, L.D. Burke
- CHED **1561**. Traditions and innovations guiding the way to success for Nittany Chemical Society at Penn State. **T. Breidenbaugh**, C.S. Mallis, K. Lan
- CHED **1562**. Onward and upward: Revitalizing a small student chapter. **J. Wells**, C.J. Forsythe
- CHED **1563**. Western Washington University Student Chapter of the American Chemical Society. **T. Clinkingbeard**, C. Grote, N.P. Bradshaw, N. Schorr, S.R. Emory, E. Raymond
- CHED **1564**. Priority of Biology & Chemistry at East LA College: Organically fun. **H. Castellanos**, M. Lopez, I. Gonzalez, K.N. Olsen, A.M. Rivera Figueroa
- CHED **1565**. Getting your chapter involved the community: Examples of community involvement by the Elmira College ACS student affiliate chapter. **A. Davenport**, C. Zorn, C.E. Stilts
- CHED **1566**. Instilling chemistry into our biggest natural resource. **A.R. Chappell**, K.N. Weeber
- CHED **1567**. Central Washington University SA-ACS 2014-2015: Development of standard operating procedures (SOPs) for the safe, educational and fun performance of chemistry demonstrations. **C. Verwey**, C.D. Carman, A. Wilson, C.E. Malmberg, N. Beebe, S. Bouche, D. Chavez, J. Siegenthaler, P.W. Swain, T.L. Sorey
- CHED **1568**. Importance of community outreach and encouragement of the sciences. **J. Kao**, K. Gensemer, B. DeMauro, S.A. Fleming
- CHED **1569**. Barry University Chemistry Club: Celebrating twenty years of excellence. **P. Nwokoye**, H. Dao, V. Hoelscher, Q. Su, J. Sanchez, G. Fisher, T. Hamilton
- CHED **1570**. How to retain members and make them feel included. **J.L. Farley**, A. Shepard, A.T. McDonald, J. Callus, M. Smoker
- CHED **1571**. Chemical demonstration program for continuing education. **C. Cookenmaster**, M. Pendleton, M. Bache, E. Milligan, D.M. Bartley
- CHED **1572**. SAACS Is Au₂ at SHU. **L. Farber**, K. Kocieczny, A. Buonaccorsi, J. Fierro, N. Doppler, J.M. Werthell, K. Scinto, K. Hess, D.N. Beier, M. Stewart, S. Bergman, C. Ruvolo, K. Campos
- CHED **1573**. Forensic chemistry division; A new outreach in our campus. **J. Chabrier Rodriguez**, E. Medina, C. Osorio Cantillo, J.I. Ramirez Domenech, E.J. Ferrer Torres
- CHED **1574**. Xavier University of Louisiana's student chapter: Enriching the legacy. **L.M. Mensah**, C. Pace, K. Lam, T.J. Harris, K. Crosby, E. Murphy, D. Johnson, M.R. Adams, J.A. Privett, C.M. Lawrence
- CHED **1575**. UTPB Chemistry Club: Promoting chemistry in west Texas. **K.A. Beran**, S. Moreno, B.J. Garcia, M. Hagle, S. Siegler
- CHED **1576**. Successful activities of the Waynesburg University ACS Chapter. **G. Strouse**, C. Petrone, K. Wilson, T. Bromenschenkel, N. Frazee, E.A. Baldauff
- CHED **1577**. Lock Haven University Chemistry Club. **J. Seidel**, J. Caffyn, K. Range
- CHED **1578**. Student Chemists Association at The College of New Jersey. **T. Maney**, H. Sajjad, C. Kirby, A.R. O'Connor, B.C. Chan
- CHED **1579**. Erskine College ACS Chapter: Not just winging it anymore. **D.A. Roe**, D.K. Gentry, A.D. Houston, T.R. Hayden, J.E. Boyd
- CHED **1580**. PLU Chemistry Club: Redistributing knowledge according to Le Châtelier's Principle. **S.D. Murphy**, S. Huang, N.A. Yakeis, A.M. Munro
- CHED **1581**. Collegiate Chemistry Bowl, Demomania, Chemagic show, eminent speaker and networking luncheon part of UT-Martin hosting the undergraduate program at SERMACS. **S.K. Airee**, K.A. Harris, K.H. McCrillis, L. Gargus
- CHED **1582**. Career development and networking for chemistry, biochemistry, engineering, and pharmacy majors: KU Chem Club. **M. Holtz**, V. Tallavajhala, A. Petruilis, C. Barrett, P.R. Hanson, R.S. Black
- CHED **1583**. Saint Vincent College Chemistry Club. **A.J. Rupprecht**, A.N. Dobracki, M. Brady, S.J. Gravelle
- CHED **1584**. Green chemistry: Prevention for a cleaner future. **R. Jimenez-Hernandez**, M. Torres-Caban, B.J. Ramos-Santana
- CHED **1585**. Forging leaders: Diamonds for society. **D.E. Morales-Mantilla**, D. Morales-Rosa, B.J. Ramos-Santana
- CHED **1586**. Stay calm and get your grizzly growl on: Georgia Gwinnett College chemistry outreach. **G.E. Rudd**, C. Fussell, S. Jiva
- CHED **1587**. Catawba College Chemistry: The fuel that will stand the test of time. **A.L. Williamson**, B. Baumgarten
- CHED **1588**. Chemistry outreach efforts at North Dakota State University. **S. Walker**, R. Hesson, M. Mann, M.J. Kleinsasser
- CHED **1589**. Fundraising methods at North Dakota State University. **J. Wraga**, T. Kim, S. Walker, M.J. Kleinsasser
- CHED **1590**. Modeling a successful student chapter. **M. Vang**, A. Lolinco, B.J. Cole, P. Ounkham, R. Espinoza, K.M. Kazaryan, I. Kuchkovskaya, N. Chhay, M.L. Golden, D. Golden
- CHED **1591**. University of Utah American Chemical Society Student Chapter: Successful student chapter poster. **C.J. White**, F. Fernandez, B. Ronna, B.L. Richeson, Z. Headman, C. Jennings, A. Jo, H. Hansen, R.Y. Chung, G. Clement, M.R. Kiley, H.L. Sebahar, J.D. Rainier, T.G. Richmond
- CHED **1592**. Truman State University Student Chapter. **J.M. McGowan**, C. Witt, E.P. Riekeberg
- CHED **1593**. Successful student chapter of the American Chemical Society, South Dakota School of Mines and Technology: Promoting chemistry and reading. **M. Braasch-Turi**, J. Meyer, M.A. Huber, P.R. Holland
- CHED **1594**. Science of service: Gordon College's student chapter of the American Chemical Society. **D. Gray**, B.J. Marshall, L.T. Walsh, E. Fjellstad, D. Andujar, M.C. Enright
- CHED **1595**. Chemistry: the final frontier: These are the chronicles of the Chemistry Club at South Texas College, its enduring mission – to spread knowledge, educate the unknowing, serve its community, and go where no chemistry club has gone before. **L. Avila**, R. Gonzalez, A.Y. Navarro, N. Salazar, A. Gonzalez

1:55 CHED **1665**. Gaining insight into visual problem solving by combining eye-tracking with multimodal data analysis. S.J. Hansen, F. Moore, P. Gordon, O. Anderson

2:15 CHED **1666**. Numerical comparisons of eye fixation sequences from chemistry problem solving. J. Baluyut

2:35 CHED **1667**. Study of self-explaining skill development in college level introductory chemistry courses via latent transition analysis. A. Villalta-Cerdas

2:55 CHED **1668**. Using an interactive simulation to support student development of expert practices for balancing chemical equations. Y. Carpenter, E.B. Moore, K.K. Perkins

3:15 Intermission.

3:30 CHED **1669**. Students' growth in scientific reasoning and the implications for chemistry instruction. J.H. Carmel, E.J. Yezierski

3:50 CHED **1670**. Characterizing students' explanations of energy change at the atomic-molecular level. N.M. Becker, K. Noyes, M. Cooper

4:10 CHED **1671**. Integrating scale-themed instruction into the undergraduate general chemistry curriculum using active learning methodologies. J.M. Trate, P. Geissinger, A. Blecking, K.L. Murphy

4:30 CHED **1672**. Exploring an inverted classroom model in General Chemistry II using POGIL style activities and undergraduate Learning Assistants. U. Swamy

4:50 CHED **1673**. Stop cheating! An evaluation of a scientific integrity writing strategy in General Chemistry I. M.L. Edwards

5:10 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Spruce

Perspectives on Climate Change Literacy and Education: Local to International

G. P. Foy, *Organizer*

K. E. Peterman, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1674**. Fracking and carbon sequestration, oh my: Connecting general chemistry students to climate change topics. K. Anderson, D.B. King, J.E. Lewis, G.H. Webster, S. Suthelmer, D.E. Latch, C.H. Middlecamp, R.S. Moog

1:55 CHED **1675**. Climate change and public health: The importance of literacy domestically and globally. N. Diklich, K.E. Peterman, G.P. Foy

2:15 CHED **1676**. Climate change impacts on biodiversity and mitigation efforts. C. King, K.E. Peterman, G.P. Foy

2:35 CHED **1677**. Energy discussions at the 20th Conference of Parties. B. Hartweg

2:55 CHED **1678**. Effects on agriculture from climate change. S. Bariana, G.P. Foy, K.E. Peterman

3:15 Intermission.

3:25 CHED **1679**. Campaign strategy, outreach, and advocacy efforts at the UN Climate Conference. R.B. Sobel

3:45 CHED **1680**. Geopolitical effects of climate change in the Arctic. K.T. O'Keefe, G.P. Foy, K.E. Peterman

4:05 CHED **1681**. How climate change will exacerbate the food, energy, and water nexus. J. McDonald

4:25 CHED **1682**. Future stance on climate change. K. Teppert, G.P. Foy, K.E. Peterman, D. Husic

4:45 Panel Discussion.

5:05 Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel
Denver

NSF Programs That Support Undergraduate Education

C. A. Burkhardt, *Organizer*

R. K. Boggess, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 Description of NSF Programs.

1:55 Question/Answer Session.

2:15 CHED **1683**. Framing the chemistry curriculum: Year 1. M.A. Griep

2:45 CHED **1684**. 49erTeach: Building capacity for teachers of chemistry and physics through NSF's Noyce teacher scholarship program. K. Asala

3:15 Intermission.

3:25 CHED **1685**. Denver Metro Chem Scholars, an NSF S-STEM program at a large urban PUI. R.D. Walker, A.J. Bonham

3:55 CHED **1686**. NSF programs that support undergraduate education. M. Cullin

4:25 CHED **1687**. Implementing and assessing the efficacy of open access ChemWiki textbook resource. G. Allen, A. Guzman, M. Molinaro, D.S. Larsen

4:55 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel
Columbine

George C. Pimentel Award in Chemical Education: Symposium in Honor of I. Dwaine Eubanks

Sputnik to Smartphones: A Half-Century of Chemistry Education

Cosponsored by HIST‡

Financially supported by ChemSource, Inc.

M. Orna, *Organizer, Presiding*

1:30 CHED **1688**. Impact of technology on chemistry instruction. R.A. Pribush

1:55 CHED **1689**. Laboratory instruction: Less verification, more discovery. L.P. Eubanks

2:20 CHED **1690**. Evolution of undergraduate research as a critical component in the education of chemistry students. B.E. Holmes

2:45 CHED **1691**. Standards and expectations. P. Smith

3:10 Intermission.

3:25 CHED **1692**. Trajectory of testing in chemistry education. T. Holme

3:50 CHED **1693**. Inquiry activities based on Simulations and Animations. J.I. Gelder, M.R. Abraham, T.J. Greenbowe

4:15 CHED **1694**. Developments in chemical education: Influences, successes, and failures in adaptations in other countries. D. Waddington, H.W. Heikkinen

4:40 CHED **1695**. Award Address (George C. Pimentel Award in Chemical Education sponsored by Cengage Learning and the ACS Division of Chemical Education). Challenges for the next generation. D. Eubanks

Section F

Sheraton Denver Downtown Hotel
Gold

Overcoming Obstacles in Student Learning in Physical Chemistry

A. L. Marsh, A. Noble, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1696**. Rethinking homework: The impact of content, format, and process on physical chemistry learning outcomes. T.D. Shepherd

1:55 CHED **1697**. Preparing students for effective engagement in group problem solving. A.R. Noble

2:15 CHED **1698**. Influences of student discourse in overcoming barriers in physical chemistry. C.L. Stanford, N.M. Becker, J.D. Byers, A.C. Moon, M.H. Towns, R.S. Cole

2:35 Intermission.

2:45 CHED **1699**. POGIL in the physical chemistry laboratory. A. Grushow, S.S. Hunnicutt, R.M. Whitnell

3:05 CHED **1700**. Quantum first physical chemistry at a regional liberal arts college. A.L. Marsh

3:25 CHED **1701**. Learning by doing: Teaching physical chemistry using guided inquiry with frequent feedback. S.S. Hunnicutt

3:45 Intermission.

3:55 Panel Discussion.

4:15 Concluding Remarks.

TUESDAY EVENING

Section A

Sheraton Denver Downtown Hotel
Gold

General Papers

S. A. Fleming, *Organizer*

C. Hamann, *Presiding*

6:00 Introductory Remarks.

6:05 CHED **1702**. Multistep synthesis of benzoyl peroxide for the second semester organic laboratory. J. Wollack

6:25 CHED **1703**. Where's the ketone: A laboratory showing the control of reaction intermediates in Grignard reactions with esters. R.D. Barrows, L. Giacomine, D. Hanson, A. Sylvester

6:45 CHED **1704**. Carbocation rearrangements in the undergraduate laboratory: GC/MS and NMR deduction of products from electrophilic aromatic substitution in a discovery laboratory experiment. M.V. Maskornick, V. Polito, I.J. Rhile, C.S. Hamann

7:05 Intermission.

7:15 CHED **1705**. Importance of sampling: The first lab in the analytical chemistry class. R. Indralingam

7:35 CHED **1706**. Organic chemistry and the native plants of the Sonoran Desert: A new model for the undergraduate laboratory. T.L. Minger, V. Nedelkova, J. Zikopoulos

7:55 CHED **1707**. Safety for chemical demonstrations. D.A. Katz

8:15 Intermission.

8:25 CHED **1708**. Synthesis and the three-separate independent purification of 3-nitroacetanilide: An exercise in recrystallization, extraction and radial chromatography in the undergraduate organic chemistry labs. R.B. Miller

8:45 CHED **1709**. Teaching research in organic chemistry with a "guided-research" laboratory experience. R. LaLonde

9:05 CHED **1710**. Investigating enzyme assays. W.A. Patton

9:25 CHED **1711**. Introduction of the professional quote format and compound screening to project-based experiments in the biochemistry laboratory. K.R. Gallagher

9:45 CHED **1712**. Design and implementation of a multi-method enzyme kinetics project for a junior-level studio laboratory. D.R. Goode, R.L. Hutcheson, C.V. Crisan, J.D. Mims

WEDNESDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Silver

Green Chemistry: Theory and Practice

Cosponsored by CE‡

Financially supported by NSF-CCI Center for Sustainable Polymers at the University of Minnesota; ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision

J. E. Wissinger, *Organizer*

E. J. Brush, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1713**. Green chemistry of biodiesel production. V. Gude, E. Martinez-Guerra

8:55 CHED **1714**. Biorefinery: A molecular design platform for green surfactants and soft materials. G. John

9:15 CHED **1715**. Greener synthesis of photochromic, fluorescent, and industrially important organic compounds for one- and two-semester organic chemistry laboratories. J. Bennett, D. Dragotta, E. Stopler

9:35 CHED **1716**. Nickel-catalyzed Suzuki-Miyaura cross-coupling in a green alcohol solvent for an undergraduate organic chemistry laboratory. N.K. Garg

9:55 Intermission.

10:05 CHED **1717**. Paper to plastics: An interdisciplinary outreach program in sustainable research. J. Byers, E. Weerapana, F.B. Tamburini, T.B. Kelly, N. Chinnaswamy, T. Fazekas

10:25 CHED **1718**. Hands-on, inquiry-based laboratory experiment for chemistry and engineering students comparing "green" and "nongreen" Noble metal nanoparticle synthesis methods. M.L. Edwards, S.A. Paluri

10:45 CHED **1719**. Green chemistry principles illustrated through the synthesis of renewable triblock copolymers: an inquiry-based experiment. J.E. Wissinger, D.K. Schneideman, M.T. Wentzel

11:05 CHED **1720**. Decision-making based on evaluation of the benefits, costs, and risks associated with the use and production of chemicals. H. Sevian, S. Cullipher, V. Talanquer

11:25 Panel Discussion.

11:45 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research

Concept Inventories

J. Barbera, N. P. Grove, *Organizers*

J. R. Raker, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **1721**. Development of a chemistry concept inventory online database. K.J. Linenberger

8:55 CHED **1722**. Student alternative conceptions of theory application during first year General Chemistry: Does anything really change? W.E. Schatzberg

9:15 CHED **1723**. Development of stereochemistry concept inventory using principles of effective test construction and results from national surveys. A. Leontyev, R.M. Hyslop

9:35 CHED **1724**. Detecting incorrect ideas in stereochemistry. A. Leontyev, R.M. Hyslop

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research

Online Homework

J. Barbera, N. P. Grove, *Organizers*

J. R. Raker, *Presiding*

10:10 CHED **1725**. Students' short and long term impressions, attitudes, perceived learning, and actual performance using two online homework systems: Embedded text vs. linked text. C. Zumalt, V.M. Williamson

10:30 CHED **1726**. Developing student-generated content in sapling learning. D.M. Zurcher, B.P. Coppola, A.J. McNeil

10:50 CHED **1727**. Form vs. function: A comparison of Lewis structure drawing tools and the cognitive loads they induce. P. Duffy, A. Coleman, T. Gamp, J.M. Tiettmeyer, N.P. Grove

11:10 CHED **1728**. How many tries are optimal for on-line homework? C.H. Atwood, J. Moody

11:30 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Spruce

Process-Oriented Guided Inquiry Learning (POGIL)

- R. S. Moog, *Organizer, Presiding*
- 8:30** Introductory Remarks.
- 8:35** CHED **1729**. Introduction to POGIL and The POGIL Project. R.S. Moog
- 8:55** CHED **1730**. High school chemistry POGIL activities on a dollar store budget. A.S. Schwab
- 9:15** CHED **1731**. Using knowledge surveys to assess student knowledge gains from POGIL activities. B.D. Gilbert
- 9:35** CHED **1732**. Quantum, spectroscopy, bonding with POGIL in first semester physical chemistry. N.E. Levinger
- 9:55** Intermission.
- 10:05** CHED **1733**. POGIL on a large scale. S.M. Taylor, C.A. LaBrake, D. Vanden Bout
- 10:25** CHED **1734**. Using POGIL in a large lecture setting: The benefits and the challenges. T.A. Madison
- 10:45** CHED **1735**. Guided inquiry in chemistry: Teaching assistant training courses for undergraduates. S.S. Hunnicutt
- 11:05** Panel Discussion.

Section D

Sheraton Denver Downtown Hotel
Denver

Instructors and Researchers: Advancing Graduate Education in Chemistry

- S. Hansen, S. Sandi-Urena, *Organizers, Presiding*
- 8:30** Introductory Remarks.
- 8:35** CHED **1736**. ETTA: Educational Training for Teaching Associates. P. Varma-Nelson, L. Easterling, J.R. Gregory
- 8:55** CHED **1737**. Orientation and teacher training programs for graduate students. M.L. Miller, R. Hirko
- 9:15** CHED **1738**. Evaluation methods and findings for interdisciplinary graduate training programs at UBC. J.J. Stewart, A.K. Bertram, L. Schafer, K.J. Knox, G. Birol, S. Burke, C. Underhill
- 9:35** CHED **1739**. Graduate teaching assistants' potential benefits and professional development associated with teaching general chemistry laboratories. S. Sandi-Urena, T. Gatlin
- 9:55** Intermission.
- 10:05** CHED **1740**. It takes a village: Transition from graduate student to practitioner. G. Bhattacharyya, G.M. Bodner, A. Verdian
- 10:25** CHED **1741**. Bringing chemical research into the undergraduate teaching lab: A graduate student perspective. J. Zhu, S. Hansen, L. Kaufman, J. Ulichny
- 10:45** CHED **1742**. How my teaching role has impacted my graduate student experience. M.L. Miller, D.P. Cartrette, O. Odeleye, T. Cox, M. Stutelberg
- 11:05** Concluding Remarks.

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.

Section E

Sheraton Denver Downtown Hotel
Columbine

Using Technology in the Undergraduate Laboratory

- A. Oxley, C. E. Stilts, *Organizers, Presiding*
- 8:30** Introductory Remarks.
- 8:35** CHED **1743**. Agent-based modeling as a tool for a discovery-based TLC experiment. D. Brownholland, M. Goodrich
- 8:55** CHED **1744**. Home-built instruments as group projects in instrumental analysis courses. M. Chia, A. Blank, A. Sabelhaus, B. Wiefeling, C.A. Morris
- 9:15** CHED **1745**. Implementation of cost-effective tablet technology for the development of electronic laboratory notebook skills and to promote active learning at the undergraduate level. R.N. Dansby-Sparks, R.M. Meier
- 9:35** CHED **1746**. Flipping the General Chemistry laboratory. A. Oxley
- 9:55** Intermission.
- 10:05** CHED **1747**. 3D printed colorimeters for use in the freshman chemistry lab. J.D. Mendez
- 10:25** CHED **1748**. Designing and implementing effective virtual laboratory experiments in general chemistry. K.J. Winkelmann, W. Keeney-Kennicutt
- 10:45** CHED **1749**. Organic lab transformation. J. Potratz
- 11:05** CHED **1750**. Electronic grading of laboratory reports to account for variation in student data. E.M. Epp, K. Nippert
- 11:25** CHED **1751**. Using QR codes and online videos in the undergraduate organic chemistry lab. C.E. Stilts
- 11:45** Concluding Remarks.

Section F

Sheraton Denver Downtown Hotel
Gold

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

- Cosponsored by PHY5*
- J. L. Sonnenberg, *Organizer*
- J. B. Foresman, *Organizer, Presiding*
- 8:30** Introductory Remarks.
- 8:35** CHED **1752**. What makes an electron a valence electron? Introducing students to computational chemistry in the POGIL-PCL framework. M.S. Reeves
- 8:55** CHED **1753**. Withdrawn.
- 9:15** CHED **1754**. Utilizing electronic structure calculations in undergraduate inorganic chemistry. J.T. York
- 9:35** Intermission.
- 9:50** CHED **1755**. Web based computational job submission for the undergraduate laboratory. M.J. Perri, S.H. Weber
- 10:10** CHED **1756**. Quantum and computational chemistry: A difficult and necessary classroom union. M.F. Tuchler
- 10:30** CHED **1757**. Gaussian-based laboratory exercises in physical chemistry. S.M. Basu
- 10:50** Intermission.
- 11:05** CHED **1758**. Computational chemistry in the physical chemistry course. T. Engel, L. Johnson
- 11:25** CHED **1759**. 15-year retrospective of computational chemistry in the undergraduate curriculum at The University of Tulsa. G.H. Purser, G.R. Medders
- 11:45** CHED **1760**. Assessment of student knowledge and opinions of computational chemistry in a physical chemistry for engineer's course. E.P. Wagner
- 12:05** CHED **1761**. Atomistic level computational chemistry for visualization and calculation in the undergraduate chemistry laboratory. L. Tribe

WEDNESDAY AFTERNOON**Section A**

Sheraton Denver Downtown Hotel
Silver

Green Chemistry: Theory and Practice

- Cosponsored by CEI†*
- Financially supported by NSF-CCI Center for Sustainable Polymers at the University of Minnesota; ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision*
- E. J. Brush, *Organizer*
- J. E. Wissinger, *Organizer, Presiding*
- 1:30** Introductory Remarks.
- 1:35** CHED **1762**. Adapting green chemistry metrics for nanoparticle synthesis. B. Reid, S.M. Reed
- 1:55** CHED **1763**. New shoots from old vines: Greening reactions in the organic chemistry laboratory. T.N. Jones, K.J. Graham, C.P. Schaller, E.J. McIntee
- 2:15** CHED **1764**. Case study: Green chemistry — theory and practice in an undergraduate laboratory. O. Oluwaniyi, S.O. Famuyiwa
- 2:35** CHED **1765**. Educating general chemistry students about green chemistry through their laboratory experience. S.A. Henrie
- 2:55** Intermission.
- 3:05** CHED **1766**. Need for green chemistry at the undergraduate level. I.T. Sidhwani, R. Sharma
- 3:25** CHED **1767**. Incorporation of green principals across a chemistry curriculum at a small liberal arts college. J. Wollack
- 3:45** CHED **1768**. Project GreenLab: A regional student-faculty collaboration in green chemistry curriculum development, research, and outreach education. E.J. Brush
- 4:05** CHED **1769**. Green chemical education in curriculum: Cracking siloed education. C.D. Jensen
- 4:25** Panel Discussion.
- 4:45** Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research Organic and Biochemistry

- J. Barbera, N. P. Grove, *Organizers*
- T. Bussey, *Presiding*
- 1:30** Introductory Remarks.
- 1:35** CHED **1770**. Acid-base topic in the context of a nursing chemistry course. C.E. Brown, M.L. Henry, R.M. Hyslop
- 1:55** CHED **1771**. Comparative study of organic chemistry representations and students' cognitive load. P. Duffy, N.P. Grove
- 2:15** CHED **1772**. Student understanding of glycolysis: Organic chemistry tasks in a biochemistry context. J.R. Raker, B.R. Van Norman
- 2:35** CHED **1773**. Biochemistry instructors' perceptions of their classroom use of analogies. T.J. Bussey, M. Orgill

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research Chemistry Majors

- J. Barbera, N. P. Grove, *Organizers*
- T. Bussey, *Presiding*
- 3:10** CHED **1774**. Concept mapping: A learning strategy for teaching Instrumental Chemical Analysis course. T. Saleh
- 3:30** CHED **1775**. Student grade perceptions throughout a chemistry program (Freshman-Master's). J.A. Webb, A.G. Karatjas
- 3:50** CHED **1776**. Investigating the enacted and stated curriculum in physical chemistry. S.E. Erhart, E.J. Yeziarski
- 4:10** Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Spruce

Research on Learning in the Laboratory

- M. J. Chrzanowski, S. Sandi-Urena, A. Villalta-Cerdas, *Organizers, Presiding*
- 1:30** Introductory Remarks.
- 1:35** CHED **1777**. Improving general chemistry students' inquiry skills and confidence with research-inspired experiments. K.J. Winkelmann, M.H. Baloga, C. Giannoulis, T. Marcinkowski, P. Cohen, G. Anquandah
- 1:55** CHED **1778**. Current research on learning in the chemistry college laboratory. S. Sandi-Urena
- 2:15** CHED **1779**. Incorporation of instructional videos to encourage students' coordination of theory and evidence in the physical chemistry laboratory. R.S. Cole, M.N. Muniz, J.A. Schmidt, E. Keuter
- 2:35** Intermission.
- 2:45** CHED **1780**. Examining student analytical reasoning in introductory chemistry laboratory. M.R. Bruce, S. Avarigli, A.E. Bruce, F.G. Amar
- 3:05** CHED **1781**. Perceptions of students and teaching assistants regarding a project-based undergraduate laboratory. S.R. Mooring, N.L. Burrows
- 3:25** CHED **1782**. Reform in general chemistry laboratory instruction: How do students experience change between an expository laboratory and a cooperative project-based laboratory? M.J. Chrzanowski, S. Sandi-Urena
- 3:45** Discussion.

Section D

Sheraton Denver Downtown Hotel
Denver

Undergraduate Research in Chemistry: Expanding Opportunities and Broadening Participation

- Models Supporting and Expanding Undergraduate Research**
- B. L. Gourley, R. M. Jones, *Organizers, Presiding*
- 1:30** Introductory Remarks.
- 1:40** CHED **1783**. First-Year Research Experience (FYRE) program: A gateway to undergraduate research and enhanced STEM development at the University of Oklahoma. N. Kothapalli, A. Burgett, R. Halteman
- 2:00** CHED **1784**. Guiding a senior undergraduate in chemical education and computational chemistry research. J.P. Beck
- 2:20** CHED **1785**. PRISM: CSUSB strengthening the scientific workforce. K.R. Cousins, Y. Kim
- 2:40** CHED **1786**. Integrating undergraduate research with teaching and learning: Unanticipated opportunities to broaden participation. L.E. Echegoyen, S.B. Aley, C.E. Botez, G. Corral, H.H. Meeuwse, D. Villagran

Section D

Sheraton Denver Downtown Hotel
Denver

Undergraduate Research in Chemistry: Expanding Opportunities and Broadening Participation

- Undergraduate Research in the Curriculum**
- B. L. Gourley, R. M. Jones, *Organizers, Presiding*
- 3:00** CHED **1787**. Freshman research immersion: Transforming freshman into researchers. M.E. Fegley, J.R. Ahey, W.E. Jones, N.E. Stamp
- 3:20** CHED **1788**. Research-based analytical chemistry laboratory: Incorporation of students' self-designed projects into curriculum. R. Gao
- 3:40** CHED **1789**. Increasing reach: Dealing with resource limitations and scalability issues by bringing collaborative research into the teaching laboratory. R.E. Bachman
- 4:00** CHED **1790**. Components of a research-rich undergraduate chemistry curriculum. T.J. Wenzel
- 4:20** Concluding Remarks.

[†] Cooperative Cosponsorship

Section E

Sheraton Denver Downtown Hotel
Columbine

Nanotechnology in Undergraduate Education and Research

D. S. Heroux, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1791. Nanotechnology experiments for inorganic chemistry laboratory. D.S. Heroux

1:55 CHED 1792. Synthesis and exploration of Au nanoparticles in an open-ended junior-level capstone lab. C.S. Seney, J.D. Mimbs

2:15 CHED 1793. Harnessing the power of partnerships and technology in nanoscience education. K.A. Pacheco, J. Ristvey

2:35 Intermission.

2:45 CHED 1794. Debating societal impacts of nanotechnology through role playing. K.J. Winkelmann

3:05 CHED 1795. Synthesis and comparative study of ZnO/Au, ZnO/Ag, MgO/Au, and MgO/Ag core-shell nanoparticles with their functionalization with antibiotics. C. Pellicier Rodriguez, M. Feliciano Sanchez, E. Medina, J.I. Ramirez Domenech, C. Osorio Cantillo, E.J. Ferrer Torres

3:25 CHED 1796. Investigating the antimicrobial properties of silver nanoparticles with respect to *Desulfovibrio* genus bacteria. J. Snitker, M. Montes

3:45 Concluding Remarks.

Section F

Sheraton Denver Downtown Hotel
Gold

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Cosponsored by PHYS

J. B. Foresman, *Organizer*

J. L. Sonnenberg, *Organizer, Presiding*

1:30 CHED 1797. Computational chemistry should start in high school. R.R. Gotwals

1:50 CHED 1798. Computational chemistry throughout the curriculum. K. Range

2:10 CHED 1799. Computational modelling across the curriculum: General, organic and physical chemistry. M.W. Ducey, D.R. Myers, J.S. Rhoad, J.N. Woodford

2:30 Intermission.

2:45 CHED 1800. Computational chemistry in an undergraduate curriculum: Strategies for deliverable skills. M.M. Ivey, J.L. Sonnenberg

3:05 CHED 1801. Examples of instructional units in computation and modeling for the undergraduate chemistry curriculum. L.S. Pelter, M.W. Pelter

3:25 CHED 1802. 20 years of computational chemistry at a public regional university: Thoughts and experiences. M. Pelter, L. Pelter

3:45 Intermission.

4:00 CHED 1803. Computational chemistry: Practical issues in leveraging the Cloud. R. Thackston, B. Kinmons, R.C. Fortenberry

4:20 CHED 1804. PSI4Education: Computational chemistry labs using free software. R.C. Fortenberry, T.D. Shepherd, A. Ringer McDonald, M. Kennedy, D. Sherrill

4:40 CHED 1805. Challenges and rewards of the computational chemistry undergraduate thesis project. R.C. Brown

5:00 CHED 1806. NCSI workshops are ready to help train faculty to use computational chemistry in the classroom. C. Metz, S.C. Sendlinger, E.T. Bell-Loncella, R. Panoff

THURSDAY MORNING**Section A**

Sheraton Denver Downtown Hotel
Gold

General Papers

S. A. Fleming, *Organizer*

C. R. Pharr, *Presiding*

8:00 Introductory Remarks.

8:05 CHED 1807. Building connections in biology and chemistry courses in the second year curriculum. S.R. Sieck

8:25 CHED 1808. Chemical analysis of paint: Development of multidisciplinary class sessions for chemistry and art students. B. Sieve, J. Hedges, C.A. Morris

8:45 CHED 1809. Interdisciplinary experimental approach for undergraduate chemistry students. C. Lobato, N. Romero-Coronio, A. Gomez-Rivera, L. Roa-De la Fuente

9:05 Intermission.

9:15 CHED 1810. Flipped classroom for large organic chemistry class. S. Xie

9:35 CHED 1811. Half flipped: Using videos and online quizzes to maximize in class problem solving time. C.R. Pharr

9:55 CHED 1812. Flipping general chemistry to improve student success. C.M. Zaleski

10:15 Intermission.

10:25 CHED 1813. Unit Conversion Literacy Project: A partnership model for driving curricular change. G. Baker

10:45 CHED 1814. Engaging science students and the public through science-themed art. D.B. Cordes

11:05 CHED 1815. Sophomore organic chemistry to synthesize that? J.K. Murray

11:25 CHED 1816. Capstone experience for the sophomore organic chemistry sequence emphasizing written and oral expression. L.R. Eller

Section B

Sheraton Denver Downtown Hotel
Century

General Papers

S. A. Fleming, *Organizer*

M. T. Mongelli, H. Stokes-Huby, *Presiding*

8:00 Introductory Remarks.

8:05 CHED 1817. Exploring DNA and protein structures with PyMOL. J.A. Himmelberger

8:25 CHED 1818. Teaching general chemistry in context using the ChemConnections Activity Workbook. K.L. Braun, H. Mernitz, S. Anthony

8:45 CHED 1819. Demonstrating the intelligence capabilities of the Q-electronic tutor. T.R. Farhat

9:05 Intermission.

9:15 CHED 1820. Polycraft: Utilizing online gaming to enable next generation polymer chemistry education. W. Voit

9:35 CHED 1821. Teaching and learning with a tablet. H. Stokes-Huby, M.T. Mongelli

9:55 CHED 1822. Incorporating peer-review homework assignments into a large enrollment freshman chemistry course. C.T. Cox, R.N. Zare, K. Murphy

10:15 Intermission.

10:25 CHED 1823. Student designed organic laboratories as an alternative research project. R.B. Lettan II, S. Sagan, S. Candiello

10:45 CHED 1824. Designing accessible interactive chemistry simulations for all students – including students with disabilities. E.B. Moore, A. Paul, K. Perkins

11:05 CHED 1825. Perceptions of competency for male and female chemistry majors: Does he receive more credit? R.P. Beeton, S. Hilmwig, T. Martinez

Section C

Sheraton Denver Downtown Hotel
spruce

General Papers

S. A. Fleming, *Organizer*

J. D. Mendez, *Presiding*

8:00 Introductory Remarks.

8:05 CHED 1826. Guided inquiry laboratory experiment water analysis and hands-on experience for K-12 students in the Advancing Mathematics and Science Skills Program. S.O. Fakayode, M. Kanipes-Spinks

8:25 CHED 1827. Collaboration between historically black colleges and universities and local school districts to promote K-12 science education, North Carolina, USA. S. Fakayode, V. Snipes, M. Kanipes-Spinks

8:45 CHED 1828. Quantitative approach to the study of the effectiveness of using the Dual Credit General Chemistry I Program at Missouri Western State University as a recruiting tool. J.L. Torres y Torres, M.W. Ducey

9:05 Intermission.

9:15 CHED 1829. Electrolytic reactions of reagent precursors for preparation and standardization of commonly used reagents in an undergraduate laboratory. S. Melaku, R. Dabke

9:35 CHED 1830. Towards increasing student engagement in the general chemistry laboratory with environmental research. R. Driscoll, J. Hall Tomasik, A. Miller, S.A. Majorski, D.J. Lecaptain

9:55 CHED 1831. Utilizing 3D printing to create demonstrative models for freshman chemistry courses. J.D. Mendez

10:15 Intermission.

10:25 CHED 1832. Integrative and exploratory junior-level studio laboratory for student-centered learning and scientific growth. D.R. Goode, D.E. Moore, C.S. Seney, A.M. Kiefer

10:45 CHED 1833. Solution concentration uncertainty: An experiment to illustrate the concepts of precision and propagation of error through measurement of the molar extinction coefficient of $\text{Cu}(\text{NH}_3)_4\text{Cl}_2$. J.J. Stankus

11:05 CHED 1834. Laboratory experiment: Carbonates and the ideal gas law. T. Hodgkins

11:25 CHED 1835. Open source drug discovery with undergraduates and high school students. A.E. Williamson, M.H. Todd, P. Willis, O. Consortium

CHAS**Division of Chemical Health and Safety**

D.M. Decker, F. K. Wood-Black and J. M. Pickel, *Program Chairs*

MONDAY AFTERNOON**Section A**

Embassy Suites Denver–Downtown Convention Center
Silverton Ballroom 1

Legalized Marijuana & Health & Safety

Cosponsored by CCS

N. R. Langerman, R. W. Phifer, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 CHAS 1. Taking care of Mary Jane's workers. J. Lieberman

2:10 CHAS 2. Safety considerations in the development of sensible workplace drug testing policies for legalized marijuana. R.W. Phifer

2:40 CHAS 3. Marijuana health and safety for licensed and regulated businesses. C. Villano

3:10 CHAS 4. State mandated testing of retail marijuana in Colorado. A. LaFrate

3:40 Intermission.

3:55 CHAS 5. Safety and health standard of cannabis extractions with an emphasis on CO₂. A. Cahoj

4:25 CHAS 6. Recent improvements in chromatography: Advancing chromatography data quality to make a safer Cannabis product. A. Rigdon, R. Lake, R. Freeman, F. Carroll, T. Kahler

4:55 CHAS 7. GC methods for Cannabis safety and potency testing. A. Rigdon, J. Cochran, C. Hilliard, W. Schroeder, C. Schroeder, T. Flood

5:25 Concluding Remarks.

MONDAY EVENING**Section A**

Colorado Convention Center
Halls C/D

Sci-Mix

J. M. Pickel, *Organizer*

8:00 - 10:00

CHAS 8. Division of Chemical Health and Safety. D.M. Decker

CHAS 9. Withdrawn.

CHAS 10. Safety survey of chemistry teaching laboratories in Nepal. B. Giri, K. Kandel

CHAS 11. Lessons learned from a hood fire and deflagration event. J.M. Pickel

CHAS 12. Increasing sample throughput of Cannabis analyses on any LC system. R. Lake, A. Rigdon, R. Freeman, F. Carroll, T. Kahler

TUESDAY MORNING**Section A**

Embassy Suites Denver–Downtown Convention Center
Silverton Ballroom 1

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

Cosponsored by AGFD, CCS and PRES

H. J. Elston, N. R. Langerman, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 CHAS 13. How hazardous can nanostructured titanium dioxide be to humans in a water purification application? P. Zuniga, J. Quesada-Kimzey

9:25 CHAS 14. Ask Dr. Safety: EH&S support of nanotechnology R&D. N.R. Langerman, H.J. Elston

10:55 Concluding Remarks.

TUESDAY AFTERNOON**Section A**

Embassy Suites Denver–Downtown Convention Center
Silverton Ballroom 1

Safety in Undergraduate Teaching

Cosponsored by CCS

F. K. Wood-Black, *Organizer, Presiding*

1:30 Introductory Remarks.

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

- 1:40 CHAS 15.** Moving from a danger culture to a safety culture. R. Stuart
- 2:00 CHAS 16.** Teaching basic technique: A view into preparing for a safer educational and work environment. F.K. Wood-Black, K. Black
- 2:20 CHAS 17.** Using traditional safety rules to teach more advanced concepts in chemical hygiene. S.B. Sigmann
- 2:40 CHAS 18.** Talk dirty to me: Teaching undergraduate students the importance of good hygiene in the teaching laboratory. L. Gallion, A.M. Wilson, M.J. Samide
- 3:00 CHAS 19.** Risk hazard assessment in the general chemistry laboratory. S.D. Wiediger, A. Hyett
- 3:20** Intermission.
- 3:35 CHAS 20.** Developing a safety synergy in the chemistry department at Stanford University. C.T. Cox, S. Chan
- 3:55 CHAS 21.** Safety Friday: Do in-class safety presentations impact student behavior and perceptions of laboratory safety? A.M. Wilson, P.M. Morgan
- 4:15 CHAS 22.** Student view of safety in the undergraduate laboratory. T. Black, F.K. Wood-Black
- 4:35 CHAS 23.** Case study: Impact of chemical safety training in undergraduate teaching. O. Oluwaniyi, O.O. Fadare
- 4:55 CHAS 24.** Nitric acid acts upon trousers: Learning about hazardous chemicals. K.P. Fivizzani
- 5:15 Concluding Remarks.

CINF

Division of Chemical Information

E. Davis, Program Chair

OTHER SYMPOSIA OF INTEREST:

Drug Discovery (see COMP, Sun, Mon, Tue, Wed)

Applications of Positron Emission Tomography in Drug Discovery (see MEDI, Sun)

New Models for Drug Discovery: Public, Private, and Non-Profit (see MEDI, Mon)

Putting Chemical Biology in Context (see BIOL, Tue)

Citizens First: Communicating Climate Science to the Public (see CHED, Tue)

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of David A. Case (see COMP, Mon, Tue)

SOCIAL EVENTS:

Reception, 6:30 PM: Sun
Harry's Party, 5:30 PM: Mon
Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

Business Meeting, 1:00 PM: Sat

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.

SUNDAY MORNING

Section A

Colorado Convention Center
Room 110

Getting to the Best Reaction: Tools for Finding a Needle in a Haystack

R. Schenck, *Organizer, Presiding*

10:00 Introductory Remarks.

10:05 CINF 1. Automated design of realistic organometallic complexes and catalysts. M. Foscatto, G. Occhipinti, V. Venkatraman, B.K. Alsborg, V.R. Jensen

10:30 CINF 2. Different needles for different tailors: How specialized reaction search algorithms support scientists working in various research areas. V. Eigner Pitto, J. Eiblmaier, H. Kraut, H. Saller, P. Loew

10:55 CINF 3. Classification of scientific journal articles for the NIST Thermodynamic Research Center. A. Dima, Y. Feng, S. Youssef, K. Kroenlein

11:20 CINF 4. Mining electronic lab notebooks for synthetic needles (or gems). P.J. McHale

11:45 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 110

Defining "Value" in Scholarly Communications: Evolving Ways of Evaluating Impact on Science

S. Rouhi, T. M. Vogel, *Organizers, Presiding*

1:00 CINF 5. Withdrawn.

1:25 CINF 6. Dynamic evaluation of impact for scholarly communications in the field of thermophysical properties. R. Chirico, V. Diky, J. Magee, A. Bazyleva, C. Muzny, K. Kroenlein

1:50 CINF 7. Impact of crystal structures over the last, and next, 50 years. S. Ward, I. Bruno, C. Groom

2:15 CINF 8. Give me kudos for taking responsibility for self-marketing my scientific publications and increase impact. A.J. Williams, W. Russell, M. Kenneway, L. Peck

2:40 Intermission.

2:55 CINF 9. How do you define the value of something if it's free? Observations on Caltech's Institutional Repository. D.T. Wrublewski, G.S. Porter

3:20 CINF 10. Redefining value: Alternative metrics and research outputs. K. Deards, R.M. Burks, S. Rouhi, W. Gunn

MONDAY MORNING

Section A

Colorado Convention Center
Room 110

Research Results: Reproducibility, Reporting, Sharing & Plagiarism

M. G. Hicks, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CINF 11. Addressing researcher Incentives for publishability over accuracy. S. Davis Bowman, B. Nosek

9:05 CINF 12. Ethics in publishing: Editorial and related experiences. P.S. Weiss

9:35 CINF 13. Data management and the research record in research misconduct investigations. K. Busch

10:05 Intermission.

10:20 CINF 14. Irreproducibility in the scientific literature or: How often do scientists tell the truth, the whole truth and nothing but the truth? R.G. Bergman

10:50 CINF 15. Interplay of prior information and new data in high-throughput small-molecule studies. P.A. Clemons

11:20 CINF 16. STRENDAs – proposing minimum information for reporting functional enzymology data. C. Kettner, M.G. Hicks

MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 110

Research Results: Reproducibility, Reporting, Sharing & Plagiarism

M. G. Hicks, *Organizer*

C. Kettner, *Presiding*

1:30 CINF 17. Reproducibility in organic synthesis. R.L. Danheiser

2:00 CINF 18. Data and models, models and data. T.R. Clark, C. Kramer

2:30 CINF 19. Reproducibility and the quality of chemical probes. A. Edwards

3:00 Intermission.

3:15 CINF 20. MIRAGE – the minimum information required for a glycomics experiment: Rationale and progress. W. York, C. Kettner, R. Ranzinger

3:45 CINF 21. Reporting and reuse of crystal structure data and knowledge. I. Bruno, S. Ward, C. Groom

4:15 CINF 22. Reproducibility and variance of literature compound structure and bioassay data. J.P. Overington

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E. Davis, *Organizer*

8:00 - 10:00

1, 3-6, 11, 20. See previous listings.

CINF 23. Chemical literature: A comparison of most important databases for searching the chemical literature from an undergraduate perspective. N. Bharti

CINF 24. From lab to the libraries: A new route for chemistry librarianship. N. Bharti

CINF 25. 3Dmol.js: Simple visualization and sharing of 3D molecular data. D. Koes, N. Rego

26, 34-37, 44. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Room 110

Research Results: Reproducibility, Reporting, Sharing & Plagiarism

M. G. Hicks, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CINF 26. Sharing and reproducibility/replication: An NIH view. P. Bourne

9:05 CINF 27. Globalization of Big Data: Access, integration, and quality control issues. S. Boyer, E. Bolton, R. Martin, E. Louie, T.D. Griffin, G. Fu, B. Yu

9:35 CINF 28. Flagging and curating erroneous chemical and biological records using cheminformatics to ensure data reproducibility. D. Fourches

10:05 Intermission.

10:20 CINF 29. Increasing open communication to facilitate reproducibility. C. Soderberg

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Room 110

Molecular & Structural 2D & 3D Chemical Fingerprinting: Computational Storing, Searching, & Comparing Molecular & Chemical Structures

R. J. Bienstock, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 30. Insights into molecular similarity from crystal structures. C. Groom, S. Ward, I. Bruno, S. Vyas, N. Feeder

2:00 CINF 31. Do chiral fingerprints and descriptors work? S. Swamidass, G.P. Miller, T. Hughes, J. Hartman, S. Cothren

2:25 Intermission.

2:40 CINF 32. Similarity to SAR – interactive navigation of similarity relationships to guide optimization. M.D. Segall, E. Champness, J. Chisholm, C. Leeding, P. Hunt, A. Elliott, S. Dowling, H. Garcia

3:05 CINF 33. Database fingerprint clustering methods using KNIME. R.J. Bienstock

3:30 CINF 34. Highly visual representation methods for comparison of chemical structures and related properties. J.W. Sager, P. Mountney, C.P. Snyder, T.E. Mansley

3:55 Concluding Remarks.

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 110

Development & Use of Data Format Standards for Cheminformatics

D. Martinsen, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 CINF 35. Overview of the analytical Information markup language. S.J. Chalk

9:35 CINF 36. Thermophysical property dissemination utilizing an XML-based standard. K. Kroenlein, R. Chirico, V. Diky, A. Bazyleva, J. Magee, C. Muzny

10:05 CINF 37. Standard data format for computational chemistry: CSX. S.J. Chalk, N.S. Ostlund, M. Sopek, B. Wang

10:35 Intermission.

10:50 CINF 38. Development of an ontology specific to computational chemistry.

M. Sopek, S.J. Chalk, B. Wang, L. Nardozi, N.S. Ostlund

11:20 CINF 39. Importance of data standards for large scale data integration in chemistry. A.J. Williams, V. Tkachenko, A. Pshenichnov, K. Karapetyan, C. Coba

11:50 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 110

Development & Use of Data Format Standards for Cheminformatics

D. Martinsen, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 40. InChI as the chemical data format standard for cheminformatics. S.R. Heller

2:05 CINF 41. Using HL7 SPL standard for modeling substance information. Y. Borodina, F.L. Switzer, G. Schadow

2:35 Intermission.

2:50 CINF 42. JCAMP-MOL: A JCAMP-DX extension to allow integrated delivery of structural models and correlated spectral data. R.M. Hanson, R.J. Lancashire

3:20 CINF 43. Communicating crystal structures: Successes, challenges, and opportunities. I. Bruno, C. Groom, S. Ward

3:50 CINF 44. Building a standard for standards: The ChAMP project. S.J. Chalk, A. Williams

4:20 Concluding Remarks.

TOXI

Division of Chemical Toxicology

A. C. Bryant-Friedrich, Program Chair

MONDAY MORNING

Forensic Toxicology of Marijuana

Sponsored by SOCED, Cosponsored by BMGT and TOXI

CHAL

Division of Chemistry and the Law

K. E. Bianco and J. J. Hasford, Program Chairs

SOCIAL EVENTS:

Luncheon, 12:00 PM: Mon

Reception, 5:00 PM: Mon

BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Sun

SUNDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

A. Berks, X. Pillai, Organizers, Presiding

10:00 CHAL 1. Review of recent Federal Circuit decisions relevant to what scientists need to know about patent filing and prosecution. X. Pillai, A. Berks

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Hot Topics in Chemical and Pharmaceutical Patent Law

J. J. Hasford, Organizer

K. E. Bianco, Organizer, Presiding

1:00 CHAL 2. Options for protecting your intellectual property. K.E. Bianco

1:30 CHAL 3. Chemistry/pharma patents AND the “unpredictable arts”– increasing restrictions on patent protection for chemical compounds and compositions. H. Tostmann

2:00 CHAL 4. Recent case law on non-obviousness of patented chemical and pharmaceutical formulations. J.J. Hasford

2:30 CHAL 5. Recent Supreme Court cases in patent law. S.P. Hasford

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

A Patent Litigation Primer

K. E. Bianco, J. J. Hasford, Organizers, Presiding

9:30 CHAL 6. Patent litigation primer: What every chemist needs to know. K.E. Bianco, J.J. Hasford

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Anti-Doping: A Unique Combination of Chemistry and the Law

J. D. Lee, J. J. McShane, Organizers, Presiding

1:00 Introductory Remarks.

1:15 CHAL 7. Evolution of the world anti-doping code. R. Young

1:55 CHAL 8. Deterring performance-enhancing drug use in sports: The role of science. L. Bowers

2:35 Intermission.

3:00 CHAL 9. Deterring performance-enhancing drug use in sports: The role of investigations. W. Bock

3:40 CHAL 10. Role of World Anti-Doping Agency accredited laboratories in the fight against doping. D. Eichner

4:20 Panel Discussion.

MONDAY EVENING

Section A

Colorado Convention Center Halls C/D

Sci-Mix

K. E. Bianco, Organizer

8:00 - 10:00

CHAL 11. Chocolate: Food of the gods. H.M. Peters, S.B. Peters

CHAL 12. New changes in the “America Invents Act” for inventors. NewSection 102. A. Berks

CHAL 13. Provisional patent applications for fun and profit! A. Berks

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Fundamental Concepts in Protecting Chemical Technologies

M. J. Incorvia, Organizer, Presiding

9:00 CHAL 14. Patent vs. trade secret protection – the benefits and pitfalls. B. Kugler, K. Pearson

9:40 CHAL 15. How to read a patent. D. Swartz, M.J. Incorvia

10:00 CHAL 16. Maintaining intellectual property protection through confidentiality and non-use agreements. D. Kellis, R. Brunelli

10:30 CHAL 17. Intellectual property ownership. H. Covell, B. Lieb, R. Brunelli

11:00 CHAL 18. Rocky Mountain Regional Office of the US Patent and Trademark Office. J. Posthumus, R. Slifer

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Legal and Business Considerations for Chemical Technologies

M. J. Incorvia, Organizer, Presiding

1:30 CHAL 19. Supreme Court/Federal Circuit patent law update. B. Lieb, R. Brunelli

2:30 CHAL 20. Global patenting strategy. D. Swartz

3:00 CHAL 21. Intellectual property issues in acquisitions and financing. J. Posthumus, R. Brunelli, D. Swartz

3:30 CHAL 22. Inventive step in the United States, Japan, and Europe. Y. Shimizu

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

WEDNESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Patenting Chemical Inventions

K. L. Berkowski, S. Danek, Organizers, Presiding

9:00 CHAL 23. You discovered something new in the lab... now what? J.C. Hayes

9:30 CHAL 24. Patent eligible subject matter in the chemical arts. S. Danek

10:00 CHAL 25. Examination of the obviousness requirement for patenting chemical compounds. K.L. Berkowski

10:30 CHAL 26. Getting from bench-to-bed-side. V. Nielsen

11:00 CHAL 27. Technology transfer and industry collaborations: A new era in cooperative and sponsored research. M. Carr

WEDNESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Intellectual Property and Natural Resources: What Can I Protect and How?

J. L. Kennedy, D. Lorentzen, Organizers, Presiding

1:00 CHAL 28. Protecting natural resources with patents. J.L. Kennedy, D. Lorentzen

2:00 CHAL 29. Intellectual property strategy for technology employing natural resources. J.L. Kennedy, D. Lorentzen

THURSDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

The Many Faces of CHAL: Where Chemistry Meets the Law

K. E. Bianco, Organizer

R. G. Bone, Presiding

9:00 CHAL 30. First inventor to file: Two years on. R.G. Bone

9:30 CHAL 31. Is your chemical process still patentable? R.R. Charney

10:00 CHAL 32. Inter partes review: The story so far. R.G. Bone

10:30 CHAL 33. Is your drug now indefinite? R.R. Charney

11:00 CHAL 34. Double patenting trouble: Why terminal disclaimers matter more than ever. R.G. Bone

11:30 CHAL 35. Separate powers, singular purpose: How Congress, the Executive, and the courts are revolutionizing pharmaceutical patent litigation. C. Ray

COLL

Division of Colloid and Surface Chemistry

R. Nagarajan, Program Chair

OTHER SYMPOSIA OF INTEREST:

Nanomaterials for Solar Energy Conversion and Storage (see ENFL, Sun, Mon, Tue, Wed, Thu)

Chemical Processes at Environmental Interfaces (see ENVR, Sun, Mon)

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, and Single Photon Level (see PHY5, Sun, Mon, Wed)

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications (see PMSE, Sun, Mon, Thu)

Stimulus-Responsive Assemblies and Materials (see PMSE, Sun, Mon, Tue)

WCC Rising Stars Awards Symposium (see WCC, Mon)

SOCIAL EVENTS:

Social Hour, 6:00 PM: Sun

Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

Executive Committee Meeting, 5:00 PM: Sat

COLL Open Business Meeting, 5:30 PM: Sun

SUNDAY MORNING

Section A

Marriott City Center Denver

Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, Organizers, Presiding

8:30 Introductory Remarks.

8:35 COLL 1. Dendronized helix bundle assemblies designed de novo. J.G. Rudick

9:05 COLL 2. Mimicry of biorecognition motifs with peptidic foldamers. S.H. Gellman

9:35 COLL 3. Functional coiled-coil peptides controlled assemblies. A. Kros

10:05 Intermission.

10:20 COLL 4. Thermodynamics of surface-tethered peptide-polymer conjugates. S.P. Carmichael, M. Shell

10:50 COLL 5. Combating diseases with peptide-polymer conjugate. H. Klok

11:20 COLL 6. Carving pi-ways into biomaterials: electronic delocalization via peptide self-assembly. J.D. Tovar

Section B

Marriott City Center Denver

Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

W. Parak, Organizer

L. Liz Marzan, Organizer, Presiding

8:30 COLL 7. Colloidal effects in virus stability. F. Stellacci

9:00 COLL 8. Self-assembly of nanoparticles in chiral and other superstructures. N. Kotov

9:30 COLL 9. Ultraflexible reconfigurable magnetic nanoparticle filaments and networks by nanocapillary lipid bridging. O.D. Velev, B. Bharti, A. Fameau, M. Rubinstein

10:00 Intermission.

10:30 COLL 10. Colloidal design and optimization for assembly of complex crystals. S.C. Glotzer

11:00 COLL 11. Selective and differential functionalization of interior surface of hollow nanoparticles for nanoreactor applications. S. Kim, D. Lee, I. Lee

- 11:20 COLL 12.** Protein-based organic/inorganic hybrid nanocapsules for *In vivo* delivery applications. Y. Nam, J. Lee
- 11:40 COLL 13.** Interface engineering for nanocrystal stability in media spanning hexane to water. L.M. Wheeler, N.J. Kramer, U.R. Kortshagen
- 12:00 COLL 14.** Design of stimuli-responsive nanogels for bioapplications. J. Ramos, A. Pikabea, G. Aguirre, J. Forcada

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, J. Zheng, *Organizers, Presiding*

8:30 Introductory Remarks.

- 8:35 COLL 15.** Shape engineering substrate-based plasmonic nanostructures. K.D. Gilroy, R.A. Hughes, D. Sil, E. Borguet, S. Neretina
- 8:55 COLL 16.** All-optical control of localized plasmonic resonance using photoalignment and liquid crystals. T.J. Bunning, L. De Sio, G. Klein, S. Serak, N. Tabirian, A. Cunningham, C. Tone, F. Ciuchi, T. Burgi, C. Umeton
- 9:15 COLL 17.** Unique temporal and spatial biomolecular emission profile on individual zinc oxide nanorods. M. Singh, J. Hahn
- 9:35** Intermission.
- 9:45 COLL 18.** Withdrawn.
- 10:05 COLL 19.** Unprecedented upconversion efficiency in lanthanide nanocrystals via uniform, optically inert shells. N. Johnson, S. He, A. Almutairi
- 10:25 COLL 20.** Creation of natural dye sensitized solar cell. J. Uddin
- 10:45 COLL 21.** Rapid and sensitive assessment of biological and environmental samples using microwave-accelerated bioassay technique. M. Mohammed, K. Aslan

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Interfacial Phenomena

S. Muralidharan, M. Nieh, A. N. Parikh, *Organizers*
N. Srividya, *Organizer, Presiding*

- 9:00 COLL 22.** Physical measurements of hydrophobin air-filled bubbles and oil-filled blobs. X. Zhang, S. Kirby, D. Gorman, Y. Chen, W. Huberty, F. Hung, S.L. Anna, L. Walker, P.S. Russo
- 9:30 COLL 23.** Interactions of aromatic compounds with water-air and water-phospholipid interfaces. R.J. Perkins, R. Rapf, S.S. Mansy, V. Vaída
- 10:00** Intermission.
- 10:10 COLL 24.** Cellular uptake mechanisms as controlled by nanostructures of a lipid mixture: Comparison between bicelles and vesicles. W. Aresh, Y. Liu, J. Sine, D. Thayer, A. Puri, Y. Huang, Y. Wang, M. Nieh
- 10:40 COLL 25.** Investigating effects of Al³⁺ on structure and fluidity of lipid membranes: FRAP and molecular dynamics. H.K. Wayment-Steele, Y. Jing, L.E. Johnson, S. Svedhem, M.S. Johal, M. Swann, B. Agnarsson, A. Kunze
- 11:10 COLL 26.** Characterization of solid-supported ultrathin films using MP-SPR. N.M. Granqvist, W.M. Albers, A. Jokinen, J.W. Sadowski

Section E

Marriott City Center Denver
Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Metal Nanomaterials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

- 9:00 COLL 27.** Production of highly dispersed silver nanoparticles recovered from photographic film wastes using a simple green method. A.M. Atta, H.A. Al-Lohedan, A. Ezzat
- 9:20 COLL 28.** AFM-based fabrication and probing of metallic nanostructures. C.L. Berrie, C.M. Edwards, S. Ulapane
- 9:40 COLL 29.** Controlling the electronic structure and chemical reactivity of small nanoparticles through atomic composition. D. Kauffman, D. Alfonso, C. Matrangola, J. Trindell, R. Jinn
- 10:00 COLL 30.** Withdrawn.
- 10:20 COLL 31.** Real time microfluidic investigation: The role of seed age on gold nanorod formation. J. Watt, R. Anderson, B. Hance, D. Huber
- 10:40 COLL 32.** Investigation of the surface effects of Ag nanoparticles in solution as a result of a NSF-TUES related funding opportunity. C.S. Seney
- 11:00 COLL 33.** Dissolution and antibacterial efficiency of silver nanoparticles: Influence of particle size, shape, and surface chemistry. Q. Zhang, W. Jang, V.L. Colvin
- 11:20 COLL 34.** Study of interparticle interactions between gold nanoparticles using liquid cell electron microscopy. Q. Chen, H. Cho, K. Manthiram, M. Yoshida, X. Ye, P. Alivisatos
- 11:40 COLL 35.** Size-focusing synthesis of gold nanoclusters with *para*-mercaptobenzoic acid. L.M. Tvedte, C.J. Ackerson
- 12:00 COLL 36.** Constructing 0, 1, and 2D silvers within interlayer spaces of titania nanotubes. S.A. Ferdousi, K.L. Young
- 12:20 COLL 37.** Iridium-triggered facet transformation of Au nanocrystals via spontaneous oxidation-reduction process. C. Yang

Section F

Marriott City Center Denver
Colorado H

Particles at Fluid Interfaces

Cosponsored by PRES

M. A. Bevan, *Organizer*

J. Frechette, *Organizer, Presiding*

- 8:30 COLL 38.** Capillary migration of spheres on curved fluid interface. K. Stebe, N. Sharif-Mood, I. Liu
- 8:55 COLL 39.** Interactions between soft microgel particles at fluid interfaces. O.S. Deshmukh, A. Maestro, D. van den Ende, M. Cohen Stuart, F. Mugele, M.H. Duits
- 9:20 COLL 40.** Molecular characterization of surfactant adsorption at the surface of emulsion particles. G.L. Richmond, J. Hensel, A. Carpenter
- 9:45 COLL 41.** Understanding Pickering emulsions using multiscale simulations. A. Striolo
- 10:10 COLL 42.** Tracking nanoparticles in 3D – techniques and applications. J. Little, S. Stavis, P. Mathai, A. Balk, L. Mair, C. Hangarter, J. Unguris
- 10:35 COLL 43.** Spontaneous emulsification and interface formation induced by colloids. W. Kegeles
- 11:00 COLL 44.** DNA-functionalized nanoparticle assembly. M. Olvera De La Cruz
- 11:25 COLL 45.** Capillary foams: A new pathway toward functional porous materials. Y. Zhang, J.C. Meredith, S.H. Behrens
- 11:50 COLL 46.** Organized assemblies of colloids formed at the interfaces of micrometer-sized droplets of liquid crystal: Enabling the synthesis of patchy and nonspherical particles. N.L. Abbott

Chemical Processes at Environmental Interfaces

Chemistry and Imaging at Air/Liquid(Solid) Interfaces of Atmospheric Systems

Sponsored by ENVR, Cosponsored by COLL

SUNDAY AFTERNOON

Section A

Marriott City Center Denver
Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, *Organizers, Presiding*

- 2:00 COLL 47.** Artificial organelles: Cellular expression and assembly of polypeptide microdomains. J.A. MacKay, Z. Li, A. Truong, J. Dhandhukia, M. Pastuszka, P. Shi, S. Hamm-Alvarez, C. Okamoto
- 2:30 COLL 48.** Self-assembling peptide materials for hydrogen sulfide delivery. J.B. Matson, J.M. Carter
- 2:50 COLL 49.** Photons, chemicals, and electric fields as functional stimuli in supramolecular materials. S.I. Stupp
- 3:20** Intermission.
- 3:35 COLL 50.** 3D cell entrapment as a function of the weight percent of peptide-amphiphile hydrogels. C.M. Scott, E. Kokkoli
- 4:05 COLL 51.** Targeting collagen strands by triple helix hybridization. S. Yu
- 4:35 COLL 52.** Design evolution of an antibacterial bioadhesive inspired by cationic peptide hydrogels. J.P. Schneider
- 5:05 COLL 53.** Self-assembling antimicrobial nanofibers based on supramolecular peptide assemblies. H. Dong

Section B

Marriott City Center Denver
Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

L. Liz Marzan, *Organizer*

W. Parak, *Organizer, Presiding*

- 2:00 COLL 54.** Ultrasonic modification and functionalization of surfaces and particle. H. Moehwald
- 2:30 COLL 55.** Functionalization of gold nanorods. C.J. Murphy
- 3:00 COLL 56.** Hybrid platforms based on metal nanoparticles-doped filter paper for sensing and catalysis. I. Pastoriza Santos
- 3:30 COLL 57.** Dynamically self-assembling nanoflasks. R. Klajn
- 4:00 COLL 58.** Compact coatings for quantum dots that resist nonspecific binding to proteins, cells, and tissues. L. Ma, A. Smith
- 4:20** Intermission.
- 4:50 COLL 59.** Functional nanoparticles: Synthesis and biomedical applications. S. Sun
- 5:20 COLL 60.** Multicoordinating amphiphilic polymers provide compact, highly stable, and reactive semiconductor and metal oxide nanocrystal-conjugates. W. Wang, A. Kapur, G. Palui, H.M. Mattoussi
- 5:50 COLL 61.** Intracellular sensing of ion concentration with nanoparticles. W. Parak

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, J. Zheng, *Organizers, Presiding*

- 2:00 COLL 62.** Smart photon management for organic photovoltaic. Y. Yang, Y. Yang, J. You, Z. Hong

- 2:30 COLL 63.** Nanoscale oxynitrides with tunable composition and absorption spectra. G. Dukovic
- 3:00 COLL 64.** Light extraction from organic light-emitting diodes using plasmonic scattering layers. L. Rothberg, C. Favaro, C. Chang
- 3:30** Intermission.
- 3:40 COLL 65.** Nanostructured plasmonic antenna systems and catalytic electrode materials for enhancing solar water splitting. S. Pan
- 4:10 COLL 66.** Molecular imprinted polymers for plasmonic sensing. A.J. Haes
- 4:40 COLL 67.** On the possibility of the para-aryl-dithiols cross-linking plasmonic nanoparticles as dithiolates. D. Zhang

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Model and Cellular Systems

S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

M. L. Longo, *Presiding*

- 2:00 COLL 68.** Air-stable droplet interface bilayers. C.P. Collier, C.I. Richards, S.A. Sarles, J. Boreyko
- 2:30 COLL 69.** From compartmentalized polymersomes to biomimetic artificial cell. M. Marguet, R. Peters, J. van Hest, S. Lecommandoux
- 3:00** Intermission.
- 3:10 COLL 70.** Probing interactions between nanoparticles and cellular membrane via single cell mechanics. G. Liu, Y. Liu, D. Anderson, A. Karsai, D. Uyeminami, L. Von Winkle, K. Pinkerton
- 3:40 COLL 71.** Rigidity signals drive differential ROCK signaling to regulate invadopodia activity. A. Parekh
- 4:10 COLL 72.** Phase separation in hybrid polymer/lipid vesicles: A rational to obtain lipid or polymer raft-like nanodomains. J. Le Meins, T. Dao, R. Salva, F. Fernandes, A. Brulet, M. Schmutz, M. Er-Rafik, M. Prieto, S. Lecommandoux, O. Sandre

Section E

Marriott City Center Denver
Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Metal Oxide Nanomaterials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

- 2:00 COLL 73.** Methods for rapid synthesis of nonaggregated nanozeolite Y. B. Wang, Y. Li, P.K. Dutta
- 2:20 COLL 74.** Design of suitable protocols to evaluate metal oxide nanoparticles in unmodified commercial sunscreens. C. Sapcharoenkun, P. Kasamechonchung, P. Kumnorkaew, P. Kopermsub
- 2:40 COLL 75.** Local and long range structure in metal oxide nanoparticles. M.A. Langell, M.A. Peck, M. Kumbier, D. Wilson
- 3:00 COLL 76.** Fabrication of abundant Zn vacancies in ZnO for p-type conductivity, room-temperature ferromagnetism and high photocatalytic activity. L. Pan, J. Song, J. Zou, S. Wang, Z. Huang, L. Wang, X. Zhang
- 3:20 COLL 77.** Application-scale size-selective fractionation of iron oxide nanoparticles using CO₂-expanded liquids. P.S. Vengsarkar, R. Xu, C.B. Roberts
- 3:40 COLL 78.** Improvements of TiO₂ nanoparticle dispersion stability in nonpolar solvents by long chain fatty acid functionalization. N. Baek, Y. Kim, S.F. Okeefe
- 4:00 COLL 79.** Mobility of antiscalant-modified BaSO₄ particles through saturated proppant pack. C. He, R.D. Vadic

- 4:20** COLL **80.** Enhanced photodecomposition activity induced by nanodimensional cerium oxide domains on titania surfaces. **C.A. Estes, M.B. Mitchell**
- 4:40** COLL **81.** Thiol adsorption on metal oxide nanoparticles and surfaces. **Y. Wang, O. Grimm, J.E. Whitten**
- 5:00** COLL **82.** Highly uniform gadolinium oxide nanoparticles as remarked remarkably enhanced MRI contrast agents for cellular MR imaging. **N. Taheri, G. Stinnett, r. pautler, P. Decuzzi, V.L. Colvin**
- 5:20** COLL **83.** Cr:ZnGa₂O₄ nanoparticles with controllable size and persistent luminescence. **Y. Mao, B. Bahadur Srivastava**
- 5:40** COLL **84.** Controlled synthesis of inorganic nanostructures using soft stretchable substrates. **S.A. Morin, J.J. Bowen, J.M. Taylor**

Section F

Marriott City Center Denver
Colorado H

Particles at Fluid Interfaces

Cosponsored by PRES

J. Frechette, *Organizer*

M. A. Bevan, *Organizer, Presiding*

- 2:00** COLL **85.** Electrostatic repulsion between colloids at the oil-water interface. **E.M. Furst**
- 2:25** COLL **86.** Janus particles as dynamically tunable solid surfactants. **D. Lee**
- 2:50** COLL **87.** Bicompartmental phase transfer vehicles based on colloidal dimers with anisotropic structural and interfacial properties. **N. Wu**
- 3:15** COLL **88.** Self-organisation of colloidal particles at liquid interfaces. **T.S. Horozov**
- 3:40** COLL **89.** Particle transport at oil/water interfaces driven by spatially varying surfactant adsorption or desorption kinetics. **R.D. Tilton, S. Garoff, T.M. Przybycien, G. Duner**
- 4:05** COLL **90.** Thermodynamics of Janus particles in 2D confinement. **S. Razavi, R.S. Tu, I. Kretzschmar**
- 4:30** COLL **91.** Remotely triggered colloidal disassembly from particle-laden microbubble. **V. Garbin**
- 4:55** COLL **92.** Measurements and models of reversible adsorption of nanoparticles at the oil-water interface. **X. Hua, M. Bevan, J. Frechette**

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer*

C. R. Kagan, *Presiding*

- 2:00** COLL **93.** Breaking Lord Rayleigh's Rule: Linked photochemical reactions that double the resolution of a lens. **C.G. Willson, R.A. Mesch, X. Gu, W. Wang, T. Kawakami, Y. Hajiwara, M. Okazaki, H. Truong, Y. Li, S. Jockusch, N. Turro**
- 2:40** COLL **94.** Designing precursors for the deposition of inorganic nanostructures by CVD, SPMCD and EBID. **L. McElwee-White**
- 3:10** COLL **95.** Dynamic substrate control: Dual-tone hydrogel photoresists. **C. Xue, D. Wong, S. Norris, A.M. Kasko**
- 3:40** COLL **96.** Chemical lift-off lithography by collapsing soft-material molds. **W. Liao, H. Jan**
- 4:10** COLL **97.** Atomic picture of nuclear decay in stable 2D radioactive films. **E.H. Sykes**

Chemical Processes at Environmental Interfaces

Chemistry and Imaging at Air/Liquid(Solid) Interfaces of Atmospheric Systems

Sponsored by ENVR, Cosponsored by COLL

SUNDAY EVENING

Section A

Colorado Convention Center
Hall B2

Fundamental Research in Colloids, Surfaces & Nanomaterials

Cosponsored by PRES

R. Nagarajan, *Organizer*

6:00 - 8:00

- COLL 98.** J-aggregate formation of cationic cyanine dyes on clay minerals. **N. Sato, T. Fujimura, Y. Ohtani, T. Shimada, S. Takagi**
- COLL 99.** Dynamics of binary mixtures of cationic and anionic microgels at the air water interface. **K. Horigome, D. Suzuki**
- COLL 100.** Solvent-free functionalization of multiwalled carbon nanotube buckypaper with amines. **I.J. Ramirez-Calera, V. Meza-Laguna, E. Abarca-Morales, V.A. Basiuk, E.V. Basiuk**
- COLL 101.** Coordination functionalization of graphene oxide and nanodiamond with nickel(II) tetraazamacrocyclic complexes. **N. Alzate-Carvajal, L.V. Henao-Holguin, V. Meza-Laguna, A. Moreno-Bárceñas, J.F. Pérez-Robles, E. Rybak-Akimova, V.A. Basiuk, E.V. Basiuk**
- COLL 102.** Characterization of covalently-functionalized mesoporous silica nanoparticles by solution-phase NMR methods. **S.E. Lehman, Y. Tataurova, S.C. Larsen**
- COLL 103.** DFT study of noncovalent complexes of phthalocyanines with spherical fullerenes and short nanotube models. **V.A. Basiuk**
- COLL 104.** Label-free detection of RNA by using liquid crystals. **Y. Liu, K. Yang**
- COLL 105.** Interaction of a Ni(II) tetraazaannulene complex with spherical and elongated fullerenes: A DFT study. **L.V. Henao-Holguin, V.A. Basiuk**
- COLL 106.** Imaging of liver cells using water soluble CdTe quantum dots. **A. Coover, T.G. Lewis, T.J. Ripley, A.L. Asunskis, D.J. Asunskis**
- COLL 107.** Effects of composition on the gradient structure and surface properties of fluorinated polyacrylates latex blends film. **H. Yuanyuan, Z. Zhaoan, Y. Chen**
- COLL 108.** Effect of chain length, number of chains, and charge on the in vitro cytotoxicity of surface coating agents used for nanoparticles. **Y. Zhang**
- COLL 109.** Fluorescent organic nanodots for sensing metals and a targeted immunofluorescence labeling. **H. Kim**
- COLL 110.** Electrochemical and photocatalytic activity analysis of TiO₂-NIO/TiO₂. **S. Buama, P. Rangsunvigit**
- COLL 111.** Studies on the mechanisms of forced transport of dye through solution modifications to a polymerized surface. **J. Siegenthaler, D. Rivera**
- COLL 112.** Adsorption of poly(vinyl alcohol) onto polydimethylsiloxane substrates: Formation of continuous films, honeycomb structures, and fractal morphologies. **B. Sharma, A. Karki, L. Nguyen, W. Chen**
- COLL 113.** Role of substrate receding contact angle in deposit patterns of sessile droplets containing stabilized gold nanoparticles. **E. Laudadio, L. Zhang, W. Chen**
- COLL 114.** Smooth and uniform thiol-functionalized substrates for bioconjugations. **T. Tabassum, S. Xu, W. Chen**
- COLL 115.** Probing the hydrodesulfurization properties of cobalt-nickel phosphides: Supported catalysts and encapsulated nanoparticles. **S. Danforth, R. Lijana, B. Ilic, P. Topalian, M.E. Bussell**
- COLL 116.** Capacitance and hydrogen evolution reaction characterization of electrodeposited nickel alloy thin films. **M. Gira, J.R. Hampton**
- COLL 117.** Quantitative characterization of methanol oxidation catalysis on dealloyed NiCu films. **M. Milliken, J.R. Hampton**
- COLL 118.** Nickel phosphide hydrotreating catalysts on phosphorus-modified oxide supports. **B.J. Morgan, S. Danforth, B. Ilic, M.E. Bussell, P. Topalian**
- COLL 119.** Total holographic characterization of colloidal suspensions. **L.A. Philips, F.C. Cheong, D.G. Grier**
- COLL 120.** Effects of shear and walls on the diffusion of colloids in microchannels. **S. Ghosh, F. Mugele, M.H. Duits**
- COLL 121.** Glutathione-coated luminescent gold nanoparticles: A surface ligand for minimizing serum protein adsorption. **R. Vinluan, J. Liu, C. Zhou, M. Yu, S. Yang, A. Kumar, S. Sun, A. Dean, X. Sun, J. Zheng**
- COLL 122.** Crystallization of proteins on iron nanocolumns using metal-assisted and microwave-accelerated evaporative crystallization for liproved size distribution. **K. Mauge-Lewis, E. Toth, D. Seifu, K. Aslan**
- COLL 123.** Crystal engineering of L-alanine in the presence of multiple amino acid additives using metal-assisted and microwave-accelerated evaporative crystallization. **A. Mojibola, E. Constance, T.E. Onuekwusi, I. Nicholson, M. Mohammed, K. Aslan**
- COLL 124.** De-crystallization of uric acid crystals in synovial fluid using gold colloids and low power microwave heating. **B. Kioko, T. Ogundolie, M. Adebisi, Y. Ettinoffe, C. Rhodes, B. Gordon, N. Thompson, M. Mohammed, K. Aslan**
- COLL 125.** Biodegradable polymer materials containing stabilized silver nanoparticles. **A. Paul, A. Vasiliev**
- COLL 126.** Characterization and bioapplication of nanoscaled materials derived from green chemistry. **P. Hanumandla, J. Dinn, N. Ngassa, D. Lopez, P. Nandakumar, J.L. Liu**
- COLL 127.** How small molecules self-assemble into nanofibers and form hydrogels. **Y. Gao, B. Hammouda, J. Douglas, F. Horkay**
- COLL 128.** Computational study of hydroxyproline-pectin cross-linkage for drug delivery. **M.H. Andersen, L. Tribe**
- COLL 129.** Tmpyp containing nanoparticles with enhanced photo-physical properties. **M. Zhu, S. Shuthanandan, H. Zhang, G.H. Aryal, J. Jayawickramarajah**
- COLL 130.** Optical characterization of purified noble metal nanoparticles. **A. Thomas**
- COLL 131.** Green synthesis of magnetic nanocomposites formulated with Indian medicine to perform cancer theranostic study. **J.L. Liu, K.Y. Amaravathi, H. Shravan, S. Bashir, X. Du**
- COLL 132.** Plasmonic nanocrystal solar cells utilizing strongly confined radiation. **P. Moroz, M. Zankov, N.N. Kholmicheva, U. Rijal, A. Razgoniaev, A. Ostrowski**
- COLL 133.** Structure and behavior relationships among semifluorinated linear, dibranched and miktoarm amphiphiles. **W. Tucker, A. McCoy, S. Fix, M. Stagg, M. Murphy, S. Mecozzi**
- COLL 134.** Effect of pH on the adsorption of cationic polyacrylamide to polyacrylic acid. **D. Seo, H. Lee, H. Youn**
- COLL 135.** Role of alpha-hemolysin's phosphocholine binding pocket and cholesterol in lipid membrane adsorption and nanopore formation. **C. McCauley, L. Keranen Burden, D. Burden**
- COLL 136.** Surface equilibrium and kinetic dynamics of alpha hemolysin on red blood cell membranes. **J. Ellingsen, A.S. Freeman, L. Keranen Burden, D. Burden**
- COLL 137.** Morphological and electrochemical characterization of Laponite/polyaniline/graphene and graphene oxide nanocomposite materials. **I. Ramphal, M.E. Hagerman**
- COLL 138.** Morphosynthetic studies of polyaniline/graphene oxide/Laponite nanocaffolds. **Y. Hu, M.E. Hagerman**
- COLL 139.** Study of selective heavy metal removal from seawater. **X. Chen, Y. Li, W. Han, K.L. Yeung**
- COLL 140.** Interaction of ligand-capped metal nanoparticles with t2D atomic layered nanomaterials. **S.S. Low, S. Gang, Y. Shon**

- COLL 141.** Gold nanoparticles size characterization using PCA and LDA techniques by UV-Vis spectroscopy. **H. Cavusoglu, Y. Danisman, H. Sakalak, M. Yilmaz, M. Yavuz**
- COLL 142.** Dynamic observation of NIH3T3 cells adhesion behaviors on binary self-assembled monolayers modified gold surfaces. **W. Kao, H. Chang, J. Shyue**
- COLL 143.** Ag nanoparticle nucleation vs. shell growth. **M. Shaughnessy, D. Khon, N. Sharma, M. Zamkov**
- COLL 144.** Improving the catalytic activity of metal semiconductor nanocomposites. **J. Bocanegra, D. Khon, E. Khon, M. Zamkov**
- COLL 145.** Preparation of highly efficient Winsor-IV type microemulsions for rapid wood penetration. **X. Du, L.A. Lucia, R.A. Ghiladi, O.J. Rojas**
- COLL 146.** Variations in intermolecular interactions in the microtubule associated protein tau revealed by atomic force microscopy. **Z. Donhauser**
- COLL 147.** First principles characterization of nontronite clay surfaces with varying Fe(II)/Fe(III) composition. **S. Ramadury, S.E. Mason**
- COLL 148.** Effect of solvent on the growth of isotropic/anisotropic core/shell nanoparticles via alternating layer techniques. **R. Tan, S.K. Roberts, Y. Shen, M.Y. Gee, A.B. Greytak**
- COLL 149.** Nanoparticle mediated remote activation of thermophilic enzymes with alternating magnetic fields. **C. Collins, C.J. Ackerson**
- COLL 150.** Template synthesis of gold nanoparticles using an organic molecular cage. **R. McCaffrey, W. Zhang**
- COLL 151.** Progress toward clonable inorganic nanoparticles. **T. Ni**
- COLL 152.** Role of surface groups in cycloaddition reactions over ZIF-8 films. **E.R. Webster, F. Tian, L.B. Benz**
- COLL 153.** Adsorption and interaction of alcohols with ZIF-8 films and the role of surface groups. **L.B. Benz, H.L. Larson, A.M. Mosier, F. Tian, E. Baxter, A. Cheetham**
- COLL 154.** Rational design and control of functional molecules on single metal nanoparticles. **Y. Zheng**
- COLL 155.** Nanoporous hydrogen-reduced bismuth vanadate coupled with electrocatalysts as high-performance photoanodes for solar fuels. **J. Gan, X. Lu, Y. Tong, Y. Zheng**
- COLL 156.** Ultrafast and temperature-dependent optical properties of Au₄₇, Au₁₀₂ and Au₄₄ clusters. **V.D. Thanthirige, K. Kwak, D. Lee, E. Sinn, R. Guda**
- COLL 157.** Fabrication of inverse opal films with stop bands in the full spectral range of visible light using co-assembly technique. **U.S. Madduma-Bandarage, Y. Vasquez**
- COLL 158.** Electric-field assembly and propulsion of chiral colloidal clusters. **F. Ma, S. Wang, D. Wu, N. Wu**
- COLL 159.** Effect of surfactants on cyclopentane hydrates: Structure and properties. **E. Brown, J. Wells, C.A. Koh**
- COLL 160.** Properties of Fe₃O₄@chitosan nanoparticles at oil/water interfaces. **A.R. Molina**
- COLL 161.** Withdrawn.
- COLL 162.** Elucidating reaction pathways for thermoelectric materials fabricated by bottom-up solution-phase solid-state synthesis. **C. Holder, E. Rugen, D. Stevens, M.E. Anderson**
- COLL 163.** New approach for scientific research on RO membrane. **J. Okabe, M. Nishida, T. Ogawa, T. Sasaki, M. Kimura**
- COLL 164.** Foundational layer formation of metal-organic coordinated thin films. **M.L. Ohnsorg, B. Bowser, L. Gentry, M.E. Anderson**
- COLL 165.** Investigation of the stability of Ag nanoparticles in solution by isothermal titration calorimetry (ITC) and zeta-potential measurements. **J.D. Mimbs, C.S. Seney, R. Vaithi, A. Weems, R.H. Goddard**
- COLL 166.** Study of fractal colloidal gels using DLS and SALS. **R. Ebini**

- COLL 167.** Effects of H₂O and H₂ plasma surface modification of SnO₂ nanowires and spiked nanowires. **C.J. Miller, E.P. Stuckert, E.R. Fisher**
- COLL 168.** Withdrawn.
- COLL 169.** Analysis of polymeric phase separation within a thermoset polymer blend for applications in high performance low gloss coatings. **S.L. Giles, J.H. Wynne, C.R. Clayton, N.W. Heller**
- COLL 170.** Controlling the unit cell lattice parameters in nanoscaled Cu₂Pd₃O by composition and crystallite size. **M. Kumbier, G.L. Christensen, M.A. Langell**
- COLL 171.** Synthesis, characterization, and imaging applications of various silver nanoparticles morphology. **D. Castillo, L.M. Hernandez, M. Forero-Shelton, W.L. Vargas**
- COLL 172.** Chemical synthesis and High temperature structural stability of monodisperse ruthenium nanostructures. **N. Chou, D. Zakharov, E. Stach, A. Harutyunyan**
- COLL 173.** Effect of doping density on current-voltage behavior and quantum yields of dye-sensitized single crystal TiO₂ electrodes. **K.J. Watkins, B.A. Parkinson, M. Spitzer**
- COLL 174.** Directed synthesis of bimetallic nanoparticles using poly(2-vinylpyridine) colloids. **A.K. Taylor, D.A. Rider**
- COLL 175.** Modulating beta amyloid (A β) aggregation with metal ions and nano-chelators. **M.R. Mackiewicz, B.D. Jorgenson, E.A. Costa**
- COLL 176.** Surface-chemistry effect on cellular response of luminescent plasmonic silver nanoparticles. **S. Sun**
- COLL 177.** Enhanced dispersion of cellulose nanocrystals for nanofibrillated cellulose nanocomposites. **W. Fang, E. Kontturi, M. Linder, P. Laaksonen**
- COLL 178.** Microscopy study of poly(3-hexylthiophene) films processed from binary mixtures of organic solvents. **M.P. Gordon, D.S. Boucher**
- COLL 179.** Distinct assembly and disassembly pathways of nanotube formed by drug amphiphile. **P. Zhang, A. Cheatham, H. Cui**
- COLL 180.** Investigation of bone growth onto titanium rods investigated with model cell membranes. **M. Gulley, A.G. Sostarecz**
- COLL 181.** Exploring the desolvation of BSA-ligand complexes using the quartz-crystal microbalance and dual polarization interferometer. **N. Stanton, J. Kang, C.R. Selassie, M.S. Johal**
- COLL 182.** Withdrawn.
- COLL 183.** Synthetic route for the growth of entirely I-III-VI semiconductor core/shell nanocrystals. **S.M. Hughes, F. Rowe, S. Dvorak**
- COLL 184.** Synthesis of micrometer-sized CdSe nanosheet via cation exchange. **P. Tongying, Y. Morozov, M. Zhukovskiy, M.K. Kuno**
- COLL 185.** Zein nanoparticles as superhydrophobic coatings: a simple and ecofriendly way to antiwetting textiles surfaces. **G. Li**
- COLL 186.** Laser-induced copper deposition from solution with the addition of non-ionic surfactants: Influence of hydrophilic properties. **S.V. Safonov, S. Araslanova, F. Sergey**
- COLL 187.** DFT study of the dissociative adsorption of chlorobenzene and 1,2-dichlorobenzene on Si(100). **E. Butson, N.F. Materer, Q. Zhu**
- COLL 188.** Ultrastrong epoxy nanocomposites containing self-assembled synthetic clay in smectic order. **P. Li, K. White, C. Lin, D. Kim, R. Krishnamoorti, A. Mullana, R. Nishimura, H. Sue**
- COLL 189.** Withdrawn.
- COLL 190.** Synthesis and characterization of homogeneous Zn₂Cu_xO solid-solutions. **D. Wilson, M.A. Langell**
- COLL 191.** Size- and shape-controlled synthesis of Gold nanoparticles using chitosan as a stabilizer. **L. Liu, J. Chaudhuri**
- COLL 192.** Influence of shelling temperature and time on the optical and structural properties of CuInS₂/ZnS quantum dots. **C. Robinson, C.D. Heyes**
- COLL 193.** Bright tunable photoluminescence in colloidal amorphous porous silicon nanostructures. **J. El Demellawi, S. Chaieb**
- COLL 194.** Topical delivery of lipophilic carbonic anhydrase inhibitors with liposomal formulations. **A. Shabana, S. Akocak, M.A. Iles**
- COLL 195.** Model system development for urban films and environmental adsorption. **J.S. Grant, S.K. Shaw**
- COLL 196.** Stretchable surface-chemical patterns. **J.J. Bowen, J.M. Taylor, S.A. Morin**
- COLL 197.** Oxidative decomposition of Au₂₅(SR)₁₈ clusters in a catalytic context. **T. Dreier, A. Wong, C.J. Ackerson**
- COLL 198.** Titania containing thin films for the detection of TATP and peroxide vapors. **N.F. Materer, T.H. James, C. Cannon, D.W. Scott, Z. Alotzman, A.W. Applett**
- COLL 199.** Synthesis of large-pore SBA-15 silica at room temperature. **T. Man, I. Stoyko, I. Nayshevsky, M. Kruk**
- COLL 200.** Surface reactions of gas-phase atomic radicals with alkanethiolate monolayers. **A. Gans, S.A. Kandel**
- COLL 201.** Stability and transport properties of magnetic nanoparticles under high temperature, high salinity aqueous conditions for oil reservoir imaging. **Y. Fei, S. Kong, E. Urena, E. Lin, V. Ngo, Y. Lu, C.J. Ellison, K.P. Johnston**
- COLL 202.** Layer-by-layer assembly of polyelectrolytes and different size and shape gold nanoparticles. **S.M. Budy, D. Hamilton, Y. Cai, M.K. Knowles, S.M. Reed**
- COLL 203.** Multivalued carbon nanotube incorporated "molecular fan" coatings for optimized thermal management applications. **T. Eyassu, T. Hsiao, K. Henderson, T. Kim, C. Lin**
- COLL 204.** Size dependence of gold nanoparticle interactions with a supported lipid bilayer: A QCM-D study. **C.M. Bailey, E. Kamaloo, K. Waterman, K. Wang, R. Nagarajan, T.A. Camesano**
- COLL 205.** Extreme-wettable nanomolecular layer. **H. Baik, S. Chae, Y. Kim**
- COLL 206.** Droplet size distributions of water-in-oil emulsions using low field NMR before and after gas hydrate formation. **A. Abdul Majid, M. Saidian, C.A. Koh**
- COLL 207.** Methane activation on ceria surfaces modified with metal nanoparticles. **M. Nolan, J. Carey, A. Van Veen**
- COLL 208.** Surface properties of hydrocolloid-stabilized magnetite Murrh capped nanoparticles. **A.M. Atta, H.A. Al-Lohedan**
- COLL 209.** Epoxy/clay nanocomposites containing clay layers in smectic long-range order. **M. Wong, P. Li, F. Lei, M. Miyamoto**
- Section B**
Colorado Convention Center
Hall B2
Interfacial Biomolecular Recognition
Cosponsored by BIOL \ddagger
Financially supported by Avanti Polar Lipids, Inc.
J. Ross, Organizer
B. E. Bowler, M. Kastantin, Organizers
- 6:00 - 8:00**
COLL 210. Isolation and investigation of distinct cytochrome c/cardiolipin interaction sites. **M. Elmer-Dixon, B.E. Bowler**
- COLL 211.** Role of lysine 72 in human cytochrome c alkaline conformational transition. **E.M. Nold, B.E. Bowler**
- COLL 212.** ¹⁹F Dendron probes for specific detection of enzyme activity. **H. Wang, K.R. Raghupathi, J. Zhuang, S. Thayumanavan**
- COLL 213.** Biomolecular patterning via chemical lift-off lithography. **H.H. Cao, W. Liao, N. Nakatsuka, S. Deshayes, A.M. Kasko, P.S. Weiss, A.M. Andrews**
- COLL 214.** Surface passivation and acidic conditions allow for the rapid synthesis of DNA-conjugated gold nanoparticles with high salt stability and DNA-binding specificity. **J. Deka, R. Mech, L. Ianeselli, H. Amenitsch, F. Cacho-Nerin, P. Parisee, L. Casalis**
- COLL 215.** Sialic acid decorated polymer@
- goldNP as biofunctional hybrids: assembly, lectin and viral binding. **Z. Zhang, B. De Geest**
- COLL 216.** Using fluorescent-labeled nanodiscs to study lipid interactions with yeast Cytochrome C. **H.B. Steele, L. McClelland, K. Stipe, M.C. Terwilliger, B.E. Bowler, J. Ross**
- Section C**
Colorado Convention Center
Hall B2
Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion
Cosponsored by PRES
Financially supported by Sigma-Aldrich
S. Pan, J. Zheng, Organizers
- 6:00 - 8:00**
COLL 217. Plasmonic enhancement of dye-sensitized solar cells using SiO₂@AuNP thin films. **B.D. Clark, E.M. Spain**
- COLL 218.** Preparation of Fe(II)-impregnated granular activated carbon for arsenate removal from water. **H. Xu**
- Section D**
Colorado Convention Center
Hall B2
Plasmonic Catalysis and Sensing
C. Matranga, Organizer
E. Borguet, Organizer
- 6:00 - 8:00**
COLL 219. Enhanced photocurrent via plasmon excitation of ultrasmall PbS quantum dots on Au/TiO₂ electrode. **X. Li, K. Suzuki, T. Toda, S. Yasuda, K. Murakoshi**
- COLL 220.** Nucleation and growth of silver nanoparticles by AB and ABC-type atomic layer deposition. **S. Masango, R.P. Van Duyn, P.C. Stair**
- MONDAY MORNING**
- Section A**
Marriott City Center Denver
Colorado A/B
Molecular Engineering of Peptide Assembly
Financially supported by Institute for Molecular Engineering, University of Chicago
H. Cui, M. V. Tirrell, Organizers, Presiding
- 8:30** **COLL 221.** Supramolecular polypeptide structures assembled from folded, globular proteins. **W. Park, J. Champion**
- 9:00** **COLL 222.** Elastin-based amphiphilic copolymers as precision building blocks for controlled self-assembly. **E. Garanger, S. Mac Ewan, A. Chilkoti, S. Lecommandoux**
- 9:30** **COLL 223.** Growth factors engineered for super-affinity to the extracellular matrix enhance tissue healing. **P.S. Briquez, M.M. Martino, J.A. Hubbell**
- 10:00** Intermission.
- 10:15** **COLL 224.** Effect of surfaces in modulating peptide assembly. **J.E. Shea**
- 10:45** **COLL 225.** Materials with desired nanostructure through peptide design and solution assembly. **D.J. Pochan**
- 11:15** **COLL 226.** Fibrillar protein and peptide co-assemblies: Design and applications in medicine. **T. Sun, G. Hudalla, C. Mora Solano, J. Collier**
- Section B**
Marriott City Center Denver
Colorado I
Functionalization of Complex Nanosurfaces
Cosponsored by PRES
W. Parak, Organizer
L. Liz Marzan, Organizer, Presiding
- 8:30** **COLL 227.** Formation of protein coronas on gold nanorods stabilized by amphiphilic ligands. **K. Hamad-Schiffert**
- 9:00** **COLL 228.** Direct delivery of proteins and nucleic acids to the cytosol using nanoparticle-stabilized capsules. **V.M. Rotello**
- 9:30** **COLL 229.** In how far can we make nanoparticles mimic molecules? **Z. Nie, C. Yi, Y. Liu, J. He**
- 10:00** **COLL 230.** Hierarchical architectures from ordered electroactive small molecules. **N. Martin, C.M. Atienza, J. López, A. Insuasty, J. López-Andarias**
- 10:30** Intermission.
- 11:00** **COLL 231.** Modification of microgel surfaces with a self-assembling peptide. **K.C. Clarke, L.A. Lyon**
- 11:20** **COLL 232.** Probing the dynamic and structure of nanoparticle protein corona by using single molecule spectroscopy. **A.D. Indrasekara, S. Dominguez-Molina, L. Kiskey, C.F. Landes, S. Link**
- 11:40** **COLL 233.** Lipid coated gold nanoparticles as models of faceted and highly curved membranes. **D. Hamilton, S.M. Budy, S.M. Reed**
- 12:00** **COLL 234.** Role of ligands in the structure and properties of molecular silver nanoparticles and their assemblies. **T.P. Bigioni**
- Section C**
Marriott City Center Denver
Colorado C/D
Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion
Sensing, Electronics, & Photophysics
Cosponsored by PRES
Financially supported by Sigma-Aldrich
S. Pan, J. Zheng, Organizers, Presiding
- 8:30** **COLL 235.** Theranostic gold nanorods for synergistic cancer treatment. **Z. Gu**
- 9:00** **COLL 236.** Determining drug efficacy using plasmonically enhanced imaging of the morphological changes of cells upon death. **M. Aioub, L. Austin, M.A. El-Sayed**
- 9:30** **COLL 237.** Functional DNA nanotechnology and its applications in environmental sensing and live cell imaging. **Y. Lu, J. Zhang, L. Li, P. Wu, K. Hwang, H. Xing**
- 10:00** Intermission.
- 10:10** **COLL 238.** Role of the protein corona in mediating nanoparticle targeting. **W. Chan**
- 10:40** **COLL 239.** Prolonged hot electron dynamics in plasmonic-metal/semiconductor heterostructures with implications for solar photocatalysis. **W. Wei**
- 11:10** **COLL 240.** Enhanced light-matter interactions in nanoparticle arrays. **T.W. Odom**
- 11:40** **COLL 241.** Renal clearable metal nanoparticles for cancer imaging. **J. Zheng**
- Section D**
Marriott City Center Denver
Denver III
Biomembrane Synthesis, Structure, Mechanics, & Dynamics
Vesicles and Related Systems
S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, Organizers
D. L. Daleke, Presiding
- 9:00** **COLL 242.** Functional reconstitution of integral membrane proteins in giant lipid vesicles by hydrogel swelling. **N. Malmstadt**
- 9:30** **COLL 243.** Membrane shape instabilities induced by BAR domain proteins. **T. Baumgart**
- 10:00** **COLL 244.** Nanoparticle-induced pore formation in lipid bilayers. **J. Schmidt**
- 10:30** Intermission.
- 10:40** **COLL 245.** Nanolipoprotein particles entrapped within nanoporous silica gel. **W. Zeno, S.H. Risbud, M.L. Longo**
- 11:10** **COLL 246.** Multiple faces of cholesterol in membrane fusion. **L.K. Tamm**
- 11:40** **COLL 247.** Designing biotinylated lipids for selective partitioning to liquid ordered phase. **D.Y. Sasaki, N. Momin, S. Lee, C. Hayden, J. Stachowiak, G.D. Bachand**

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

C. Matranga, *Organizer*
E. Borguet, *Organizer, Presiding*

8:30 COLL **248**. Photoinduced dynamics at metallic and semiconducting nanoparticles: time-domain ab initio studies. O.V. Prezhdo

9:05 COLL **249**. Plasmons, hot electrons, and artificial photosynthesis. M. Moskovits

9:40 COLL **250**. Ligand effects on the aqueous plasmonic catalysis by alloyed gold-copper nanorods. S.V. Jenkins, J. Chen

10:00 Intermission.

10:15 COLL **251**. Surprisingly efficient plasmon-induced hot electron transfer and photochemistry in semiconductor-Au nanostructures. T. Lian

10:50 COLL **252**. Characteristics of reaction intermediates at plasmon-induced water oxidation processes. K. Suzuki, S. Yasuda, K. Murakoshi

11:25 COLL **253**. Surface-enhanced spectroscopies by rational nanoantenna design. N.J. Halas

Section F

Marriott City Center Denver
Colorado H

Particles at Fluid Interfaces

Cosponsored by PRES

M. A. Bevan, J. Frechette, *Organizers*
N. Wu, *Presiding*

8:30 COLL **254**. Synthesis of hybrid dumbbells with combined compositional and interfacial asymmetries. S. Wang, N. Wu

8:50 COLL **255**. Synthesis and characterization of chemically and physically bonded Janus particles. L.M. Hernandez, S. Razavi, I. Kretzschmar, W.L. Vargas

9:10 COLL **256**. Salt-induced detachment of non-touching colloidal particles from oil-water interfaces. N. Elbers, J. van der Hoeven, A. van Blaaderen

9:30 COLL **257**. Direct view of the nanobio interface. F. Geiger

9:50 COLL **258**. Carbon dioxide-in-water foams stabilized with interfacially active nanoparticles and surfactants. A.J. Worthen, P.S. Parikh, T.R. Dickey, D.A. DiCarlo, M. Prodanovic, S.L. Bryant, C. Huh, K.P. Johnston

10:10 COLL **259**. Studying the molecular orientation and behavior of ionic liquid films at solid-liquid interface. R.S. Anaredy, S.K. Shaw

10:30 COLL **260**. Interactions and ordering of soft microgels at oil-water interfaces. W. Richtering

10:50 COLL **261**. Synthesis of monodisperse, colloidal microcapsules, and their use in controlled encapsulation and release studies. N. Elbers, J. Jose, A. Imhof, A. van Blaaderen

11:10 COLL **262**. Nanoparticle induced charge redistribution of the air-water interface and its role in regulating nanoparticle spatial distributions. M.A. Brown

11:30 COLL **263**. Inverted pendant drop set-up for X-ray absorption spectroscopy of electrolyte solutions and their surfaces. M.K. Bera, M.R. Antonio

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer, Presiding*

9:00 COLL **264**. Plasmonic gold nanoparticles in the cancer cell: Following cell cycle, cell death, drug delivery dynamics and efficacy. M.A. El-Sayed

9:40 COLL **265**. Chemically modified 2D nano-electronic heterostructures. M. Hersam

10:20 COLL **266**. Surface chemistry and interface engineering for high performance perovskite solar cells. A.K. Jen

11:00 COLL **267**. Adaptive wavelet approach for signal/image processing. J. Gilles

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

Chemical Processes at Environmental Interfaces**Chemistry at Aqueous/Mineral(Solid) Interfaces**

Sponsored by ENVR, Cosponsored by COLL

MONDAY AFTERNOON**Section A**

Marriott City Center Denver
Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, *Organizers, Presiding*

2:00 COLL **268**. Periodically sequenced peptides: A new tool for nanoscale materials synthesis. M. Kubillus, R.S. Tu

2:30 COLL **269**. Design of 3-helix micelles as viable nanocarriers. T. Xu

3:00 COLL **270**. Molecular design of peptide nucleic acid amphiphiles as self-assembled probes for electrophoretic miRNA detection. J.W. Schneider, B.A. Armitage, D.H. Ly, J.M. Goldman

3:30 Intermission.

3:45 COLL **271**. Multistimuli responsive polypeptides and stimuli responsive hydrogels. T.J. Deming

4:15 COLL **272**. Molecular engineering of peptide and protein therapeutics. M.J. Webber, D.G. Anderson, R. Langer, S.I. Stupp

4:35 COLL **273**. Biomimetic silica formation probed at the molecular level using SFG spectroscopy and MD simulation. H. Lutz, J. Baio, V. Jaeger, A. Roehrich, J. Pfleandtner, G. Drobny, T. Weidner

4:55 COLL **274**. Engineering mitochondria-penetrating peptides. S.O. Kelley

Section B

Marriott City Center Denver
Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

L. Liz Marzan, *Organizer*
W. Parak, *Organizer, Presiding*

2:00 COLL **275**. Charge shuttling across membranes by functionalized gold nanoparticles. M. Brust

2:30 COLL **276**. Hyaluronic acid-modified Fe₃O₄@Au core/shell nanostars for multimodal imaging and photothermal therapy of tumors. J. Li, Y. Hu, J. Yang, P. Wei, W. Sun, M. Shen, G. Zhang, X. Shi

2:50 COLL **277**. Nanostructured gold model catalysts on thin film substrates. W.C. McKee, M. Patterson, D. Huang, L. Liu, R. Kurtz, P. Sprunger, Y. Xu

3:10 COLL **278**. Nonwettability, oxidation stable, brightly-luminescent silicon nanocrystal film. C. Qian, W. Sun, G.A. Ozin

3:30 COLL **279**. Enzyme multilayer coatings prevent bacterial biofilm formation on urinary catheters. K. Ivanova, M. Fernandes, A. Francesko, T. Tzanov

3:50 Intermission.

4:20 COLL **280**. Chemical and structural transformations in colloidal inorganic nanocrystals. L. Manna

4:50 COLL **281**. Dithiocarbamate-anchored ligands on smooth and nanostructured gold surfaces. A. Wei

5:20 COLL **282**. Mesoporous membranes, zwitterionic monomers, and iniferter-initiated polymerization: Where does the polymerization proceed? L. Sillies, H. Ditzoleit, C. Hess, B. Stühn, A. Brunsten

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion**Spectroelectrochemistry, Imaging, & Surface**

Cosponsored by PRES

Financially supported by Sigma-Aldrich

J. Zheng, *Organizer*
S. Pan, *Organizer, Presiding*
W. Wei, *Presiding*

2:00 COLL **283**. Spectroelectrochemistry and electrochemiluminescence of mixed-thiolate protected Au130 clusters. G. Wang, D. Wang, J. Padelford, T. Ahuja, T. Wang

2:30 COLL **284**. Imaging nanoscale energy transfer at the limits of temporal resolution and spatial accuracy. K.L. Knappenberger, J.W. Jarrett, S. Biswas, X. Lui, P.F. Nealey, R. Vaia

3:00 COLL **285**. Tailoring optical and plasmon resonances in core-shell and core-multishell nanowires for plasmonic light harvesting. C. Yang

3:30 Intermission.

3:40 COLL **286**. Single-particle photoelectrocatalysis. P. Chen

4:10 COLL **287**. Aqueous growth of fluorescence-tunable gold nanoclusters capped with lipoic acid-polyethylene glycol ligands. D. Mishra, F. Aldeek, G. Palui, H.M. Mattoussi

4:40 COLL **288**. Vivid, full-color plasmonic pixels. S. Link

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics**Dynamics**

S. Muralidharan, M. Nieh, A. N. Parikh, N. Sridivya, *Organizers*
D. Y. Sasaki, *Presiding*

2:00 COLL **289**. Substrate specificity of the plasma membrane phosphatidylinositol flippase. D.L. Daleke

2:30 COLL **290**. Anionic phospholipid asymmetry and translocation in lipid membranes. J.C. Conboy

3:00 Intermission.

3:10 COLL **291**. Infrared study of membranes and membrane proteins. F. Gai

3:40 COLL **292**. Molecular transport through living cell membranes: Effects of molecular structure, membrane structure, and electrolyte composition. H. Dai

4:10 COLL **293**. Molecular interactions at model cell membranes. Z. Chen

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

E. Borguet, *Organizer*
C. Matranga, *Organizer, Presiding*

2:00 COLL **294**. Plasmonic hetero-oligomer nanoparticle arrays for hydrogen sensing. T.W. Odom

2:35 COLL **295**. Optical gas sensors based on localized surface plasmon resonance. A. Martucci

3:10 COLL **296**. Localized surface plasmon resonance (LSPR) optical detection of hydrogen. D. Sil, K.D. Gilroy, S. Syla, S. Neretina, E. Borguet

3:30 Intermission.

3:45 COLL **297**. Thermal energy harvesting plasmonic based chemical sensors.

M. Carpenter, N. Karker, G. Dharmalingam

4:20 COLL **298**. Plasmonic spectroscopy and photochemistry on highly damping platinum group metals. K. Ikeda

4:55 COLL **299**. Nanocomposite fiber optic pH sensor for high temperature applications. C. Wang, P. Ohodnicki, X. Su

Section F

Marriott City Center Denver
Colorado H

Advances in Formulations Science & Technology

Cosponsored by PRES

R. Y. Lochhead, *Organizer, Presiding*

2:00 COLL **300**. Advances in targeted multifunctional inhalation aerosols with nanotechnology and solid-state particle engineering design. H.M. Mansour

2:30 COLL **301**. Effects of formulation on the affinity of an SPD peptide fragment toward hair keratin: Experimental and molecular dynamics data. A. Cavaco-Paulo

3:00 COLL **302**. Design of thermal gelling polymer formulations for spray applications. J.L. Curtis-Fisk, M. Knarr, R. Adden, S.L. Jordan, T. Rogers

3:30 COLL **303**. Novel parameter to replace HLB. K. Sakamoto

4:00 COLL **304**. Watching paint age. M.H. Keefe, M. Linsen, M. Clark, J. Calderaio, J. Refiner

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer*

Y. Zheng, *Presiding*

2:00 COLL **305**. Development of multifunctional nano carrier platforms for cancer treatment. A. Nel

2:30 COLL **306**. Enabling biomolecule selection by small molecule-functionalized substrates: A decade of collaborative progress. A.M. Andrews, H. Cao, N. Nakatsuka, S. Deshayes, A. Vaish, M.J. Shuster, L.S. Slaughter, W. Liao, A.M. Kasko, P.S. Weiss

3:00 COLL **307**. Nanoparticle-mediated sorting of circulating tumor cell subpopulations. S.O. Kelley

3:30 COLL **308**. Graphene integration by molecular assembly. P. Han, K. Akagi, F. Federici Canova, H. Mutoh, S. Shiraki, K. Iwaya, P.S. Weiss, N. Asao, T. Hotsugai

4:00 COLL **309**. Reactions and functionalizations of graphene and surfaces. K.N. Houk

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

MONDAY EVENING**Section A**

Colorado Convention Center
Halls C/D

Sci-Mix

R. Nagarajan, *Organizer*

8:00 - 10:00

8, 26, 53, 64, 74-75, 78, 82, 106, 119, 164, 174-175, 191, 212, 220, 232-233, 243, 262, 269, 272-273, 302-303. See previous listings.

310- 311, 322, 341, 351, 365, 367, 378, 380-382, 390, 400, 411, 413, 419, 423, 430, 434, 437, 455, 458, 465, 468-469, 492, 502-503, 518, 521, 523-524, 535, 545-546, 549-550. See previous listings.

TUESDAY MORNING

Section A

Marriott City Center Denver
Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, *Organizers, Presiding*

8:30 COLL 311. Protein analogous micelles: Versatile, modular nanoparticles. M.V. Tirrell

9:00 COLL 312. Enzymatic transformation and self-assembly of peptides for future cancer therapy. B. Xu, J. Zhou, X. Du, J. Shi, Y. Kuang

9:30 COLL 313. Designability of peptide-based materials. V.P. Conticello

10:00 Intermission.

10:15 COLL 314. Tumor-penetrating peptides in the targeting of drugs and theranostic nanoparticles. E. Ruoslahti

10:45 COLL 315. Peptide-guided drug assembly. H. Cui

11:15 COLL 316. Engineering underwater adhesives: Leveraging cation- π interactions to govern peptide cohesion. M.A. Gebbie, W. Wei, A.M. Schrader, T.R. Cristiani, J. Waite, J.N. Israelachvili

11:35 COLL 317. Peptide-polymer amphiphiles as programmable synthons for biologically-responsive nanomaterials. N.C. Gianneschi

Section B

Marriott City Center Denver
Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

L. Liz Marzan, *Organizer*

W. Parak, *Organizer, Presiding*

8:30 COLL 318. Interaction of colloidal nanoparticles with mammalian cells: Correlation of uptake and toxicity with physicochemical properties, such as surface coating. N. Feliu, S. Ashraf, C. Carrillo-Carrion, P. del Pino, B. Pelaz, W. Parak

8:50 COLL 319. Impact of gold nanoparticles on cells: PEGylation's type matters. P. del Pino, W. Parak

9:20 COLL 320. Silanization of layer-by-layer assemblies: Mechanisms and application for the fabrication of superhydrophobic surfaces. A. Dirani, A. Fernandes, P. Lipnik, C. Poleunis, B. Nysten, K. Gilnel, A.M. Jonas

9:40 COLL 321. Verification of anti-icing/icephobic properties of different chemical modified superhydrophobic surfaces. Y. Wang, Q. Wang, Q. Chen

10:00 Intermission.

10:30 COLL 322. Super-high resolution of control assembled fluorescent-TMV using microlens. R. Balaraman, C. Zhou, P. Kohli

10:50 COLL 323. Surface-enhanced Raman scattering nanoparticles as optical labels for imaging cell surface proteins. G.C. Walker, C. MacLauglin

11:20 COLL 324. Surface modification of inorganic nanoparticles for biomedical applications. B. Pelaz, M.G. Soliman, P. del Pino, W. Parak

11:40 COLL 325. Engineering the optical properties of gold nanoparticles by assembling into highly packed 2D arrays of different structure. M.A. Mahmoud

12:00 COLL 326. Protein resistant nanoparticle surfaces designed for the assembly of biodegradable plasmonic gold nanoclusters. R. Stover, A.K. Murthy, S.P. Gourisankar, M. Martinez, A. Issac, T. Truskett, K. Sokolov, K.P. Johnston

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Biosensing, Energy Conversion & Catalysts

Cosponsored by PRES

Financially supported by Sigma-Aldrich

J. Zheng, *Organizer*

S. Pan, *Organizer, Presiding*

C. Yang, *Presiding*

8:30 COLL 327. Metallic nanocomposites of carbon nanotube and their bioconjugates: effective antimicrobials? A. Chaudhari, S. Singh, S. Pillai

9:00 COLL 328. Au/CdS plasmonic photocatalytic nanostructures constructed using P22 virus-like particles for enhanced photoactivity. A. Gupta, Z. Zhou, S. Palchoudhury, G. Bedwell, R. Li, P.E. Prevelige

9:30 COLL 329. Scalable metal-semiconductor nanostructure integration for multimode gas sensing at high temperature. P. Gao

10:00 Intermission.

10:10 COLL 330. Plasmonic enhancement characteristics of multilayered metallic nanostructures. D.D. Evanoff, E.R. Butcher, J.P. Cook

10:40 COLL 331. Exotic Au nanostructures: structure solution, properties, and applications. Y. Han

11:10 COLL 332. Ultrasensitive detection using SERS and SEHRS: From nonlinear optical properties to nuclear forensics. J.P. Camden

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Structure and Interactions

S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*
F. Gai, *Presiding*

9:00 COLL 333. Conformation and dynamics of endogenous cannabinoid ligand 2-AG in a lipid matrix and its interaction with cannabinoid type II receptor. T. Kimura, M. Mihailescu, D.L. Lynch, P.H. Reggio, A.A. Yeliseev, K. Gawrisch

9:30 COLL 334. Studying the mechanism of coiled coil mediated membrane fusion. A. Kros

10:00 COLL 335. Exploring the interactions of ions with supported lipid membranes. P.S. Cremer

10:30 Intermission.

10:40 COLL 336. Dynamic reorganization and correlation among lipid raft components probed by imaging mass spectrometry. S.G. Boxer

11:10 COLL 337. Functionalized lipid-nucleic acid nanoparticles for delivery applications. C.R. Safinya, R.N. Majzoub, K.K. Ewert

11:40 COLL 338. Nanometric gap structure between substrate-supported model membrane and silicone elastomer. K. Morigaki

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

C. Matranga, *Organizer*

E. Borguet, *Organizer, Presiding*

8:30 COLL 339. Super-resolution imaging of plasmonic nanostructures. K.A. Willets

9:05 COLL 340. Plasmonic efficiency enhancement for up-hill photocurrent generation at gold electrode modified with self-assembled monolayer. K. Uosaki, K. Ikeda

9:40 COLL 341. Localized surface plasmon (LSPR) based optical detection of ions in aqueous solution. D. Sil, K. Gilroy, C. Murphy, S. Sylla, R.A. Hughes, S. Neretina, E. Borguet

10:00 Intermission.

10:15 COLL 342. Nanogap plasmonic structures for Raman studies of single molecules and heating. D. Natelson, Y. Li, P. Zolotavin

10:50 COLL 343. Ultrabright luminescent metallic nanoparticles. H. Dai

11:25 COLL 344. Hybrid core-shell and coupled nanostructures: Design and applications. S. Hunyadi Murph

Section F

Marriott City Center Denver
Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL \ddagger

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*

B. E. Bowler, M. Kastantin, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COLL 345. Nanoparticle assembly and gelatin binding mediated by collagen mimetic peptide hybridization. S. Yu

9:05 COLL 346. Supercritical angle fluorescence (SAF) microscopy with nanometer resolution investigating the interaction and aggregation of proteins at lipid bilayer. S. Seeger

9:35 COLL 347. Fibrinonection conformation and integrin binding on crowded surfaces. M. Kastantin, N. Grover, D.F. Marruecos, D.K. Schwartz, J. Kaar

10:05 Intermission.

10:20 COLL 348. Docking model of synaptotagmin 7 C2A via electron paramagnetic resonance. A. Boo, J.R. Osterberg, F. Maynard, N.L. Chon, H. Lin, J. Knight

10:45 COLL 349. Lateral diffusion of synaptotagmin 1 and 7 on supported lipid bilayers: Assessing the frictional additivity of C2A-C2B tandem domains. D.T. Giardina, J. Vasquez, J.D. Knight

11:10 COLL 350. Molecular dynamics simulations of PEGylated dendron-based micelles adsorption on biological membranes. S. Sen, P. Kral

11:35 COLL 351. Xanthan/magnetite scaffolds for neuronal adhesion, proliferation and differentiation of embryonic stem cells. D. Petri, T. Glaser, V. Bueno, H. Ulrich

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer*

A. K. Jen, *Presiding*

9:00 COLL 352. Programmable atom

equivalents from nucleic-acid modified nanostructures: constructing a new "Table of Elements". C.A. Mirkin

9:40 COLL 353. Colloidal nanocrystal building blocks for large-area optical metamaterials. C.R. Kagan, A.T. Fafarman, S. Hong, W. Chen, X. Ye, T. Paik, H. Caglayan, C.B. Murray, N. Engheta

10:20 COLL 354. Surface chemistry of DNA at the single molecule level: Plenty of room at the bottom? T. Ye

10:50 COLL 355. Molecular photonics for materials science, energy and healthcare. Y. Zheng

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Sponsored by GEOC, Cosponsored by COLL

TUESDAY AFTERNOON

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer*

M. Hersam, *Presiding*

2:00 COLL 356. Surface chemistry in solar energy harvesting materials. E. Sargent

2:40 COLL 357. Anomalous nanocolloids defying the likes dissolves likes rule. N. Kotov, J. Bang, B. Yeom

3:10 COLL 358. Dimensional control of chemical interfaces using polymerizable amphiphiles. S.A. Claridge

3:40 COLL 359. Award Address (ACS Award in Colloid and Surface Chemistry sponsored by Colgate-Palmolive Company). Assembly and measurements of isolated and coupled functional molecules. P.S. Weiss

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Sponsored by GEOC, Cosponsored by COLL

WEDNESDAY MORNING

Section A

Marriott City Center Denver
Colorado A

Natural Resource Capture, Storage & Energy Conversion

Theory, Synthesis, Hybrid/Soft Materials, Catalysts, MOFs and Related Application (TSHSCMA)

S. Bashir, *Organizer*

J. Liu, *Organizer, Presiding*

J. Uddin, *Presiding*

8:30 COLL 360. Light-activated multicomponent materials for tandem catalysis. M.R. Knecht, E.M. Zahran, M.A. Nguyen, N. Bedford, Y. Chang, B.S. Gupton, R.R. Naik, L. Bachas

9:00 COLL 361. Zn-MOFs with pyridine-based organic linkers and their carburized, N-doped carbons analogues as CO₂ capture adsorbents. J. Kim, A.G. Oliver, G.T. Neumann, J.C. Hicks

9:25 COLL 362. Synthesis of VTMS(X)-HMS-3 mesoporous ordered silica for hydrogen storage. Y. Mao, D. Owens, A. Han, L. Sun

9:50 COLL 363. Insights in sol-gel matrix diffusion methodology in the synthesis of soft materials from second group (Ca²⁺, Ba²⁺, Mg²⁺) earth alkaline metals. T. Chavez-Gil

10:15 COLL 364. Synthesis of Pt-based catalysts for DMFCs by microfluidic reactors. D. Zhang, F. Wu, X. Wang, D. Xia, J.L. Liu, G. Guo

10:40 COLL 365. Design of polymeric solid acid catalyst for efficient biofuel production. X. Sun, X. Qian

11:05 COLL 366. Metal-organic frameworks for on-board storage of hydrogen and natural gas. J.A. Mason, E.D. Bloch, M.T. Kapelowski, M.K. Taylor, J. Oktawiec, K. Sumida, M.I. Gonzalez, D. Gygi, W. Queen, J.R. Long

Section B

Marriott City Center Denver
Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL \ddagger

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*

B. E. Bowler, M. Kastantin, *Organizers, Presiding*

8:30 COLL 367. Detecting biomolecular interactions and photodynamics in solution by suppression of Brownian motion. W.E. Moerner, Q. Wang, G. Schlau-Cohen, H. Yang

9:00 COLL **368**. Super-resolution imaging and reaction mapping of P450 3A4 and P450 reductase in heterogeneous biomimetics: Starry night. **J.A. Brozik**, S.C. Humphreys, C. Barnaba, A.O. Barden, J.P. Jones

9:30 COLL **369**. Stimuli-responsive chymotrypsin conjugates synthesized using polymer-based protein engineering. **C.S. Cummings**, H. Murata, A.J. Russell

10:00 Intermission.

10:15 COLL **370**. Cytochrome c: An electrostatically bound peripheral membrane protein. **P.K. Kinnunen**

10:45 COLL **371**. Interfacial exposure, recognition, and signaling by mitochondrial cardiolipins. **V. Kagan**

11:15 COLL **372**. Conformational diversity of cytochrome c on cardiolipin containing liposomes probed by fluorescence and circular dichroism spectroscopy. **R. Schweitzer-Stenner**, L.A. Pandiscia, L. Serpas, D. Malyskha

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Biosensing, Catalysts, & Electrochemistry

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, Organizer

J. Zheng, Organizer, Presiding

B. Nelson, Presiding

8:30 COLL **373**. Template free fabrication of vertically aligned Ag nanorods for surface plasmon enhanced photocatalytic reactions and Raman spectroscopy. **J. Wang**, S. Pan

8:50 COLL **374**. Copper plasmonics and catalysis: Role of electron-phonon interactions in dephasing localized surface plasmon. **Q. Sun**, Y. Ding, S.M. Goodman, H.H. Funke, P. Nagpal

9:10 COLL **375**. Electrodeposited alloy thin films for catalysis applications. **M. Gira**, M. Milliken, K. Tkacz, **J.R. Hampton**

9:30 COLL **376**. Block copolymer template-directed synthesis of mono- and bimetallic nanoparticle catalysts. **D.A. Rider**, K. Mikkelsen, A. Taylor, D.S. Perez

9:50 Intermission.

10:00 COLL **377**. Rational design of nanocatalysts for oxygen reduction reaction. **S. Guo**

10:20 COLL **378**. Tunable plasmonic nanoparticles for enhancing photocatalytic reactions. **C. Li**, T. Lee, T. Lee

10:40 COLL **379**. Enhanced photocatalytic activities of chemical vapor deposited hematite films for solar water splitting by Au NPs in embedded configuration. **A. Panikar**, N. Pachauri, Z. Shan, S. Pan, A. Gupta

11:00 COLL **380**. Electrochemical investigation of nanoparticles modified glassy carbon electrode and its application for ketoconazole determination. **M. Alshalafeh**, K. Alqaad, **T.A. Saleh**

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Structure and Modeling

S. Muralidharan, A. N. Parikh, N. Srividya, Organizers

M. Nieh, Organizer, Presiding

9:00 COLL **381**. Biomembrane structure using neutron scattering and molecular labeling. **J.D. Nickels**, S. Chatterjee, J.G. Elkins, F.A. Heberle, R.F. Standaert, D.A. Myles, **J. Katsaras**

9:30 COLL **382**. Experiment and simulation reveal the bending properties of nanoscopic lipid domains. **J. Nickels**, M. Ohl, X. Cheng, F. Heberle, C.B. Stanley, M. Feygenson, J. Neuefeind, P. Zolnierczuk, B. Mostofian, B. Linder, R.F. Standaert, J. Katsaras

10:00 COLL **383**. Shear flow-induced de-registration of compositional domains in supported lipid bilayer membranes. **M. Haataja**

10:30 Intermission.

10:40 COLL **384**. Determination of membrane bending moduli from fully atomistic simulations. **F.L. Brown**

11:10 COLL **385**. Nanoscale structure of sphingolipid containing liquid-ordered phases. **E. Lyman**, A. Sodt, R. Pastor

11:40 COLL **386**. Withdrawn.

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

E. Borguet, Organizer

C. Matraga, Organizer, Presiding

8:30 COLL **387**. Enhancing catalytic efficiency of hollow palladium nanoparticles by photothermal heating of added gold nanoparticles to their cavity: palladium-gold nanorattles. **M.A. Mahmoud**, M.A. El-Sayed

9:05 COLL **388**. Plasmon resonant enhancement of photocatalytic processes. **S. Cronin**, J. Qiu, G. Zeng

9:40 COLL **389**. Visible-light, plasmonic, heating for catalytic CO₂ conversion applications. **C. Matraga**

10:00 Intermission.

10:15 COLL **390**. Photochemical reactions on plasmonic metal nanostructures. **S. Lincic**

10:50 COLL **391**. Active control of surface chemistry on plasmonic nanomaterials. **C.F. Landes**

11:25 COLL **392**. Plasmon-driven CO oxidation in Au-SrTiO₃ nanostructures at room temperature. **B.C. Sweeny**, K. Qian, J.S. DuChene, J. Qiu, A.C. Johnston-Peck, D. Su, E.A. Stach, W.D. Wei

Section F

Marriott City Center Denver
Colorado H

Elucidation of Mechanisms & Kinetics on Surfaces

Cosponsored by CATL and ENVR

A. Savara, Organizer, Presiding

9:00 Introductory Remarks.

9:10 COLL **393**. Elucidation of reaction mechanisms in complex catalytic networks. **T. Bligaard**

9:30 COLL **394**. Isolated metal active site concentration controls catalytic CO₂ reduction selectivity. **J. Matsubu**, P. Christopher, V. Yang

9:50 COLL **395**. Mechanism and kinetics of surface limitations in MF1 ezolite catalysts. **A.R. Teixeira**, C. Chang, W. Conner, W. Fan, **P.J. Dauenhauer**

10:10 Discussion.

10:20 COLL **396**. Hydrogenation of butadiene on Pt in realistic hydrogen pressure: mechanistic insights from DFT. **P. Sautet**, S. Gautier

10:40 COLL **397**. Kinetics and mechanisms of oxidation reactions on metal oxide surfaces. **S.L. Scott**, D.H. Collier

11:00 COLL **398**. Differences in the reaction mechanisms of hydrodeoxygenation (HDO) of m-cresol on platinum and ruthenium catalysts. **D.E. Resasco**, Q. Tan, G. Wang, L. Nie

11:20 COLL **399**. Theoretical studies of oxygenates derivatives by metallic heterogeneous catalysts. A micro-solvation approach. **C. Michel**, P. Sautet

11:40 Discussion.

11:50 COLL **400**. Thermodynamics and kinetics of oxygen induced chain-like reconstructions on the Pt(111) surface. **L. Herder**, W.F. Schneider

12:10 COLL **401**. Adsorbate-adsorbate interaction model for microkinetic trend studies and catalyst screening. **B. Yang**, T. Khan, Y. Xu, A. Lausche, J.K. Norskov, T. Bligaard

12:30 Discussion.

Section G

Marriott City Center Denver
Colorado B

Basic Research in Colloids, Surfactants & Nanomaterials

Amphiphilic Systems

Cosponsored by PRES

R. Nagarajan, Organizer, Presiding

8:30 COLL **402**. Long chain alkylimidazole switchable surfactants. **W. Qiao**, M. Chai

8:50 COLL **403**. Interfacial characterization of chemically modified sphorolipid derivatives. **A. Koh**, R.A. Gross

9:10 COLL **404**. Bilayer self-assembly from single-chain amphiphiles during the origins of life. **S.E. Maurer**

9:30 COLL **405**. Monitoring the effect of surfactant type and process condition on sebum removal from CNF/PET surfaces in an aqueous solution using QCM/SPR technique. **A.H.M. Tayeb**, O.J. Rojas, C.L. Salas, K. Ghosh, M.A. Qudus

9:50 COLL **406**. Study of surfactant influence on the low-pH stability of polyolefin dispersions. **Q. Wan**, M. Crimmins, S.L. Jordan, R. Yan, M. Hus

10:10 COLL **407**. Solutes stabilized by brush amphiphiles: A study of solutes induced morphological transitions of brush amphiphile micelles. **H. Luo**, M. Herrera-Alonso

10:30 COLL **408**. Aqueous delivery of π-π conjugated polymer solutions through a network formed by a fungal Janus-like surfactant. **C. Rosu**, N. Kleinheinz, D. Choi, P.S. Russo, E. Reichmanis

10:50 COLL **409**. Self-assembly of novel fluoro-surfactants with polyoxometalates (POMs) as polar component in acetonitrile/water solution. **B. Zhang**

11:10 COLL **410**. Characterization of a chelating surfactant: Solution behavior and application prospects in ion flotation. **I. Svanelid**, **M. Norgren**, E. Edlund

11:30 COLL **411**. Properties of novel bio-inspired glycolipid surfactants: Tailoring function by disaccharide headgroup and alkyl tail length. **L. Kegel**, L. Szabo, R. Polt, **J.E. Pemberton**

11:50 COLL **412**. CO₂-reactive surfactant ionic liquids for reversible control of colloidal morphology and DNA compaction. **P. Brown**, T. Hattton

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Sponsored by GEOC, Cosponsored by COLL

WEDNESDAY AFTERNOON

Section A

Marriott City Center Denver
Colorado A

Natural Resource Capture, Storage & Energy Conversion

Theory, Synthesis, Hybrid/Soft Materials, Catalysts, MOFs and Related Application (TSHSCMA)

J. Liu, Organizer

S. Bashir, Organizer, Presiding

X. Wang, Presiding

2:00 COLL **413**. Vapor-assisted crystallization synthesis of a microporous (Ti) MIL-125 exhibiting significant mesoporosity. **N.D. McNamara**, J.C. Hicks

2:30 COLL **414**. Synthesis and electromagnetic absorption properties of core-multishell MWCNT/Fe₃O₄/PANI/Au hybrids. **Y. Xu**, C. Liu, Z. Wang

2:55 COLL **415**. Computational discovery of metal-organic frameworks gas capture and storage. **D. Siegel**

3:20 COLL **416**. Enhancement of optical absorptions in oxide nanostructures: Insight from a TDDFT study. **M. Huda**

3:45 COLL **417**. Selective reduction of CO₂ to formate by a homogeneous Iron electrocatalyst in water between pH 5 and 13. **L.A. Berben**, A. Taheri

4:10 COLL **418**. Nanoparticles and nanomaterials for electrochemical conversion of oxygen and carbon dioxide. **A.A. Gewirth**, C. Tse, T. Hoang, K.G. Schmitt

4:35 COLL **419**. Optical response of molecule — semiconducting nanoparticle hybrids. **A. Keller**, V. Mujica

Section B

Marriott City Center Denver
Colorado H

Interfacial Biomolecular Recognition

Cosponsored by BIOL†

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, Organizer

B. E. Bowler, M. Kastantin, Organizers, Presiding

2:00 COLL **420**. Cytochrome c unfolding at cardiolipin-rich membrane surfaces. **E.V. Pletneva**

2:30 COLL **421**. Conformational dynamics of cytochrome c related to peroxidase activity during apoptosis. **L. McClelland**, S. Bandi, T. Mou, S.R. Sprang, **B.E. Bowler**

3:00 COLL **422**. Artificial virus nanoparticles to control cellular processes at the virus-host interface. **B.M. Reinhard**, X. Yu, S. Gummuluru

3:25 Intermission.

3:40 COLL **423**. Tracking amyloids with fluorescent oligo(p-phenyleneethynylene) electrolytes. **P. Donabedian**, T. Pham, D.G. Whitten, E.Y. Chi

4:05 COLL **424**. Super-resolving the dynamics of a membrane-bound virulence regulator in *Vibrio cholerae*. **J.S. Biteen**

4:35 COLL **425**. Proximity energies and their consequences in living systems. **T. Laue**

5:05 COLL **426**. Molecular basis of high-affinity membrane binding by the C2A domain of granuphilin. **A. Watson-Siriboe**, T. Lyakhova, **J. Knight**

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Fabrication for Biosensing, Energy Conversion & Catalysts

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, J. Zheng, Organizers, Presiding

2:00 COLL **427**. Gold nanoparticle assembly for selective two photon scattering imaging of cancer cell. **P.C. Ray**

2:20 COLL **428**. Size selective SERS analysis using nanorattles with porous polymer shell and entrapped gold nanoparticles. **Y. Jia**, S. Shmakov, E. Pinksassik

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.

- 2:40 COLL 429.** Ultrafast laser induced synthesis of narrowly distributed sub-5 nm surfactant-free Au-Pd nanoparticles. D. Sil, K. Moore Tibbetts, J.H. Odnher, R.J. Levis, E. Borguet
- 3:00 COLL 430.** Fabrication of plasmonic nanoantenna arrays on flexible substrates via colloidal lithography for biosensing. A. Bohoulou, V.L. Colvin
- 3:20** Intermission.
- 3:30 COLL 431.** Withdrawn.
- 3:50 COLL 432.** Enhancement of enzymatic colorimetric response by silver island films on high throughput screening microplates. B. Abel, K. Aslan
- 4:10 COLL 433.** Development of polymer-metal colloid hybrid platforms for bioassays with improved dynamic range. E. Bonyi, K. Aslan
- 4:30 COLL 434.** Surface plasmon enhanced photoelectrochemical performance of core-shell Ag@Ag₂S nanoparticles decorated TiO₂ nanowire electrodes. Z. Shan, S. Pan, A. Panikar, A. Gupta
- 4:50** Concluding Remarks.

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Structure and Mechanics

- S. Muraidharan, M. Nieh, N. Sridivya, *Organizers*
A. N. Parikh, *Organizer, Presiding*
- 2:00 COLL 435.** Probing cellular mechano-sensitivity using biomembrane-mimicking cell substrates of adjustable stiffness. C. Naumann, Y. Lin, L. Lautscham, Y. Ge, W. Goldmann, B. Fabry
- 2:30 COLL 436.** Evaluation of drug mediated changes in rhythmic contractile activity of cardiomyocytes. S. Zou
- 3:00** Intermission.
- 3:10 COLL 437.** Changes in the cell surface during progression to cancer of human cervical epithelial cells. I. Sokolov, M. Dokukin, N. Guz, C. Woodworth
- 3:40 COLL 438.** Probing the coupling between polybasic peptides and PIP₂ lipids in asymmetric supported lipid bilayers. A.W. Smith, X. Shi, X. Li
- 4:10 COLL 439.** Oncogene induced stiffening of living cells. N. Nordgren, L.Z. Rathje, T. Pettersson, D. Rönnlund, J. Widengren, P. Aspenström, A.K. Gad

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

C. Matrajan, *Organizer*

E. Borguet, *Organizer, Presiding*

- 2:00 COLL 440.** Electronic structure models of plasmon-enhanced processes. G.C. Schatz
- 2:35 COLL 441.** Ultrafast size-dependent electronic interactions in metal clusters. N. Del Fatti, T. Stoll, P. Maioli, A. Crut, F. Vallee
- 3:10 COLL 442.** Plasmon-driven growth of gold nanoprisms with implications for photocatalysis. Y. Zhai, J.S. DuChene, Y. Wang, A.C. Johnston-Peck, B. DiCiaccio, K. Qian, E.W. Zhao, J. Qiu, F. Ooi, D. Hu, D. Su, E. Stach, Z. Zhu, W.D. Wei
- 3:30** Intermission.
- 3:45 COLL 443.** Plasmon enhanced sensing and catalysis. P.J. Nordlander
- 4:20 COLL 444.** Unique properties of metal nanocrystals for driving photocatalysis. P. Christopher
- 4:55 COLL 445.** Analysis of 2- and 3D plasmon coupling between nanoparticles on cellular and viral surfaces. B.M. Reinhard, X. Yu, A. Feizpour

Section F

Marriott City Center Denver
Colorado H

Elucidation of Mechanisms & Kinetics on Surfaces

Cosponsored by CATL and ENVR

A. Savara, *Organizer, Presiding*

- 2:00 COLL 446.** Impact of self-assembled monolayers on (oxidized) cobalt for Si-based molecular electronic junctions. C.A. Hacker, S. Pookpanratana
- 2:20 COLL 447.** Dynamics of self-assembled monolayers on Au(111) studied by time-resolved scanning tunneling microscopy. H. Wu, K. Soththwes, P.M. Schön, G.J. Vancso, H. Zandvliet
- 2:40 COLL 448.** Polyurethane degradation and characterization of aerospace coatings. J.H. Wynne, N.K. Weise, A.E. Mera, D. Bellevou
- 3:00 COLL 449.** Cyclic azasilanes: A kinetic approach to rapid silane surface modification. A.F. Maddox, J.G. Matsons, M.P. Singh, J. Zazyczny, B. Arkles
- 3:20** Discussion.
- 3:30** Intermission.
- 3:40 COLL 450.** Pyridinium as the electrocatalyst in carbon dioxide reduction on polycrystalline gold electrodes. A.J. Lucio, S.K. Shaw
- 4:00 COLL 451.** Rapid formation of reactive initiator monolayers for conjugated polymer brushes using electrochemical reduction of Ni(II). A. Roy, J.J. Locklin
- 4:20 COLL 452.** Vibrational sum frequency generation studies for elucidating mechanisms and kinetics at surfaces. F. Geiger
- 4:40** Discussion.

- 4:50 COLL 453.** Advancements in the determination of membrane zeta potential at high ionic strengths: Specific application to semipermeable polymeric membrane. B.D. Coday, T. Luxbacher, A. Childress, N. Almaraz, T.Y. Cath
- 5:10 COLL 454.** Nucleation and crystallization kinetics of initial apatite nanocrystal formation within biological templates. D. Kim, B. Lee, S. Thomopoulos, Y. Jun
- 5:30 COLL 455.** Three column series approach to investigate role of desorption rates in colloid-facilitated transport of americium, cesium, and plutonium: Experiments and modeling. T.M. Ditttrich, H. Boukhalfa, P.W. Reimus
- 5:50** Discussion.

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Sponsored by GEOC, Cosponsored by COLL

THURSDAY MORNING

Section A

Marriott City Center Denver
Colorado A

Natural Resource Capture, Storage & Energy Conversion

Biofuels, Fuel Cells, Membranes, Electrolytes, & Batteries (BFCMEB)

- S. Bashir, *Organizer*
J. Liu, *Organizer, Presiding*
J. Uddin, *Presiding*
- 8:30 COLL 456.** Structure-function relationships into layered solid oxide fuel cell cathode material. S. McIntosh
- 9:00 COLL 457.** Tailoring the structure of active materials for solar thermochemical fuel production through templating. A. Stein, C. Malonzo, S. Rudisill, N. Petkovich, J. Davidson, R. DeSmith, L. Venstrom
- 9:25 COLL 458.** Reducing cracks in photoanode of dye-sensitized solar cells based on binder-free TiO₂ nanoparticles by 1D electrospun metal oxide nanofibers. X. Wang, M. Xi, H. Fong, Z. Zhu

- 9:50 COLL 459.** Metabolic characterization of nonmodel microalgae for sustainable biofuel production. G. Atilla-Gokumen, E. Matich, E. Camgoz, M. Ghafari, B.A. Pfeifer, B.Z. Haznedaroglu
- 10:15 COLL 460.** Pore collapse and regrowth in silicon electrodes for rechargeable batteries. S. DeCaluwe, B. Dhar, J. Dura, H. Wang
- 10:40 COLL 461.** Fast charging of dual lithium-ion-insertion cells. R. Chandrasekaran

Section B

Marriott City Center Denver
Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL†

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*

B. E. Bowler, M. Kastantin, *Organizers, Presiding*

- 8:30 COLL 462.** Hierarchical view of DNA based recognition, and the role of flexibility and shape. J.J. De Pablo
- 9:00 COLL 463.** Withdrawn.

- 9:30 COLL 464.** Entropic and electrostatic effects on the folding free energy of a surface-attached biomolecule: An experimental and theoretical study. K. Plaxco, H. Watkins
- 10:00** Intermission.

- 10:15 COLL 465.** Surface-mediated DNA hybridization. J. Monserud, D.K. Schwartz
- 10:45 COLL 466.** Single molecule view of conformational changes and hybridization of DNA on dynamic surfaces. T. Ye
- 11:10 COLL 467.** Quantitative single-molecule imaging of DNA hybridization at capture surfaces with sequence specificity. E.M. Peterson, M.W. Manhart, D. Kriech, J.M. Harris
- 11:35 COLL 468.** Using nonlinear optical spectroscopy to monitor DNA molecular recognition and structure at the buried silica/aqueous interface. J. Gibbs-Davis

Section C

Marriott City Center Denver
Colorado C/D

Basic Research in Colloids, Surfactants & Nanomaterials

Polymeric Materials

Cosponsored by PRES

R. Nagarajan, *Organizer*

J. Jahnke, *Presiding*

- 8:30 COLL 469.** Rapid synthesis of faujasite/polyethersulfone composite membrane and application for CO₂/N₂ separation. B. Wang, L. Zhao, W. Ho, P.K. Dutta
- 8:50 COLL 470.** Relationship between polyelectrolyte bulk complexation and kinetics of their layer-by-layer assembly. P.S. Desai, A. Salehi, J. Li, R.G. Larson
- 9:10 COLL 471.** Adsorption of bacteria into electrospun cellulose nanofiber mats: Development of a dynamic model. K. Rieger, R. Thyagarajan, M. Hoen, D.M. Ford, J.D. Schifman
- 9:30 COLL 472.** Multilayer chromophore thin film fabrication via layer by layer deposition technique. M. Zhu, G.H. Aryal, H. Zhang, J. Jayawickramarajah
- 9:50 COLL 473.** Modulating the uptake of dextran coated SPIONs in stem cells: The effect of surface charge. M. Barrow
- 10:10 COLL 474.** Effect of membrane structural dopants on charge transport through conjugated oligoelectrolyte modified phospholipid bilayers. J. Jahnke, G. Bazan, J. Sumner
- 10:30 COLL 475.** Uniform cross-linked cellulase aggregates prepared in millifluidic reactors. L. Nguyen, K. Yang
- 10:50 COLL 476.** Self-healing and disruption of arboral fibrils. G. Parkinson, J. Sun, P.S. Russo
- 11:10 COLL 477.** Two-photon absorption properties of chromophores in polyelectrolytes. M. Hatshan, R. Guida

Section D

Marriott City Center Denver
Denver III

Basic Research in Colloids, Surfactants & Nanomaterials

Biomolecular Materials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

- 8:30 COLL 478.** Substrate mediated stability of DNA origami at elevated temperatures and in diverse solvent environments. M.A. Pillers, M. Lieberman
- 8:50 COLL 479.** Exploring biomedical applications of nanoparticles by their surface functionalization. K. Rashwan, G. Sereda, P. Jampani, B. Burum, D. Christianson, E. Brakke, K. Kaufman, C. Pap
- 9:10 COLL 480.** DNA nanotubes and nanotapes via self-assembly of ssDNA-amphiphiles. T.R. Pearce, B. Waybrant, E. Kokkoti
- 9:30 COLL 481.** Connections between nanoparticle (NP) surface chemistry and protein corona formation: Influence of the corona on small ($d_{\text{corona}} < 5.0$ nm) NP-supported lipid bilayer interactions. S.E. Lohse, E. Melby, J. Park, B. Putans, R.J. Hamers, J.A. Pedersen, C.J. Murphy
- 9:50 COLL 482.** New generation of well-defined lipid-based magnetic nanoparticles for theranostics. S. Biswas, J.A. Kulkarni, Y.C. Tam, P.R. Cullis
- 10:10 COLL 483.** Robust and tailored wet adhesion in biopolymer thin film with wet adhesion and toughness superior to wet adhesion in bone. T. Pettersson, S. Pendergraph, S. Utset, A. Marais, E. Gustafsson, L. Wagberg
- 10:30 COLL 484.** Chiral recognition and selection during the self-assembly process of protein-mimic macroanions: The effect of long-range electrostatic interactions. P. Yin, T. Liu
- 10:50 COLL 485.** Synergistic DNA delivery with pyridinium amphiphiles with different packing parameters – toward composite DNA delivery systems. M.A. Ilies, A. Kizewski
- 11:10 COLL 486.** Distinct Adsorption Configurations and Self-assembly characteristics of elongated proteins on chemically uniform and alternating surfaces. S. Song, J. Hahn

Section E

Marriott City Center Denver
Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Basic Research on Surfaces and Interfaces

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

- 8:30 COLL 487.** Superhydrophobicity and oleophobicity via increased modified surface topography. K.T. Flynn, M.D. Tustison, C. Zhou, K. Jiao
- 8:50 COLL 488.** Reconfigurable anisotropic coatings via magnetic field-directed assembly and translocation of locking magnetic chains. A. Tokarev, Y. Gu, A. Zakharchenko, O. Trotsenko, I.A. Luzinov, K. Kornev, S. Minko
- 9:10 COLL 489.** Assembly of surface-anchored metal-organic frameworks: Controlling deposition conditions to tune film morphology. M.L. Ohnsorg, B. Bowser, L. Gentry, M.E. Anderson
- 9:30 COLL 490.** Estimating sorption kinetics from the transient shape of a pendant drop. A.R. White, T. Ward
- 9:50 COLL 491.** Probing the effect of the HC-FC dipole on the properties of thin films formed from hydrocarbon-terminated perfluorinated alkanethiols. O. Zenasni, M.D. Marquez, T. Lee
- 10:10 COLL 492.** Synthesis and characterization of partially fluorinated self-assembled monolayers having an inverted surface dipole. M.D. Marquez, O. Zenasni, T. Lee

- 10:30** COLL **493**. Analysis of interactions at fluid-solid interface: Exploring the complete slip boundary condition. S.L. Nania, S.K. Shaw
- 10:50** COLL **494**. Multilayered metallic nanostructures with an embedded internal standard as surface enhanced Raman substrates. E.R. Butcher, D.D. Evanoff
- 11:10** COLL **495**. X-ray photoelectron spectroscopy at the liquid-nanoparticle interface: Opportunities for colloidal science. M.A. Brown
- 11:30** COLL **496**. Interfacial liquids, Most soft surfactants probed by AFM. H. Onishi
- 11:50** COLL **497**. Selenium: The better anchor group for self-assembled monolayers (SAMs) on gold? A. Terfort, M. Zhanikov, P. Gymer
- 12:10** COLL **498**. Withdrawn.

Section F

Marriott City Center Denver
Colorado H

Basic Research in Colloids, Surfactants & Nanomaterials

Basic Research on Colloids

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

- 8:30** COLL **499**. Dynamic adhesion forces between microparticles and substrates in water. Q. Xu, Z. Xia, M. Li, L. Zhang, J. Niu
- 8:50** COLL **500**. Formation of luminescent inorganic precipitation tubes. P.J. Fryogle, E.J. Nelson, J.J. Pagano
- 9:10** COLL **501**. Incorporation of nanoparticles into tunable, highly-ordered, porous silica films. Y. Vasquez, M. Kollé, L.A. Mishchenko, B.D. Hattton, J. Aizenberg
- 9:30** COLL **502**. Ionic and molecular modifiers of calcium oxalate crystallization: Tailoring interfacial interactions. B.G. Almani, J. Chung, J.D. Rimer
- 9:50** COLL **503**. Colloidal particle dispersions for the synthesis of full color electrophoretic inks. K. Belsey, C. Topping, L. Farrand, S.J. Holder
- 10:10** COLL **504**. Selecting the swimming mechanisms of colloidal particles: Bubble propulsion vs. self-diffusiophoresis. S. Wang, N. Wu
- 10:30** COLL **505**. Characterization and dispersion behavior of quaternary ammonium encapsulated polyoxometalates in polyurethane. J. Lundin, S.L. Giles, P. Fulmer, R.F. Cozzens, J.H. Wynne
- 10:50** COLL **506**. Janus particles for probing and manipulating immune functions. Y. Yu, Y. Gao, L. Sanchez, Y. Jia
- 11:10** COLL **507**. Intra-phase mixing in binary drops translating through corrugated microchannels. T. Ward
- 11:30** COLL **508**. Molecular dynamics simulations of colloidal nanoparticles solvation. S. Sen, P. Kral
- 11:50** COLL **509**. Theoretical description of architectures of nanoparticles. N. Almora Barrios, N. Lopez

THURSDAY AFTERNOON

Section A

Marriott City Center Denver
Colorado A

Natural Resource Capture, Storage & Energy Conversion

Biofuels, Fuel Cells, Membranes, Electrolytes, & Batteries (BFCMBE)

J. Liu, *Organizer*

S. Bashir, *Organizer, Presiding*
X. Wang, *Presiding*

- 2:00** COLL **510**. Understanding abiotic:biotic interface: Molecular-level insights into the behavior of enzymes covalently immobilized on surfaces. T. Ogorzalek, Y. Liu, S. Wei, C.L. Brooks, Z. Chen, N. Marsh

- 2:30** COLL **511**. Direct synthesis of single layer layered double hydroxide nanosheets. J. Yu, B.R. Martin, J.E. Sims, L. Sun
- 2:55** COLL **512**. Silyl electrolytes for lithium-ion battery applications. L.J. Lyons
- 3:20** COLL **513**. Withdrawn.
- 3:45** COLL **514**. Creation of natural dye sensitized solar cell by using nanostructured titanium oxide. J. Uddin, S.S. Jenny, A. Ahmed, S. Yadav, M. Jiru
- 4:10** COLL **515**. Amphiphilic functionalization of cathode catalyst to advance electrochemical reactivity of fuel cells. D. Gaona, S. Bashir, J.L. Liu

Section B

Marriott City Center Denver
Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL \ddagger

Financially supported by Avanti Polar Lipids, Inc.

R. Ross, *Organizer*

B. E. Bowler, M. Kastantin, *Organizers, Presiding*

- 2:00** COLL **516**. Aiding developments of single-molecule force spectroscopy for biosensing via molecular simulation. Z.E. Hughes, K.L. Drew, T. Walsh
- 2:25** COLL **517**. Use of surface-specific spectroscopy techniques to unravel molecular recognition in biosensing. O.N. Oliveira
- 2:50** COLL **518**. New roles for antifreeze proteins in recognizing non-ice surfaces. X. Wen
- 3:15** Intermission.
- 3:30** COLL **519**. Studying receptor-mediated liposome fusion kinetics at aqueous/liquid crystal interfaces. K. Macri, P. Noonan, D.K. Schwartz
- 3:55** COLL **520**. Effect of nanoparticle surface chemistry and salt concentration on binding to RNA and DNA. J.A. Nash, A. Singh, N.K. Li, Y.G. Yingling
- 4:20** COLL **521**. Ultrasound biosensing techniques based on biomolecule-induced aggregation of nanodroplets. R. Chattaraj, P. Mohan, J.D. Besmer, C.M. Livingston, A.P. Goodwin
- 4:45** COLL **522**. Impedimetric biosensors for detecting VEGF based on PEDOT carboxylic acid/PEDOT copolymer. M. Kim, R. Iezzi, D.C. Martin
- Section C**
- Marriott City Center Denver
Colorado C/D
- Basic Research in Colloids, Surfactants & Nanomaterials**
- Carbon and Organic Materials**
- Cosponsored by PRES
- R. Nagarajan, *Organizer, Presiding*
- 2:00** COLL **310**. Artificial light harvesting system composed of organic dyes and clay minerals. S. Takagi, Y. Ishida, T. Shimada
- 2:20** COLL **523**. SiC porous materials derived from apple for high-performance electromagnetic interference shielding. Z. Wang, C. Liu, Y. Xu
- 2:40** COLL **524**. Modeling fullerene aggregation in electrolyte solutions: A combined deterministic-stochastic framework. S. Mortuza, S. Banerjee
- 3:00** COLL **525**. Synthesis of carbon-based nanoscale composite particles for imaging applications. M.J. Meziani, M.A. Mottaleb, B. Yoo, Y. Sun
- 3:20** COLL **526**. Label-free two photon imaging of live cells using graphene dots. P.C. Ray
- 3:40** COLL **527**. Developing carbenes as surface modifiers. M. Macleod, J.A. Johnson
- 4:00** COLL **528**. Carbon dots preparation and effect on protein fibrillation. S. Li, R.M. Leblanc
- 4:20** COLL **529**. Conductance and rectification through asymmetric biphenyl molecule systems. J.E. Meany, S.A. Woski

- 4:40** COLL **530**. Electron transfer and molecular binding to nanostructured carbon for super-capacitor materials. D. Banks, J. Mitchell, I. Shcherbakov, J.C. Poler

Section D

Marriott City Center Denver
Denver III

Basic Research in Colloids, Surfactants & Nanomaterials

Functionalized Nanoparticles

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **531**. Withdrawn.

2:30 COLL **532**. Withdrawn.

2:40 COLL **533**. Phase transport of citrate stabilized gold nanoparticles using nonspecifically adsorbed polymers. L.B. Thompson, A.M. Alkilyani, A. Caravana

3:00 COLL **534**. Highly efficient poly-lysine functionalization of gold surfaces by dual click reactions utilizing dithiol adsorbates. A. Shakiya, A.C. Jamison, T. Lee

3:20 COLL **535**. Toward understanding electronic and optical properties of colloidal germanium nanocrystals as a function of size and surface ligand. A.L. Holmes, J. Hütiges, A. Reckmann, E. Muthuswamy, K. Meerholz, S. Kauzlarich

3:40 COLL **536**. Withdrawn.

4:00 COLL **537**. Orthogonal functionalization of patchy particles. X. Zheng, Y. Wang, Y. Wang, D. Pine, M. Weck

4:20 COLL **538**. Strong hydrophobizer: Laterally chemisorbed low-molecular-weight polydimethylsiloxane. T. Lee, S. Chae

4:40 COLL **539**. Elucidating structure/property relationships of peptide-decorated Au nanoparticles using advanced molecular simulations. Z.E. Hughes, T. Walsh

Section E

Marriott City Center Denver
Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Semiconductor Materials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **540**. Optical signatures of crystal phase in semiconductor nanocrystals. S. Lim, A. Schleife, A. Smith

2:20 COLL **541**. Shape controlled narrow-gap tin chalcogenide nanostructures. S. Guo

2:40 COLL **542**. Colloidal synthesis and photocatalytic properties of orthorhombic AgGaS₂ nanocrystals. C. Fan, M. Regulacio, M. Han, A. Xu

3:00 COLL **543**. Careful control of confinement potential and interfacial lattice strain in colloidal quantum dots to improve radiative recombination and fluorescence blinking. C.D. Heyes

3:20 COLL **544**. Size characterization and alternative synthesis of monolayer-protected quantum dots. A.E. Conner, L.R. Tinoco, W.L. Wright, S.C. Francone, E.V. Aguilar, F.E. Acosta, D.T. Miles

3:40 COLL **545**. Excited state dynamics in doped quantum dots. C. Tuinenga, P.V. Kamat

4:00 COLL **546**. Withdrawn.

4:20 COLL **547**. Characterization of the transformation of colloidal CdSe quantum dots into ferroelectric particles. T. Wrenn, J. McBride, J. Mares

4:40 COLL **548**. Formation of 1D-nanostructures using surface-directed vapor-liquid-solid growth process. B. Nikoobakht, A. Herzog

Section F

Marriott City Center Denver
Colorado H

Basic Research in Colloids, Surfactants & Nanomaterials

Colloidal Assembly and Gels

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **549**. Electric field-directed nanowire assembly. S.J. Boehm, L. Lin, C.D. Keating, T.S. Mayer

2:20 COLL **550**. Designing a super-assembly using mixed biological and synthetic nanostructures. J. Reyes, R. Balaraman, N.D. Becerra-Mora, J.B. Fiske, P. Kohli

2:40 COLL **551**. Bifurcation in the equilibrium height of colloidal particles near an electrode in oscillatory electric fields. T. Woehl, B. Chen, K. Heatley, N. Talken, C. Dutcher, S. Bukosky, W. Ristenpart

3:00 COLL **552**. Self-assembly of colloidal nanoparticles into chiral ribbons and hollow capsules. P. Kral

3:20 COLL **553**. Self-assembly of nanometer scaled macroions in dilute solution. J. Zhou, T. Liu

3:40 COLL **554**. Direct nanoscale visualization of the kinetics of colloidal gold nanoparticle chain assembly. T. Woehl, T. Prozorov

4:00 COLL **555**. Withdrawn.

4:20 COLL **556**. Magnetoactive hydrogels for dynamic modulation of pro-angiogenic signaling from mesenchymal stem cells. K.A. Kilian, A. Abdeen

4:40 COLL **557**. Monodisperse polymeric ionic liquid microgels by post modifications and their versatile biomedical applications. N. Sahiner, A.O. Yasar, S. Yildiz, S. Demirci, N. Aktas

5:00 COLL **558**. Supercooled water in nanoconfinement: Molecular simulation study of single-molecule and collective dynamics. N.J. Kwon, A.A. Milischuk, B.M. Ladanyi

5:20 COLL **559**. Ionic liquids and water: the surprising connection. M.A. Gebbie, H.A. Dobbs, M. Valtner, J.N. Israelachvili

COMP

Division of Computers in Chemistry

E. Esposito and S. Wildman, *Program Chairs*

BUSINESS MEETINGS:

Business Meeting, 3:00 PM: Sat

SUNDAY MORNING

Section B

Colorado Convention Center
Mile High Ballroom 1E

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Cosponsored by PHYS

M. Halls, *Organizer*

G. B. Fitzgerald, *Organizer, Presiding*

8:30 COMP **1**. Using Gaussian to aid in π -conjugated semiconducting polymer design for organic photovoltaics. C.K. Luscombe

9:00 COMP **2**. Computational description of donor-acceptor π -conjugated materials for organic photovoltaics applications. J.E. Bredas

9:30 Intermission.

9:45 COMP **3**. High-throughput computational design of semiconducting polymers: Predictions and rational guidance from DFT calculations. B.M. Wong

10:15 COMP 4. Application of density functional theory in the design of organic molecules for intramolecular singlet fission. Q. Wu, E. Busby, J. Xia, J. Low, R. Song, J.R. Miller, X. Zhu, L.M. Campos, M. Sfeir

10:45 COMP 5. Atomistic simulations of donor-acceptor polymer morphologies for high-efficiency organic photovoltaic. T.W. Kemper, R.E. Larsen, D.C. Olson

Section C

Colorado Convention Center
Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Dynamics

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

8:30 COMP 6. Nonadiabatic molecular dynamics of singlet fission and charge separation. O.V. Prezhdo

9:00 COMP 7. First principles ultrafast charge transfer dynamics in solution: A time-domain TDDFT approach coupled with dielectric relaxation. F. Ding, D. Lingerfelt, B. Mennucci, X. Li

9:30 COMP 8. Modeling inter-domain electron tunneling in copper monooxygenases. A. Migliore, D.N. Beratan

10:00 Intermission.

10:15 COMP 9. Time-dependent two-component electronic structure methods for modeling spin dynamics. X. Li, F. Ding, J. Goings

10:45 COMP 10. Pseudopotential approach to electronic structure of anionic species on metallic surfaces. A.F. Izmaylov

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Cosponsored by MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP 11. Structural informatics modeling of Daclatasvir and analogs reveals asymmetric binding to HCV-NS5A: Dual mechanisms responsible for picomolar activity and acquired resistance. J.H. Nettles, R. Stanton, J. Brojde, F. Amblard, H. Zhang, L. Zhou, J. Shi, T. McBrayer, T. Whitaker, S.J. Coats, J.J. Kohler, R.F. Schinazi

9:00 COMP 12. Structure-based discovery and de novo design of HIV fusion inhibitors. W.J. Allen, R.C. Rizzo

9:30 COMP 13. Dual layer QM/MM binding study of antimicrobial oligomer-viral capsid complexes. T. Martin, E.H. Hill, D.G. Whitten, E.Y. Chi, D.G. Evans

10:00 Intermission.

10:00 COMP 14. Fungicides and exploration of chemical spaces: Homology modeling of lanosterol 14- α -demethylase. L. Nitsch Velasquez

10:30 COMP 15. Identification and characterization of allosteric site(s) for dihydrogambogic acid (DHGA) and trans- β -caryophyllene (TBC) as cannabinoid CB₂ allosteric modulators. P. Pandey, K.K. Roy, R.J. Doerksen

11:00 COMP 16. Molecular docking screens for the discovery of novel A₂A adenosine receptor agonists: Are there any in chemical libraries? D. Rodríguez, Z. Gao, S.M. Moss, K.A. Jacobson, J. Carlsson

Section E

Colorado Convention Center
Mile High Ballroom 4F

Molecular Mechanics

Proteins

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP 17. Computational approach to enzyme design. S. Sirin, W. Sherman

9:00 COMP 18. Molecular dynamics simulations on the periplasmic-open state lactose permease. X. Zhuang, J.B. Klauda

9:30 COMP 19. Investigating the structure and dynamics of the PI3CA wild-type and H1047R oncogenic mutant for potential allosteric modulation. P. Gkeka, A. Papafotika, S. Christoforidis, Z. Cournia

10:00 Intermission.

10:15 COMP 20. Structural insight into ROS1/ALK kinase conformational dynamics. N.A. Vellore, J. Wagner, C.A. Edie, M.W. Deininger, B.J. Druker, T. O'Hare, M.A. Davare

10:45 COMP 21. Computational study of pH-dependent conformational changes in proteins. N. Di Russo, A.E. Roitberg

11:15 COMP 22. cAMP modulation of the hyperpolarization-activated cyclic nucleotide-gated 2 ion channels. F. Tofeleanu, B. Brooks

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Accurate Energies for Dynamics

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid β : Structures and Molecular Interactions

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Advances in Simulation Methodology

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Sponsored by PHYS, Cosponsored by COMP

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1D

Molecular Mechanics

Methodology

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

1:30 COMP 23. Correcting for the free energy costs of bond or angle constraints in molecular dynamics simulations. G. Koenig, B. Brooks

2:00 COMP 24. Importance of sugar pucker correction to QM/MM simulation of RNA systems. M. Huang, D.M. York

2:30 COMP 25. Improving efficiency in SMD simulations through a hybrid differential relaxation algorithm. C.L. Ramirez, A. Zeida, G.E. Jara, A.E. Roitberg, M.A. Marti

3:00 Intermission.

3:15 COMP 26. Enhancing constant-pH simulation in explicit solvent with a two-dimensional replica exchange method. J. Lee, B. Miller, A. Damjanovic, B. Brooks

3:45 COMP 27. Toward a virtual chemist: Application to asymmetric catalyst discovery. J. Pottel, M. Bezanson, N. Moitessier

4:15 COMP 28. Computer-aided molecular design of neutral lanthanide extractants. B.W. McCann

Section B

Colorado Convention Center
Mile High Ballroom 1E

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Cosponsored by PHYS

G. B. Fitzgerald, *Organizer*
M. Halls, *Organizer, Presiding*

1:30 COMP 29. Finding polymorphs of organic semiconductors. P. Clancy, K.M. Lenn, P. Frazier

2:00 COMP 30. Coarse-grained simulations of benzodithiophene-thienopyrrolodione copolymer film structure for organic photovoltaics. E. Jankowski, D.C. Olson

2:30 COMP 31. Molecular dynamics of prototypical organic photovoltaic materials. S. Yerusu, V.K. Kuppa

3:00 Intermission.

3:15 COMP 32. High throughput computational approaches to materials discovery and development for organic electronics. M.E. Thompson, P. Saris, P.I. Djurovich, L. Martin

3:45 COMP 33. Efficient knowledge discovery of optoelectronic materials using evolutionary strategies. T.F. Hughes, Y. Cao, J. Gavartin, D.J. Giesen, A. Goldberg, M.D. Halls, S. Kwak

4:15 COMP 34. Charge percolation in non-crystalline molecular materials. N. Jackson, L.X. Chen, M.A. Ratner

Section C

Colorado Convention Center
Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Embedding: QM/QM and QM/MM

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

1:30 COMP 36. Embedded descriptions of condensed phases. G.K. Chan

2:00 COMP 35. Embedding from multiscale chemical problems to crystal energetics. F.R. Manby

2:30 COMP 37. Embedded correlated wavefunction theory: Advances and applications. E.A. Carter

3:00 Intermission.

3:15 COMP 38. Molecular fragments as a tool for electronic structure. T.A. Van Voorhis

3:45 COMP 39. High-level QM/MM free energy simulations at affordable computational costs. P.S. Hudson, G. Koenig, F.L. Kearns, S. Boresch, H.L. Woodcock

4:15 COMP 40. MoD-QM/MM structural refinement method: Characterization of hydrogen bonding in the Oxytricha nova G-quadruplex. J. Ho, C.M. Ragain, J. Gascon, E.R. Batista, J. Loria, V.S. Batista

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Cosponsored by MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP 41. Structure-focused modeling approach to identify family-specific kinase inhibitors. S. Ravichandran, B.T. Luke, J.R. Collins

2:00 COMP 42. Computational analysis of the binding specificity of DMH1 to Alk2, Alk5, and VEGFR2 kinases. A. Alsamraah, J. Hao, Y.L. Luo

2:30 COMP 43. Chemical fragments positively interact with protein side chains: An analysis of PDB and CSDB database. M. Tu

3:00 Intermission.

3:15 COMP 44. Knowledge based conformation sampling algorithms and its application in Foldit drug design game. S.K. Kothiwale, J. Mendenhall, S. Combs, J. Meiler

3:45 COMP 45. X-ray fragment screening for allosteric sites. M. Verdronk

4:15 COMP 46. Withdrawn.

Section E

Colorado Convention Center
Mile High Ballroom 4F

Quantum Chemistry

Methodology

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP 47. Fast calculation of two-electron integrals. A numerical approach. P.E. Lopes

2:00 COMP 48. Advances in local RI methods for SCF calculations. S. Manzer, E. Epifanovsky, M.P. Head-Gordon

2:30 COMP 49. Exploiting sparsity to enable petascale applications in material science and quantum chemistry. M. Keceli, H. Zhang, P. Zapol, D.A. Dixon, A.F. Wagner

3:00 Intermission.

3:15 COMP 50. Accurate and efficient propagator methods for calculating electron binding energies of large molecules: Applications to fullerenes and other large acceptors. J.V. Ortiz

3:45 COMP 51. Learning non-local kinetic energy functionals for hydrocarbons with computers. J. Parkhill, K. Yao

4:15 COMP 52. Simulating plasmon-molecule interactions in the time domain. A.E. DePrince

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Gas-phase Kinetics and Dynamics

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid Precursor Protein, Origin of Amyloid β

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Classical and Quantum Descriptions of Protein Function

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Sponsored by PHYS, Cosponsored by COMP

MONDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1D

Molecular Mechanics

Force Field Development

Cosponsored by PHYS

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP 53. Multistate reweighting as an effective tool for force field parameterization. M.R. Shirts, L. Naden, B. Zimmerman, H. Palwal

9:00 COMP 54. Wolf_Pack: A scientific workflow and molecular database for force-field optimization. K.N. Kirschner, O. Krämer-Fuhrmann, M. Hülsmann, D. Reith

9:30 COMP 55. Residue-specific force fields based on protein coil library and their applications. F. Jiang, C. Zhou, S. Xun, Y. Wu

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

- 2:45 COMP 172.** Tunable luminescence in CdSe quantum dots doped by Mn impurities. **Y. Dahnovsky, V. Proshchenko**
- 3:15 COMP 173.** Highly-reduced corannulene: The influence of alkali metals on the structure and formation of aggregates. **A.Y. Rogachev**
- 3:45 COMP 174.** Quantum mechanical study of structural and electronic dilution effects in paramagnetic chemical exchange saturation transfer agents. **W.A. Miller, P.B. Moore**
- Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease Prions and Beyond**
Sponsored by *PHYS*, Cosponsored by *COLL* and *COMP*
- Modeling Excited States of Complex Systems**
Electronic Structure
Sponsored by *PHYS*, Cosponsored by *COMP*
- TUESDAY EVENING**
- Section A**
Colorado Convention Center
Hall B2
NVIDIA GPU Award
M. E. Berger, R. Gomperts, *Organizers*
- 6:00 - 8:00**
- COMP 175.** Ligand-specific conformational changes in CCR7 coupled to signaling pathway selection. **Z. Gaieb, D.D. Lo, D. Morikis**
- COMP 176.** Theoretical view of the C3d-CR2 binding controversy. **R. Mohan, R.D. Gorham, D. Morikis**
- COMP 177.** Entropically driven CK-ASB9 interaction: How GPU-enabled computing provided unique insight into an intrinsically disordered 116 kDa protein complex. **J. Schiffer, J. Parnell, E.A. Komives, R.E. Amaro**
- COMP 178.** GPU-enabled real-time electron dynamics of large light-harvesting systems in explicit solvent. **B.M. Wong, M. Oviedo**
- COMP 179.** GPU-accelerated implementations of advanced electronic structure methods in Q-Chem. **K. Nanda, E. Epifanovsky, A. Krylov**
- Section A**
Colorado Convention Center
Hall B2
Poster Session
E. X. Spósito, S. A. Wildman, *Organizers*
- 6:00 - 8:00**
- COMP 180.** Possible mechanisms for interconversion of polar forms for the ferroelectric diisopropylammonium halides. **K.R. Cousins**
- COMP 181.** Numerical modeling of carbon condensation in detonation products. **C. Mader**
- COMP 182.** Identification of a new class of potential antimalaria agents using in-silico methodology. **R. Richardson**
- COMP 183.** DFT and MP2 analysis of ligand selectivity in the catechol-O-methyltransferase enzyme. **A.K. Hatstat, M. Morris, L. Peterson, M.L. Cafiero**
- COMP 184.** Effects of implicit solvation, relaxed amino acid side chains, and point mutations on the MP2 and DFT calculations of ligand-protein structure and interaction energies of dopaminergic ligands in the SULT1A3 enzyme active site. **D. Bigler, L. Peterson, M.L. Cafiero**
- COMP 185.** MP2 and DFT analysis of the ligand selectivity of a sulfotransferase enzyme: SULT 1A. **A.H. Weems, M.L. Cafiero, L.W. Peterson**
- COMP 186.** Study of the translocation of chloride ions through *Escherichia coli* transporters using the combined QM/MM method. **C. Davis, S. Pezeshki, C. Garza, H. Lin**
- COMP 187.** Weighing energetics against best fit in development of RNA structure prediction models. **D. Bell, Z. Xia, P. Ren**
- COMP 188.** Interactions between amino acid and graphene oxide: Experiments and theoretical calculations. **L. Huang, K.E. Gubbins**
- COMP 189.** Applying intelligent design to biocatalyst engineering. **J. Pottel, A. Tomberg, C. Bendell, N. Moitessier**
- COMP 190.** Interfacial force field parameterization in CHARMM for the accurate representation of peptide adsorption free energy on high-density polyethylene. **T. Abramyan, J. Snyder, J.A. Yancey, S. Stuart, R.A. Latour**
- COMP 191.** Anions and computation: A match made in chemical heaven. **R.C. Fortenberry**
- COMP 192.** Multiscale approach to decipher enzymatic processing and selectivity of lipids. **L. Riccardi, J. Arencibia, A. Armiroti, M. Devivo**
- COMP 193.** In silico discovery of FKBP52 inhibitors as a prospective therapy for prostate cancer. **H. Li, N. Guy, M.B. Cox, A. Cherkasov**
- COMP 194.** Withdrawn.
- COMP 195.** Identification of 'dynamic hotspots' for lead discovery using MD simulation and spatiotemporal cluster analysis. **A. Arakawa, O. Ichikawa, K. Yamazaki, K. Fujimoto, M. Okada, A. Yamada, S. Okazaki**
- COMP 196.** Density-based energy decomposition analysis. **Q. Wu**
- COMP 197.** Prioritizing high throughput screening hits using a filtering workflow implemented in KNIME and QSAR models for antimalarial drug discovery. **S. Capuzzi, D. Fouches, A. Tropsha**
- COMP 198.** Simulating X-ray, UV, and VIS absorption spectra with orthogonality constrained density functional theory. **F.A. Evangelista, W.D. Derrickotte**
- COMP 199.** Fast and reliable first principles approaches for the prediction of electro-mechanical properties in organic "smart" materials. **K. Werling, B. Albrecht, D. Lambrecht**
- COMP 200.** Towards accurate parameterization for pyrrolidinium-based ionic liquids in lithium-ion batteries. **H. Torabifard, G.A. Cisneros**
- COMP 201.** Withdrawn.
- COMP 202.** Investigation of the effects of water in the binding site on protein-ligand interaction energy. **H. Sato, A. Matsuura**
- COMP 203.** Insights into cobalt oxide water oxidation catalysts: A theoretical perspective from model dimer and cubane complexes. **A. Fernando, C.M. Aikens**
- COMP 204.** Molecular modeling of dielectric constant of EC/DMC mixtures. **I. Daniels, Z. Wang, B. Laird**
- COMP 205.** Site of reactivity models predict molecular reactivity of diverse chemicals. **T.B. Hughes, G.P. Miller, S. Swamidass**
- COMP 206.** Molecular dynamics study of the confinement of alkane guests in an octa-acid dimer. **J. Barnett, H. Ashbaugh, B.C. Gibb**
- COMP 207.** Robust and efficient coupled cluster-polarizable solvation methods for electronic molecular properties in the condensed phase. **M. Caricato**
- COMP 208.** Pharmacophore-based similarity scoring method for DOCK. **L. Jiang, R.C. Rizzo**
- COMP 209.** Mechanistic analysis of water oxidation catalyzed by a mononuclear copper(II) polypeptide in aqueous solutions. **W.C. Isley, C.J. Cramer**
- COMP 210.** Development and in silico evaluation of large-scale metabolite identification methods using functional group detection for metabolomics. **J.M. Mitchell, T.W. Fan, A.N. Lane, H.N. Moseley**
- COMP 211.** Nanoscale structure and dynamics of the liquid ordered phase of lipid bilayers. **E. Lyman**
- COMP 212.** Strength, not depth: An exploration of differential membrane binding kinetics of Synaptotagmin-1 and Synaptotagmin-7 C2 domains. **J. Vermaas, E. Tajkhorshid**
- COMP 213.** Withdrawn.
- COMP 214.** Tolerance-dependent algorithm for core-constrained ligand docking with glide. **I. Tubert-Brohman, J.L. Banks, M.P. Repasky**
- COMP 215.** Quartic force fields for electronically excited states: Theoretical ro-vibronic spectra. **W.J. Morgan, R.C. Fortenberry**
- COMP 216.** Comparison of local correlation methods applied to chiroptical properties and excited states. **H. McAlexander, T. Crawford**
- COMP 217.** Bond length alternation of conjugated oligomers: Performance of recent double-hybrid functionals. **M. Wykes, N.Q. Su, X. Xu, C. Adamo, J.C. Sancho-García**
- COMP 218.** Supramolecular engineering via fragment-based design. **B.P. Hay, B. McCann**
- COMP 219.** Molecular mechanism of gated ligand binding. **Y. Li, Z. Dong**
- COMP 220.** Validation of a tuned interfacial parameter set using dual-force-field CHARMM for the accurate simulation of protein adsorption on a silica glass surface. **J. Snyder, T. Abramyan, J.A. Yancey, S. Stuart, R.A. Latour**
- COMP 221.** Implementation of the generalized internal coordinates for molecular geometry, energy gradients, and force constants. **A.V. Marenich, H.P. Hratchian, J.L. Sonnenberg, M.J. Frisch**
- COMP 222.** Price of admission: Exploring the transition from straight chain to first cycle in sesquiterpene biosynthesis using quantum chemical calculations. **C.S. Hamann, M.W. Lodewyk, D.J. Tantillo**
- COMP 223.** Photoionization of water in gas phase and in bulk: Insight from equation-of-motion coupled-cluster Dyson orbitals. **S. Gozem, A. Krylov**
- COMP 224.** Exploring rovibrational states of floppy molecules using diffusion Monte Carlo. **J. Ford, A.B. McCoy**
- COMP 225.** Scientific and technological advances in the quantum chemistry package Jaguar. **A.D. Bochevarov, T.F. Hughes, L.D. Jacobson, D.M. Philipp, M.A. Watson**
- COMP 226.** DFT study of structural evolution of gold clusters. **Aur_n**, with n= 40-50. **S. Pande, X.C. Zeng**
- COMP 227.** Quantum chemistry for X-ray photoelectron spectroscopy: Computation of XPS chemical shifts in amino acids and simple polypeptides. **I. Tolbatov, D.M. Chipman**
- COMP 228.** In silico prediction of charge carrier mobility in organic semiconductors. **S. Kwak, A. Goldberg, D. Giesen, M. Halls**
- COMP 229.** Withdrawn.
- COMP 230.** Distinguishing the protonation states of the histidine ligands of the Rieske iron-sulfur cluster by ¹⁵N isotopic substitution and vibrational frequency shifts. **B.R. Jagger, A.M. Koval, R.A. Wheeler**
- COMP 231.** Nucleation mechanisms of γ D-crystallin protein aggregates found in cataracts. **S.A. Richards, R.A. Wheeler**
- COMP 232.** Computed chemical properties for the functional sorting of the haloacid dehalogenase superfamily. **E.M. Mozur, M. Touch, M.J. Ondrechen**
- COMP 233.** Gold nanoparticle-nucleic acid modeling using GPU-accelerated molecular dynamics. **J.A. Nash, A.L. Kwansa, Y.G. Yingling**
- COMP 234.** Withdrawn.
- COMP 235.** Development of OPLS-AA Force Field Parameters for Ionic Liquids. **S.M. Gathiaka, B. Li, O. Acevedo**
- COMP 236.** Accelerating DFT and hybrid DFT in VASP Using GPUs. **P. Fleurat-Lessard, M. Hutchinson, M. Widom, A. Anciaux-Sedrakian, T. Guignon, D. Stosic, J. Bedorf, S. Tariq**
- COMP 237.** Simulations of fluorescence solvatochromisms in substituted *p*-phenylene vinylene oligomer derivatives: Excited state molecular dynamics with implicit solvent. **J. Bjorgaard, K. Velizhanin, S. Tretiak**
- COMP 238.** First-principle study of the structural and electronic properties of graphene on Zn(II) phthalocyanine tetrasulfonic acid adsorption. **R. Li, D. Nicholls, M.R. Hoffmann, N. Oncol**
- COMP 239.** Quantum mechanical molecular interactions for calculating excitation energy in molecular environments: A first-order interacting space approach. **K. Yanai, K. Ishimura, J. Hasegawa**
- COMP 240.** Nitrogen dopants and vacancy defects in graphene nanoflakes: Theoretical study of size-dependent electronic excitation properties. **C. Lin**
- COMP 241.** Free energy study of small molecules to RNA with multiple binding poses. **Y. Tanida, A. Matsuura**
- COMP 242.** Uncovering topological signatures of instability and metastability. **J. Miorelli**
- COMP 243.** Molecular dynamics of metalloporphyrins. **J. Coda, W.M. Ames**
- COMP 244.** Computational insights into intramolecular hydrogen migration via agostic-type interactions. **J. Duchimaza, K. Yan, A. Ellern, A.D. Sadow, M.S. Gordon**
- COMP 245.** Predictive methods for CO₂ solubilities in reactive ionic liquids. **Q. Sheridan, T. Lee, E. Maginn, W.F. Schneider**
- COMP 246.** Theoretical study of (hetero) aromatic fluorination catalyzed by palladium. **P. Fleurat-Lessard, J. Roger, C. Testa, J. Hierso**
- COMP 247.** Computer simulations of forward osmosis for desalination. **O. Lee**
- COMP 248.** Withdrawn.
- COMP 249.** Computational insight into origins of Z-selectivity and enantioselectivity of asymmetric ring-opening/cross-metathesis catalyzed by a stereogenic-at-Ru complex. **J.W. Nelson, H.D. Pham, X. Wang**
- COMP 250.** Coordination number and molecular geometry influences on methanethiol binding strength and acidity in [(imidazole)_nZinc(II)-S(H)CH₃] complexes. **D.P. Linder, K.R. Rodgers**
- COMP 251.** DFT study of the rate determining steps of carbon chain growth on Co. **D. Petersen, L. Arnadottir**
- COMP 252.** Theoretical study on the fluorescent spectrum of enhanced green fluorescent protein. **Y. Uchida, M. Higashi, S. Hayashi**
- COMP 253.** Identification of a pKa-regulating motif stabilizing imidazole modified double stranded DNA. **D. Buyst, V. Gheeraerdijn, J. van den Begin, A. Madder, J.C. Martins**
- COMP 254.** Alpha-hydrogen bonding stereochemical consequences in alpha,beta-unsaturated aldehydes complexed with chiral menthoxyaluminum dichloride Lewis acid catalysts in Diels-Alder reactions. **B. Vernier, A.N. Ahmed, J. Rohde, J.D. Evanseck**
- COMP 255.** Calculation of the association trajectories of oseltamivir and sialic acid to wild type and H274Y viral neuraminidase. **R.W. Wenzner, L.M. Krause, J.F. Graziadei, P.F. Marris, A.W. Van Wynsberghe**
- COMP 256.** Effect of surface defects on the optical properties of silicon quantum dots. **N.K. Dandu**
- COMP 257.** Targeted delivery of peptidoglycan immunomodulators using liposomal carriers: MD study of the lipid encapsulation. **K. Feher**

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.

- COMP 258.** Semantic web and computational chemistry. **N.S. Ostlund**, B. Wang
- COMP 259.** Reparameterization of gold thiolate ReaxFF. **B.M. Barngrover**, E.M. Kinder, T.J. Manges, T.J. Cobb, C.M. Aikens
- COMP 260.** Online parameter and property database for the TraPPE force field. **A. Sunnarborg**, A. Bliss, H. Stern, B.L. Eggimann, J.J. Siepmann
- COMP 261.** Elucidating a chemical defense mechanism of Antarctic sponges. **S.K. Vankayala**, **F.L. Kearns**, B.J. Baker, H.L. Woodcock
- COMP 262.** Characterization of fullerene structure and electronic properties using DFT and EPR parameters: Charge localization in polymer-fullerene composite solar cells. **J.N. Webb**, J. Nikias, O. Poluektov, K. Mardis
- COMP 263.** Quantum chemical studies of gas hydrates. **P. Warier**, C.A. Koh
- COMP 264.** Nature of the β -cyclodextrin-graphene interface: A quantum chemical analysis. **P. Jaiyong**, R.A. Bryce
- COMP 265.** Investigation of different binding kinetics among the neuraminidase inhibitors. **G. Kang**, D.J. Mermelstein, R.B. Clayton, A.W. Van Wynsberghe
- COMP 266.** Interaction of aqueous ammonium chloride with *Helicobacter pylori* urease. **M. Minkara**, M.N. Weaver, K.M. Merz
- COMP 267.** Iron pyridine-2,6-diimine (PDI) scaffolds: A new model with MRMP2. **J. McNeely**, A.Y. Rogachev
- COMP 268.** Density functional analysis of donor-acceptor complexes formed between ethers and sulfur trioxide or sulfur dioxide. **G. Van Den Driessche**
- COMP 269.** Human pepsin 3A hydrolysis reaction mechanism. **A.N. Mascarenas**, E. Cowles, J.J. Stewart, S.B. Braun-Sand
- COMP 270.** Substrate binding of human MTH1 protein. **H.E. Ryan**, M. Carter, J.J. Stewart, S.B. Braun-Sand, P. Stenmark
- COMP 271.** Ab initio computations of nuclear quadrupolar coupling constants: Why they don't work, and how to fix them. **G.S. Harbison**
- COMP 272.** Characterization of carbene intramolecular reactivity with various substituents through computer modeling. **M. Roth**, W.M. Ames
- COMP 273.** Withdrawn.
- COMP 274.** Using TD-DFT and NTOs to model photocatalysis. **C.M. Midkiff**, A.K. Rappe
- COMP 275.** First principle study on optimizing conditions for charge transfer in quantum dots through dye functionalization. **P. Cui**, S. Kilina
- COMP 276.** SO₂ – yet another two-faced ligand. **J. Li**, A.Y. Rogachev
- COMP 277.** Impact of substituent size and electronegativity on the band gap of TiO₂ polymorphs. **A.J. Glaid**, M.N. Srnc, J.A. Aitken, J.D. Madura
- COMP 278.** Enrichment of computational chemistry data with the semantic web. **B. Wang**, L. Nardozi, S.J. Chalk, M. Sopek, N.S. Ostlund
- COMP 279.** HK propagator uniformized along a 1D manifold. **L. Kocia**, E.J. Heller
- COMP 280.** Structural determinants of promiscuous and specific binding in protein-protein complexes using component analysis techniques. **A. Sherani**, Y.Y. Zhang, M.L. Radhakrishnan
- COMP 281.** Q-Chem: An engine for innovation. **Z. Gan**, E. Epitanovsky, **Y. Shao**
- COMP 282.** Adsorption of O₂ on neutral/charged Au_n (n = 1-3) clusters: A comparative study between DFT and coupled cluster calculations. **Y. Zhao**, **N.S. Khatri**, H. Li, Y. Gao, X.C. Zeng
- COMP 283.** Exploring the mechanisms of enantioselective organocatalytic reactions: A DFT study. **K.E. Blise**, D.L. Kohen, G.E. Hofmeister, D.G. Alberg, M. Cvitkovic
- COMP 284.** Molecular simulations of fluorescent sensors with amyloid- β protein aggregates. **J. Thompson**, E.H. Hill, E.Y. Chi, D.G. Whitten, D.G. Evans
- COMP 285.** Constrained heuristic optimization of NLO chromophores. **C.B. Rinderspacher**, J. Elward
- COMP 286.** Modeling of a bench-scale biomass pyrolyze: An experimentalist's viewpoint. **R.J. French**
- COMP 287.** Modeling some features of the reaction mechanism of chymotrypsin using semiempirical methods. **W.C. Kelly**, S.B. Braun-Sand, J.J. Stewart, **B.M. Guerrero**
- COMP 288.** Visualizing the interplay of delocalization and strong correlation in catalysis. **B.G. Janesko**
- COMP 289.** Ab initio dynamics of the unfolding and decarboxylation of pseudo-chair carboxyphosphate in aqueous solution. **E. Jesikiewicz**, S. Boesch, S.M. Firestine, J.D. Evanseck
- COMP 290.** Carboxyphosphate formation from the reaction of bicarbonate and ATP in ATP-dependent carboxylases. **S.E. Kochanek**, T. Clymer, V. Pakkala, S.M. Firestine, J.D. Evanseck
- COMP 291.** Analysis of the components of halogen bonding. **M. Billman**, A.K. Rappe
- COMP 292.** GPU-accelerated stochastic evaluation of second-order many-body perturbation energies. **R. Brewster**, S. Willow, S. Hirata
- COMP 293.** Molecular modeling of the binding interaction of RGD-functionalized poly(ethylene glycol) hydrogels with lipid bilayer surface. **Y. Lin**, G. Chen, F. Rytkin
- COMP 294.** Ab initio study of halocarbons. **K.R. Jorgensen**
- COMP 295.** Computational study of activation energies in 1,3-dipolar cycloadditions. **P. Esemio**, H.A. Trujillo
- COMP 296.** Microscale multiphysics simulations of intra-particle transport phenomena and pyrolytic conversion using biomass particle models with realistic morphology and resolved microstructure. **P. Ciesielski**, M.F. Crowley, B. Donohoe, M.R. Nimlos, T. Foust
- COMP 297.** Theoretically determined mechanism for the formation of guanine C8 adducts from arylamine derived carcinogens. **A.S. Dutton**, J. Bautista, S. Shrestha
- COMP 298.** Feedstocks thermal and compositional effects on pyrolysis yields. **D. Robichaud**
- COMP 299.** Theoretical study of criegee biradical molecule in the atmosphere. **S. Alhworthy**
- COMP 300.** Modeling non-covalent interactions in biomolecules: An ab initio based fragmentation approach. **D. Kosenkov**
- COMP 301.** Exploring novel energetic materials: A constrained search approach. **J.M. Elward**, C.B. Rinderspacher
- COMP 302.** Withdrawn.
- COMP 303.** Chemist view on reaction pathways. **N. Chéron**, R. Ramozzi, R. Grüber, **P. Fleurat-Lessard**
- Section A**
Colorado Convention Center
Hall B2
The Chemical Computing Group Excellence Award for Graduate Students
Financially supported by Chemical Computing Group
- C. L. Simmerling, Organizer**
6:00 - 8:00
COMP 304. Time-dependent nonequilibrium dynamics in QM/continuum approaches. **F. Ding**, D. Lingerfelt, B. Mennucci, X. Li
- COMP 305.** MD-generated volume profiles as a tool for probing transition states of conformational changes. **H. Wiebe**, N. Weinberg
- COMP 306.** Theoretical investigations of the fumarate addition reaction: Implications for the biological stability of future fuels and opportunities for bioremediation of hydrocarbon contaminated areas. **V.S. Bharadwaj**, C.M. Maupin, A.M. Dean
- COMP 307.** Simulations of the self-assembly of polyelectrolyte block copolymers using dissipative particle dynamics with an implicit solvent ionic strength (ISIS) method. **N.K. Li**, W.H. Fuss, Y.G. Yingling
- COMP 308.** Sum frequency generation spectra of the air/water interface from first principles-based models. **G.R. Medders**, F. Paesani
- Section A**
Colorado Convention Center
Hall B2
The OpenEye Outstanding Junior Faculty Award
Financially supported by OpenEye Scientific Software
C. L. Simmerling, Organizer
6:00 - 8:00
COMP 309. Physically-motivated first-principles force fields for molecular simulation: Theory and applications. **J.R. Schmidt**, J.G. McDaniel
- COMP 310.** RNA design rules through internet-scale social computing and high-throughput chemistry. **E. Participants**, J. Lee, W. Kladwang, M. Lee, D. Cantu, M. Azizyan, H. Kim, L. Alex, S. Yoon, A. Treuille, **R. Das**
- COMP 311.** Development of electron-hole explicitly correlated wave function based method with pseudopotential theory for investigation of optical properties of quantum dot-protein complexes. **A. Chakraborty**
- COMP 312.** Benchmarking the adsorption energies on carbon nanotubes. **D.G. Smith**, **K. Patkowski**
- Section A**
Colorado Convention Center
Mile High Ballroom 1D
Molecular Mechanics
Applications
E. X. Esposito, S. A. Wildman, *Organizers, Presiding*
8:30 COMP 313. Temperature effects on the spatial distribution of electrolyte mixtures at the aqueous liquid-vapor interface. **B.L. Eggimann**, A. Sunnarborg, J.J. Siepmann
9:00 COMP 314. Molecular simulation of surface density effects on heterogeneous DNA hybridization. **J.M. Stubbs**, S. Cooper, W. Scamman, M. van den Berg
9:30 COMP 315. Structural properties of DNA basepair mismatches. **A. Kingsland**, **L. Maibaum**
10:00 Intermission.
10:15 COMP 316. Quantum mechanical molecular mechanical calculations using amoeba force fields. **Y. Shao**, A.C. Simmonett, Y. Mao, F.C. Pickard, G. Koenig, B. Brooks, J. Herbert, T.L. Head-Gordon, M.P. Head-Gordon
10:45 COMP 317. Molecular dynamics by flexible-boundary QM/MM: On-the-fly partial charge transfer between QM and MM subsystems. **S. Pezeshki**, H. Lin
- 11:15 COMP 318.** Quantum Drude oscillator model for linear scale atomistic simulation – a coarse grained electronic structure allowing for high environmental transferability. **G.J. Martyna**
- Section B**
Colorado Convention Center
Mile High Ballroom 1E
Quantum Chemistry
Quantum Dynamics & Monte Carlo Simulations
Cosponsored by PHY5
E. V. Patterson, Organizer, Presiding
8:30 COMP 319. Second-quantized surface hopping. **A.V. Akimov**, O.V. Prezhdo
9:00 COMP 320. Systematically improvable models in excited-state dynamics calculations. **A. Molina**, A. Chien, T.G. Goodson, P.M. Zimmerman
9:30 COMP 321. Real-time electron transport from parity-time symmetric quantum mechanics. **J. Elenewski**, **H. Chen**
10:00 Intermission.
10:00 COMP 322. Ring polymer molecular dynamics: New quantum dynamical method for calculating chemical reaction rates. **Y. Suleymanov**
10:30 COMP 323. Direct dynamics simulations of steroidal ring-closing events. **R.P. Pemberton**, D.J. Tantillo
- Section C**
Colorado Convention Center
Mile High Ballroom 1F
Computational Pyrolysis & Upgrading of Bio-Oils
Bonding and Kinetics
Cosponsored by MPPG
D. Robichaud, Organizer
R. Surendran Assary, R. S. Weber, *Organizers, Presiding*
8:30 Introductory Remarks.
8:35 COMP 324. Molecular-level kinetic modeling in biomass thermochemical conversions: Software tools and their applications. **M.T. Klein**
9:20 COMP 325. Toward automated mechanism generation of lignin pyrolysis models: Development of group additivity parameters for aromatic species. **H.H. Carstensen**, A. Ince, M. Reyniers, G.B. Marin
9:50 COMP 326. First-principles study of phenol hydrogenation on Pt and Ni catalysts in aqueous phase. **R. Rousseau**, D. Mei, Y. Yoon, R.S. Weber, J.A. Lercher
10:20 Intermission.
10:25 COMP 327. Charting elementary steps in the cellulose pyrolysis reaction network. **H. Mayes**, X. Zhou, G. Beckham, L.J. Broadbelt
11:05 COMP 328. In silico zeolite catalyzed carbon-carbon coupling reactions for furan upgrading. **C. Liu**, L. Cheng, R. Surendran Assary, L.A. Curtiss
11:35 COMP 329. Mechanistic study of furan formation in HZSM-5 using quantum mechanical modeling. **S. Kim**, D. Robichaud, C. Mukarakate, L. Bu, T. Evans, G. Beckham, R.S. Paton, M.R. Nimlos
12:05 Concluding Remarks.
- Section D**
Colorado Convention Center
Mile High Ballroom 4E
Drug Discovery
Ligand-Based
Cosponsored by CINF and MEDI
Y. Tseng, S. A. Wildman, *Organizers, Presiding*
8:30 COMP 330. Halogen bonds in drug design. **S. Sirimulla**
9:00 COMP 331. Highly visual workflow for designing, selecting and enumerating new compounds for assay. **J.W. Sager**, T.E. Mansley, P. Mounteney
9:30 Intermission.

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

- 9:45 COMP 332.** Discovery of new and diverse TLR9 receptor antagonists for regulating innate immune reactions. **A. Goldblum**, A. Burger-Kentscher, A. Mattes, M. Zatsopin
- 10:15 COMP 333.** In silico design, synthesis, and assays of specific substrates and peptidomimetic inhibitors for proteinase 3. S. Narawane, C. Grauffel, A. Schillinger, B. Haug, N. Reuter
- 10:45 COMP 334.** Ligand based drug design of novel pyrimidine derivatives as Tankyrase inhibitors for the treatment of colorectal cancer. **A.P. Patel**, H.G. Bhatt

Section E

Colorado Convention Center
Mile High Ballroom 4F

Computational Study of Water

D. J. Sindhikara, *Organizer, Presiding*

- 8:30 COMP 335.** Advanced potential energy surfaces for water simulations. T.L. Head-Gordon
- 9:00 COMP 336.** Development and implementation of an advanced density based potential for water. R.E. Duke, O.N. Starovoytov, J.A. Piquemal, G.A. Cisneros
- 9:30 COMP 337.** Effects of three-body nonadditive exchange and induction forces in liquid water. **O. Akin-Ojo**, K. Szalewicz
- 10:00** Intermission.
- 10:15 COMP 338.** Microscopic structure, equilibrium density, and local environment in liquid water: A highly accurate ab initio path-integral molecular dynamics study. **R.A. Distasio**, B. Santra, H. Ko, F. Martelli, M. Ceriotti, R. Car
- 10:45 COMP 339.** Ice nucleation on graphene surface supports the classical theory of heterogeneous nucleation. **R. Cabriolu**, T. Li
- 11:15 COMP 340.** Direct calculation of the rate of homogeneous nucleation of ice for TIP4P/ICE from massively parallel molecular simulations. **A. Haji-Akbari**, P.G. Debenedetti

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Properties and Processes in Solvated Systems

Sponsored by *PHYS*, Cosponsored by *COMP*

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Modeling of Macromolecular Structure and Function

Sponsored by *PHYS*, Cosponsored by *COMP*

Modeling Excited States of Complex Systems

Electronic Structure

Sponsored by *PHYS*, Cosponsored by *COMP*

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1D

Symposium Organizer Selections

SOS

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

- 1:30 COMP 341.** Multi-scale computational investigations of the cAMP activation-mechanism of Protein Kinase A RI₁ using Brownian Dynamics and Molecular Dynamics simulations. **S.P. Hirakis**, R. Malnstrom, R.E. Amaro
- 2:00 COMP 342.** Water dynamics at protein-protein interfaces: A molecular dynamics study of virus-host receptor complexes. **P. Dutta**, M. Botlani, S. Varna
- 2:30 COMP 343.** Homology modeling and molecular dynamics study of ALKBH1 enzyme. **P. Silvestrov**, T. Müller, K. Clark, R. Hausinger, G.A. Cisneros
- 3:00** Intermission.

- 3:15 COMP 344.** Partitioning of nitroaromatic compounds through lipid bilayer. **A. Golius**, O. Isayev, L. Gorb, F. Hill, J.R. Leszczynski
- 3:45 COMP 345.** Bondalyzer: A tool for the discovery of charge density property relationships. **T.R. Wilson**, M. Eberhart, T. Jones
- 4:15 COMP 346.** Field-dependent peak shift in real-time time-dependent density functional theory. **M. Provorse**, B. Habenicht, C. Isborn

Section B

Colorado Convention Center
Mile High Ballroom 1E

Membranes

- S. A. Wildman, *Organizer, Presiding*
- 1:30 COMP 347.** Surface-functionalized nanoparticle permeation triggers lipid displacement and water and ion leakage. **P.A. Oroskar**, S. Murad, C. Jameson
- 2:00 COMP 348.** Investigating the forces governing the peripheral membrane association and dissociation of a bacterial phospholipase C (*BtPI-PLC*). **H.M. Khan**, C. Grauffel, B. Yang, T. He, R. Mary, A. Gershenson, N. Reuter
- 2:30 COMP 349.** Partitioning of anionic nanoparticles in cholesterol-containing membranes occurs via local disordering and cholesterol depletion. **P. Gkeka**, P. Angelikopoulos, L. Sarkisov, Z. Cournia
- 3:00** Intermission.
- 3:15 COMP 350.** Lateral organization and transverse coupling in asymmetric biomembranes. **X. Cheng**, J. Nickels, F. Heberle, J. Katsaras
- 3:45 COMP 351.** Investigating lipid phase changes from liquid crystalline to ripple to gel phases with all-atom molecular dynamics simulations. **P. Khakbaz**, J.B. Klauda
- 4:15 COMP 352.** Spatial organization of cellular membranes. **K. Sapp**, S. He, L. Maibaum

Section C

Colorado Convention Center
Mile High Ballroom 1F

Computational Pyrolysis & Upgrading of Bio-Oils

Reaction Engineering

Cosponsored by *ENFL* and *MPPG*

R. S. Weber, *Organizer*
D. Robichaud, R. Surendran Assary, *Organizers, Presiding*

1:30

- 1:35 COMP 353.** Impact of H₂ addition on formation of PAH during anisole pyrolysis. **Y. Koirala**, S. Villano, A.M. Dean, H.H. Carstensen, M. Reyniers, G.B. Marin
- 2:20 COMP 354.** Insights into the hydrodeoxygenation mechanisms for lignin upgrade. **D.G. Vlachos**
- 2:50 COMP 355.** Role of solid, liquid, and gaseous phases during pyrolysis of biomass. **R.C. Brown**
- 3:20** Intermission.

3:35 COMP 356. Strike a happy medium: Identifying appropriate reaction conditions for upgrading bio-oil. **M.R. Nimlos**, R.S. Weber

4:05 COMP 357. Reactor simulations for catalytic upgrading of pyrolysis vapors. **J. Ziegler**, S. Pannala, T. Foust, M.R. Nimlos, D. Robichaud

4:35 COMP 358. Multiscale/multiphysics modeling of biomass fast pyrolysis and vapor phase upgrading reactors. **S. Pannala**, E. Ramirez, J. Ziegler, D. Robichaud, M.R. Nimlos, T. Foust, C. Daw

5:05 Panel Discussion: What is Needed to Advance the State of the Art in Biomass Conversion and Upgrading?

5:35 COMP 359. Thermal properties of pine, poplar, and fir blocks from room temperature to 500°C. **D.M. Stevens**, T.L. Westover, C.L. Williams

6:05 Concluding Remarks.

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Ligand-Based

Cosponsored by *CINF* and *MEDI*

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP 360. Small molecule crystal structures in drug discovery and development. **C. Groom**, S. Ward, S. Vyas, I. Bruno

2:00 COMP 361. QSAR modeling independent of input tautomers. **M. Waldman**, R. Fraczekiewicz, R. Clark

2:30 COMP 362. General applicability of template CoMFA to prospective bioactivity prediction. **R.D. Cramer**

3:00 COMP 363. Exploring conformational search protocols for ligand-based virtual screening and 3D QSAR modeling. **D. Cappel**, S. Dixon, W. Sherman, J. Duan

3:30 Intermission.

3:45 COMP 364. Experimentally derived interaction fields as a basis for ligand-based virtual screening. **C. Groom**, J. Cole, I. Giangreco, O. Korb, S. Gothe, I. Bruno

4:15 COMP 365. Alignment of diverse ligands for a protein: a solved problem? **T. Cheeseright**, P. Tosco, M. Mackey

4:45 COMP 366. Exhaustive pairwise overlays: the gold standard for molecular alignment? **P.C. Hawkins**, R.W. Tolbert

Section E

Colorado Convention Center
Mile High Ballroom 4F

Quantum Chemistry

Applications

Cosponsored by *PHYS*

E. V. Patterson, *Organizer, Presiding*

1:30 COMP 367. Importance of a nonlocal description of electron-electron interactions in modeling the dissociative adsorption of H₂ on Cu(100). **F. Goettl**, C. Houriez, M. Guitou, G. Chambaud, P. Sautet

2:00 COMP 368. Density functional investigation of 2-alkyl-anthraquinone hydrogenation on a palladium cluster. **E. Yuan**, L. Wang, F. Ren

2:30 COMP 369. Theoretical prediction of the effects of substitution on the efficacies of ruthenium water oxidation catalysts. **A.B. League**, M. Ertem, P. Miro Ramirez, C.J. Cramer

3:00 Intermission.

3:15 COMP 370. DFT study of dehydrogenation of ethanol on alkaline earth metal oxides. **Y. Izumi**, H. Kamata, H. Ushiyama

3:45 COMP 371. Stereospecific zirconium catalyzed cycloamination of 4-penteneamine. **W.C. Everett**, T.L. Windus, A.D. Sadow

4:15 COMP 372. Reversible olefin binding to nickel dithiolenes and a variety of related complexes. **E.N. Brothers**, M.B. Hall

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Nonadiabatic Dynamics

Sponsored by *PHYS*, Cosponsored by *COMP*

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Folding and Aggregation

Sponsored by *PHYS*, Cosponsored by *COMP*

Modeling Excited States of Complex Systems

Electronic Structure

Sponsored by *PHYS*, Cosponsored by *COMP*

ENFL

Division of Energy and Fuels

A. Park, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Computational Pyrolysis and Upgrading of Bio-Oils (see *COMP, Wed*)

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas Oxidation (see *CATL, Tue, Wed, Thu*)

SOCIAL EVENTS:

Dinner, 7:30 PM: Tue

SUNDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by *MPPG*†

R. T. Koodali, Y. H. Ng, N. Wu, *Organizers*
Y. H. Hu, Y. Wu, *Organizers, Presiding*

8:00

Introductory Remarks.

8:05 ENFL 1. Nanocarbons for optoelectronic applications. **D. Guldi**

8:45 ENFL 2. Plasmonic metal-semiconductor nanostructures for solar fuel generation. **N. Wu**

9:15 ENFL 3. Uniform doping of metal oxide nanowires using solid state diffusion for photoelectrochemical water oxidation. **J. Resasco**, N.P. Dasgupta, J. Roque-Rosell, J. Guo, P. Yang

9:35 ENFL 4. Impact of humidity in the preparation of CoTiO₃ perovskites: Effective ABO₃ type catalysts for O₂ evolution. **S. Rasalingam**, R.T. Koodali

9:55 Intermission.

10:00 ENFL 5. Chalcogenide nanostructured precursors in fabrication of polycrystalline absorber layers in thin-film photovoltaics. **D.R. Radu**

10:30 ENFL 6. Light management in extremely thin photoelectrode architectures. **I. Thomann**

11:00 ENFL 7. Sustainable inorganic nanocrystals for solar energy conversion and storage applications. **K. Ramasamy**, R. Gupta, H. Sims, S. Nanov, A. Gupta

11:20 ENFL 8. Tailoring zinc oxide nanostructures for solar cell applications. **K. Sakar**, E.V. Braden, L. Song, M. Rawolle, S.V. Roth, P. Mueller-Buschbaum

11:40 ENFL 9. Structural studies of solution-grown iron pyrite (FeS₂) nanoparticles via synchrotron and neutron diffraction. **R.C. Miller**, D. Agocs, S. Fredrick, J.R. Neilson, A.L. Prieto

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

New Materials/Systems

A. A. Gewirth, A. Manivannan, *Organizers*
Y. Shao, D. Wang, *Organizers, Presiding*

8:00

Introductory Remarks.

8:05 ENFL 10. From nanomaterials to energy storage systems. **J. Liu**

8:35 ENFL 11. Flexible high-energy Li-ion batteries with fast-charging capability. **J. Cho**

9:05 ENFL 12. Enable high energy-density lithium-ion battery conversion cathodes based on iron fluorides using integrated in situ experimental and computational approaches. **S. Jin**, L. Li

Section F

Colorado Convention Center
Mile High Ballroom 4D

Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR and Novel Approaches

Cosponsored by MPPG†

G. Gadikota, A. G. Stack, *Organizers*
L. Anovitz, M. Kidder, *Organizers, Presiding*

8:00 ENFL 156. Density functional theory calculations of CO₂ and CH₄ interactions with clay surfaces. M.D. Kilmer, L. Tribe

8:20 ENFL 157. Study of pressure effects on borate cross-linked hydraulic fracturing fluids by small angle X-ray scattering. R.E. Winans, S. Lee, T. Li, R.J. Klingler, S. Seifert, R. Hutchins, M. Parris

8:50 ENFL 158. Phase equilibria and growth phenomena of CO₂ mixed gas hydrates. Z.T. Ward, Z.M. Aman, E.F. May, M.L. Johns, C.A. Koh

9:10 ENFL 159. Shale gas fracturing fluids containing additives of low environmental impact. M.H. Bell, A. Viswanath, B.C. Benicewicz

9:30 ENFL 160. Phase equilibrium and miscibility study of CO₂ and mixed gas in Tensleep oil for enhanced oil recovery. R. Borgohain, S. Xie, H. Jiang

9:50 ENFL 161. Investigation of chemical and morphological changes in shale-supercritical CO₂-water systems for sustainable unconventional hydrocarbon extraction. G. Gadikota, S. Yip, A. Park

10:10 Intermission.

10:20 ENFL 162. Potential microorganisms for enhance oil recovery in a low permeability oil reservoir. D. Hao, M. Zhang, H. Dong, S. Sun, Z. Zhang, D. Gao, Z. Song, Z. Zhang

10:40 ENFL 163. Alcohol-to-jet renewable jet fuel: Characterization, development of a surrogate fuel mixture, and diesel engine combustion. D.J. Luning Prak, M.H. Jones, J. Cowart

11:00 ENFL 164. Evaluating the leachability of residual solids generated from hydraulic fracturing in Marcellus shale. C. Swann, G.D. Boardman, J. Parks, R. Hammack

11:20 ENFL 165. Pyrolysis characteristics of Longkou oil shale under optimized condition. W. Wang, S. Li, Q. Shi, S. Liu, J. Wu, Y. Ma

11:40 ENFL 166. Formulating mixtures of nanoparticles, polymers, and surfactants to stabilize high viscosity high internal phase CO₂-in-water foams. Z. Xue, I. Ketchum, S.L. Bryant, C. Huh, M. Prodanovic, K.P. Johnston

12:10 ENFL 167. Switchable amine surfactants for CO₂ foams in high temperature enhanced oil recovery. A. Elhag, Y. Chen, J. Noguera, P. Reddy, G.J. Hirasaki, Q. Nguyen, K.P. Johnston

12:30 ENFL 168. Biogenic methane production from Bowen Basin coal waste materials using environmental microbial consortium. H. Zheng, T. Chen, V. Rudolph, S. Golding

Nanotechnology: Delivering on the Promise Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, COPA, CCS, CHAS, COLL, COMSCI, CORP ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Biomass to Fuel and Products

Sponsored by SOCED, Cosponsored by CELL, ENFL and MPPG

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG†

Y. H. Hu, N. Wu, Y. Wu, *Organizers*
R. T. Koodali, Y. H. Ng, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 169. Technical and operational perspective on the DOE Energy Innovation Hub and Fuels from Sunlight, the Joint Center for Artificial Photosynthesis. N.S. Lewis

1:45 ENFL 170. Hybrid nanomaterials for photovoltaics and photocatalysis. D. Ma

2:15 ENFL 171. Surface enhanced Raman spectroscopy for real-time observation of intermediates for photocatalytic reactions. R. Yan, P. Yang

2:35 ENFL 172. Exploration of solar hydrogen evolution using cobalt-doped titanium dioxide. L.J. Mahoney, R. Peng, C. Wu, J. Baltrusaitis, R.T. Koodali

2:55 Intermission.

3:00 ENFL 173. Exploring the role of defects on charge transport in organic semiconductors. K.M. Pelzer, M.K. Chan, S.K. Gray, S.B. Darling

3:30 ENFL 174. Repurposing Blu-ray movie discs as low-cost, quasi-random nanoimprinting templates for photon management. J. Huang

4:30 ENFL 175. Self-adapting layer of robust single-crystal earth-abundant nanoparticles catalyzing oxygen evolution. H. Chen

4:00 ENFL 176. Semiconductor materials for efficient photoelectrochemical water splitting: The PEC working group. H. Wang, T.F. Jaramillo, E.L. Miller

5:00 ENFL 177. Plasmon-enhanced Cu₂O photocathodes for solar water splitting. J. DuChene, B. Williams, A.C. Johnston-Peck, J. Qiu, D. Su, E. Stach, W. Wei

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Li-O₂ & Li-S

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
J. Lu, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 178. Water as promoter and catalyst in dioxigen electrochemistry at aqueous and organic electrified interfaces. N. Markovic, J. Jirkovsky, D. Strmcnik, L.A. Curtiss, J. Moore, K.R. Zavadil, V. Stamenkovic, K. Harrison, R. Surendran Assary, R. Subbaraman, B. Genorio, C. Diesendruck

1:35 ENFL 179. In situ fabrication of porous carbon supported α -MnO₂ nanoparticles at room temperature: Application for rechargeable Li-air battery. J. Lu, K. Amine

2:05 ENFL 180. Rechargeable K-Air battery: Principle and mechanism. Y. Wu

2:35 ENFL 181. Li-air battery with ionic liquid based electrolyte flow: Overview and perspectives. E. Paillard, S. Passerini

3:05 Intermission.

3:15 ENFL 182. Computational studies of the stability of lithium superoxide and its role in charge and discharge chemistries in lithium-oxygen batteries. L.A. Curtiss, K. Lau, U. Das, R. Surendran Assary, P. Redfern

3:45 ENFL 183. Li-ion and Li-O₂: exploring hybrid electrode/electrocatalyst materials. A. Kinaci, L. Trahey, S. Kirkin, C. Wolverton, M.M. Thackeray, M.K. Chan

4:15 ENFL 184. Modeling the electron transfer reaction at the lithium metal anode-liquid electrolyte interface in lithium-air batteries. S. Kazemiannavi, P. Dutta, S. Banerjee

4:35 ENFL 185. Establishing the relationship between lithium polysulfides and Li-S cell performance. R. Xu, J. Lu, I. Belharouak, K. Amine, Y. Ren, X. Zhang, A. Nie, R. Shahbazian Yassar, J.C. Li

4:55 ENFL 186. Towards a molecular level understanding of reactions in Li-S electrical energy storage systems. R. Surendran Assary

5:15 ENFL 187. Hierarchical porous carbon materials as electrodes for lithium sulfur batteries. S. Kaskel

5:35 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 4D

ENFL Distinguished Researcher Award: Symposium in Honor of James Burrington

J. Brazil, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ENFL 188. Important fundamental principles of selective heterogeneous oxidation catalysis ("7 pillars of oxidation catalysis"). R. Grasselli

1:40 ENFL 189. Mechanism and kinetics of propene oxidation and ammoxidation on bismuth molybdate-based catalysts. A.T. Bell

2:10 ENFL 190. Solid state mechanisms in selective oxidation by metal oxide catalysts. J.F. Brazil

2:40 Intermission.

2:50 ENFL 191. Mechanism in selective oxidation catalysis by metal oxides. J.D. Burrington

3:30 ENFL 192. Detailed reaction mechanisms for selective transformation of alkanes to oxygenates by heterogeneous transition metal oxide catalysts. W.A. Goddard

4:00 ENFL 193. Compositional inhomogeneity and lattice dynamics in the M1 catalyst: Implications concerning active sites for propane oxidation. D. Buttrey, D. Blom, T. Vogt, W. Ueda

4:30 ENFL 194. Mechanistic insights for propane ammoxidation over Mo-V-Te-Nb-O M1 phase from density functional theory calculations. Y. Xu, V.V. Gullants

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

G. Yu, *Organizer*
L. Hu, Y. Lin, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 195. Intercalation of 2D materials. L. Hu

1:35 ENFL 196. Insights into the solution synthesis of 2D metal chalcogenide nanostructures. D.D. Vaughn, D. Sun, R.E. Schaak

2:15 ENFL 197. Liquid phase exfoliation: A versatile route to materials for energy storage and production. K. Paton, J.N. Coleman

2:45 Intermission.

2:55 ENFL 198. Reversible zero-valent intercalation chemistries for 2D layered materials. K.J. Koski

3:15 ENFL 199. Enhancement of the chemical activity of 2D transition metal dichalcogenides via phase engineering. M. Chhowalla

3:55 ENFL 200. Preparation of new layered and 2D materials with basic science and energy applications. T. McQueen

4:25 ENFL 201. Bioelectrochemical oxidation of graphite drives graphene oxide production and electrosynthesis. Z. Ren, L. Lu, C. Zeng, L. Wang, X. Yin, S. Jin, J. Bunch

4:45 ENFL 202. Withdrawn.

Section E

Colorado Convention Center
Mile High Ballroom 4C

Hybrid Functional Porous Materials for Sustainable Energy: Carbon, MOF & Conductive Polymers

Energy Storage

V. Pol, *Organizer*
J. L. Lutkenhaus, S. K. Nune, *Organizers, Presiding*

1:00 ENFL 203. Advanced energy-storage devices of high-voltage symmetric supercapacitors fabricated with N-containing carbon materials. Y. Mei, Z. Zhou

1:30 ENFL 204. Peanut shell hybrid sodium ion capacitor with extreme energy: Power rivals lithium ion capacitors. D. Mitlin

2:00 ENFL 205. Nanoscale modifications in quantum dot solar cells. S. Bhattacharyya

2:20 ENFL 206. Energy applications of (photo) electrochemically prepared organic/inorganic hybrid semiconductor assemblies. C. Janaky, D. Hursan, G. Samu, C. Visy, K. Rajeshwar

2:40 ENFL 207. Poly(vinylidene fluoride) nanocomposites with enhanced energy density by filling with a small loading of surface-fluorinated Ba_{0.8}Sr_{0.2}TiO₃ nanofibers. L. Shaohui, J. Zhai, Z. An

3:00 Intermission.

3:10 ENFL 208. Block copolymer directed functional ordered mesoporous materials for energy devices: From functional materials to hierarchical materials. J. Lee

3:40 ENFL 209. Die creation and implementation to increase manufacturability in PEM fuel cell electrodes. K.M. McClung, S. Mahmoodi, R.S. Besser

4:00 ENFL 210. Methodology for stable but reactive catalysts (with λ -scale tunability). S. Das

4:20 ENFL 211. Fabrication of energy efficient conductive composites using nonconducting polymeric materials. R. Gill, Q. Nadeem, M. Rizwan

4:40 ENFL 212. Element strategy for new nanomaterials. H. Kitagawa

5:00 ENFL 213. Semitransparent DSSC cathodes based on thin layer tetraaminophthalocyanine polymers. K.J. Klunder

5:20 ENFL 214. Organic-inorganic hybrid materials for gas separation applications: Do MOFs really have any future for practical gas separations? S.K. Elsaïdi, M.H. Mohamed, P.K. Thallapally, B. Space, M.J. Zaworotko

5:40 ENFL 155. Method for direct measurement of adsorbed gas redistribution in metal-organic frameworks. Y. Chen, H. Zhou

Nanotechnology: Delivering on the Promise Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, COPA, CCS, CHAS, COLL, COMSCI, CORP ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Sustainability in the 21st Century: Optimizing Complex Interdependent Systems

Sponsored by SOCED, Cosponsored by CELL and ENFL

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.

† Cooperative Cosponsorship

- ENFL **282.** Azeotropic volatility behavior of hydrous ethanol gasoline mixtures. **B. Patz**, B. Windom
- ENFL **283.** Enhancement of methane hydrate formation with the presence of tetrahydrofuran and surfactants. **A. Siangsai**, C. Singer, **P. Rangsunvigit**, B. Kitiyanana, S. Kulprathipanja
- ENFL **284.** Effects of surfactants and treatments on co-based nanoparticles in Fischer-Tropsch synthesis reaction. **F. Gou**
- ENFL **285.** Nickel sulfides as competent hydrogen evolution catalysts in water. **N. Jiang**, Y. Sun
- ENFL **286.** Graphene-semiconductor 3D hybrid nanomaterials for sensitized solar cells. **C. Chaves-Villarreal**, T.M. Terse, A. Hernández-Valle, A.K. Mulchandani
- ENFL **287.** Electroless deposition of Co-P-Mo alloys. **E. Norkus**, I. Stankeviciene, A. Jagminiene, B. Sebekka, J. Vaiciuniene, Z. Sukackiene, A. Selskis, L. Tamasauskaite-Tamasiunaite
- ENFL **288.** Decoration of fiber structure cobalt with gold nanoparticles for application in fuel cells. **A. Zabielaite**, L. Tamasauskaite-Tamasiunaite, A. Balciunaite, S. Lichusina, I. Stalioniene, A. Jagminiene, A. Zieliene, **E. Norkus**
- ENFL **289.** Facile synthesis of exfoliated TiS₂ for all-solid-state lithium batteries. **D. Oh**, Y. Nam, K. Park, Y. Jung
- ENFL **290.** Effect of fuel evaporation on the gas-phase kinetics in the mixing region of a hydrocarbon reformer. **S. Kim**, A.M. Dean
- ENFL **291.** Improved molecular characterization of petroleum vacuum residues by FT-ICR MS analysis of their molecular distillation fractions. **D.C. Palacio**, J.P. Arenas, X. Ramirez, J.A. Orengo-Ruiz, A. Guzman, R. Cabanzo, **E. Mejia-Ospino**
- ENFL **292.** Voltage charging enhances ionic conductivity in gold nanotube membranes. **P. Gao**
- ENFL **293.** Withdrawn.
- ENFL **295.** Synthesis of Pt@ZSM-5 nanoparticles within hierarchically porous ZSM-5/SBA-15 material with high hydrogenation property. **D. Gao**, X. Dai, Y. Yang, H. Sun, Y. Qin, A. Duan, H. Wang, **X. Zhang**
- ENFL **297.** Platinum-cobalt nanocrystals prepared under different atmosphere for high catalytic performance of the methanol electro-oxidation. **Y. Qin**, X. Dai, Y. Yang, H. Sun, D. Gao, H. Wang, **X. Zhang**
- ENFL **298.** Single device that converts carbon dioxide to energy via formate. **T. Vo**, **B. Biggs**, A. Miller, K. Purohit, J. Chamin, J. Haan
- ENFL **299.** Multiscale experimental determination of cellulose pyrolysis reaction chemistry and transport phenomena. **C. Krumm**, A. Paulsen, P.J. Dauenhauer
- ENFL **300.** Textile growth of multilayer graphene from cellulose for the fabrication of photovoltaic devices. **M. Dasari**
- ENFL **301.** Synthesis of amphiphilic copolymers as additive for coal water slurry and their effect on rheology. **Y. Chang**, C. Cui, K. Huang, K. Meng, **X. Guo**, L. Li
- ENFL **302.** How comb-type polymer additives affect the rheology of coal water slurry. **C. Cui**, J. Huang, T. Wang, J. Xu, L. Li, **X. Guo**
- ENFL **303.** Recharge mechanisms of Mg-O₂ batteries. **J. Naruse**, G. Vardar, J. Smith, A.E. Sleightholme, C.W. Monroe, D.J. Siegel
- ENFL **304.** Reaction of styrene epoxide with H₂O_s(CO)_g. **J.M. Hahn**, M. Thomas, A. Bird
- ENFL **305.** Chemical modifications of polybenzimidazoles leading to enhanced properties and performance. **K. Fishel**, G. Qian, B. Benicewicz
- ENFL **306.** Investigations on the heat transfer security of endothermic hydrocarbon fuels in a heat-exchanger passage. **L. Yue**, W. Fang
- ENFL **307.** Continuing investigations into the photodegradation of poly(methylmethacrylate)-capped aluminum nanoparticles. **W. Zeng**, P.A. Jelliss, S.W. Buckner
- ENFL **308.** Withdrawn.
- ENFL **309.** Electrochemical investigations of layered double hydroxides for electrocatalysis. **B. Weintraub**
- ENFL **310.** Synthesis and evaluation of sustainable construction materials via mineralization of CO₂ from energy production cycles. **G. Gadikota**, X. Zhou, A. Park, S. Jiang
- ENFL **311.** Novel nanotube-like electrocatalysts of cobalt-tungsten carbonitride with highly active hydrogen evolution reaction. **Z. Li**, K. Du, **X. Dai**, H. Sun, Y. Yang, Y. Qin, D. Gao, X. Zhang
- ENFL **312.** Photoelectrochemical reduction of CO₂ on Cu-CO₂ nanotube arrays. **Q. Shen**, G. Zhao
- ENFL **313.** Optical sensor for the detection FAME/biodiesel. **R.A. Federico-Perez**, J.K. Fong, **Z. Xue**
- ENFL **314.** Investigation of nanocrystal heterostructures for photochemical hydrogen production. **A.N. Grennell**, M.B. Wilker, K.A. Brown, P.W. King, G. Dukovic
- ENFL **315.** Tunable anatase-brookite TiO₂ bipyramidal for enhanced CO₂ photocatalytic reduction to fuels. **H. Zhao**, L. Liu, Y. Li
- ENFL **316.** Catalyzed-cleavage of the bridged bond of coal model compounds over magnetic solid acid. **C. Zhao**, **W. Zhao**, K. Zhou, J. Fang, Y. Ren, J. Zhao, Q. Lei, Z. Zong, X. Wei
- ENFL **317.** Emulsification and performance measurement of pyrolysis oil/diesel. **J. Zhao**, W. Zhao, Q. Lei, Y. Ren, **C. Zhao**, K. Zhou, J. Fang, Z. Zong, X. Wei
- ENFL **318.** Catalytic ethanolysis of wheat stalk over coal cinder. **W. Zhao**, J. Fang, C. Zhao, Q. Lei, K. Zhou, Y. Ren, J. Zhao, Z. Zong, X. Wei
- ENFL **319.** Effect of electrolyte anion on charge/discharge rate capability for organic radical battery. **T. Shimoyama**, T. Nishi, S. Iwasa
- ENFL **320.** Sequential thermal dissolution of extraction residue from Zaozhuang bituminous coal. **S. Li**, X. Wei, T. Wang, C. Liu, J. Lv, Z. Zong
- ENFL **321.** Poplar liquefaction in water-methanol co-solvent. **H. Yan**, Z. Zong, Z. Li, X. Wei
- ENFL **322.** Catalytic hydroliquefaction of sawdust into high-value small-molecular chemicals over a novel magnetic solid superbase catalyst. **X. Li**, **Z. Zong**, W. Ma, X. Wei
- ENFL **323.** Fuel properties of heptadecene isomers prepared via tandem isomerization-decarboxylation of oleic acid. **B.R. Moser**, R.E. Murray, K.M. Doll
- ENFL **324.** Redox cofactor-apptamer complexes as possible catalysts for biofuel cells. **I. Emahi**, P.R. Gruenke, M.P. Mitchell, D.A. Baum
- ENFL **325.** Improving sugar yields and reduce enzyme loadings of DDR (deacetylation and disc refining) process through Szego milling and its techno economic analysis. **X. Chen**, W. Wang, P. Ciesielski, S. Park, O. Trass, M.P. Tucker
- ENFL **326.** Production of biodiesel from free fatty acids and triglycerides by reaction with high temperature methanol. **S. Thote**
- ENFL **327.** Low-temperature catalytic reforming of volatiles from biomass pyrolysis. **J. Cao**, C. Song, X. Zhao, X. Wei
- ENFL **328.** Optimum conditions to produce triacetanamine from fast pyrolysis of sewage sludge. **X. Huang**, **J. Cao**, **X. Zhao**, **X. Wei**
- ENFL **329.** Molecular characteristics of a Chinese subbituminous coal using HPLC/MS. **C. You**, **X. Fan**, A. Zheng, X. Wei, Y. Zhao, J. Cao, W. Zhao, Z. Zong, J. Zhu, L. Chen
- ENFL **330.** Two mass spectrometers for the analysis of high-temperature coal tar. **J. Zhu**, **X. Fan**, S. Wang, X. Wei, Y. Zhao, J. Cao, W. Zhao, Z. Zong, C. You, L. Chen
- ENFL **331.** CO-liquefaction of Shenmu bituminous and white pine sawdust in sub- and supercritical ethanol. **Y. Tian**, Y. Zhao, H. Yang, S. Chen, **X. Fan**, J. Cao, Z. Zong, X. Wei
- ENFL **332.** Electric-field assisted coating of nanoparticles for photon management nanostructures. **J. Gong**, N. Wu
- ENFL **333.** From fields to fuels: Setting the target for oxygenates in liquid fuels. **M. Menart**, A. Robinson, R.M. Richards, J.W. Medlin, J. Hensley
- ENFL **334.** Re-examination of Na₂V₂(PO₄)₃ as novel anode material for sodium-ion batteries. **Z. Jian**, Y. Sun, Y. Hu, X. Ji
- ENFL **335.** Thermogravimetric analysis of nitrogen containing material. **A. Hopson**, A.C. Sacco, P. Ponnada, N.P. Rath, R.J. Moser, G.K. Balendiran
- ENFL **336.** Aminodiborane: Structure, formation mechanism, and properties. **H. Li**, N. Ma, **X. Chen**, J. Zhao
- ENFL **337.** TiO₂ conformal coating on carbon nanotubes as lithium-ion battery anode. **L. Yan**, M. Zhou, G. Chen, S. Deng, H. Luo
- ENFL **338.** Control of methane and carbon dioxide concentrations in the effluent of a catalytic partial oxidation reactor for hydrogen production from natural gas. **A. Al-Musa**, S. Shabunya, M. Al-Johani, V. Martynenko, M. Al-Saleh, A. Al-Zahrani, V. Kalinin
- ENFL **339.** Catalytic conversion of monosaccharides into 5-hydroxymethylfurfural using aluminum complexes supported by bidentate phenoxy-amine ligands. **D.S. Saangonyo**, F.T. Ladipo
- ENFL **340.** Mechanism of light hydrocarbons adsorption in metal organic framework from direct structural evidence. **A.M. Plonka**, X. Chen, D. Banerjee, W.R. Woerner, J.B. Parise
- ENFL **341.** Excess thermopower and the theory of thermopower waves. **J.T. Abrahamson**, **S.G. Mahajan**, B. Sempere, M. Walsh, J.M. Forman, F. Sen, S. Sen, G.L. Paulus, Q. Wang, W. Choi, M.S. Strano
- ENFL **342.** High pressure catalytic conversion of n-pentane on H-ZSM-5. **E.P. Schreiner**, S. Teketel, R.F. Lobo
- ENFL **343.** Polydopamine-based carbon nanowires for wire-type supercapacitor. **W. Lee**, Y. Oh, Y. Lee, N. Kim
- ENFL **344.** Ion mobility and PetroOrg software: Novel techniques for petroleomics investigations. **E. Riches**, Y. Corilo, R.P. Rodgers, M. O'Leary, **D. Stevens**
- ENFL **345.** Cyclic voltammetric studies of the interactions between ferrocene mediators and glucose oxidase. **D. Bamber**, D.T. Glatzhofer
- ENFL **346.** Exploring alfalfa hay's potential as an alternative non-food source of biofuel. **J.B. Belay**, B. Gikonyo
- ENFL **347.** Treatment of phenanthrene using sodium persulfate activated by modified diatomite. **C.K. Silva Rackov**, M.M. Vianna, O. Chiavone-Filho, C.A. do Nascimento
- ENFL **348.** Organic oxygen transformation during pyrolysis of Baiyinhua lignite. **X. Zhao**, X. Feng, J. Cao, X. Wei
- ENFL **349.** Nickel oxide/activated carbon composite electrodes for electrochemical capacitors. **X. Zhao**, S. Huang, J. Cao, **X. Wei**
- ENFL **350.** Anomalous rising of input current induced in the transformer of inverter. **O. Ide**
- ENFL **351.** Consideration of the cause of inverter noise called ringing. **O. Ide**
- ENFL **352.** Characteristics of DC power output from an Inverter driven by sharp spike pulse. **O. Ide**
- ENFL **353.** Pyrolysis of powdered examination gloves at 340 °C and 440 °C. **N. Hamidi**, M. Marcanikova, M. Ghaili, R. Massoudi
- ENFL **354.** What's the "rub" with your salt: A case history of quality assurance for potassium chloride. **A. Evans**, A. Jensen, S. Nguyen, P. Carman, D.A. Castillo, M. Usie
- ENFL **355.** What is this "stuff", where did it come from, and how can we get rid of it? Case histories of analytical laboratory methods and instrumental analyses applied to requests for identification of oilfield "unknown material" samples. **A. Evans**, A. Jensen, S. Sun, D. Wang, A. Koch, M. Wilson, D.A. Castillo
- ENFL **356.** Temperature and injection gas composition influence on CO₂ miscibility by interfacial tension measurement. **Q. Shang**, S. Xia, M. Shen, P. Ma
- ENFL **357.** Treated bio-oils upgraded in a fixed-bed continuous reactor with sulfided CoMo/γ-Al₂O₃ catalysts. **Y. Luo**
- ENFL **358.** Improved characterization and fractionation of vacuum residues of heavy crude oils using supercritical fluid extraction. **A.Y. Leon Bermudez**, A. Guzman, L.J. Hoyos, E. Mejia, O. Corredor, D. Laverde
- ENFL **359.** Arid lands biofuel. **B.P. Neupane**
- ENFL **360.** Synthesis of multiwalled carbon nanotubes doped titania for desulfurization of model fuel. **T.A. Saleh**, **M.N. Siddiqui**
- ENFL **361.** Porous membrane assisted-solvent brat microextraction for elemental sulfur in crude oil. **I.M. Al-Zahrani**, B. Chanbasha, **M.N. Siddiqui**
- ENFL **362.** PbS and PbSe quantum dot solar cells: Ion exchange synthesis and metal halide surface passivation for high efficiency devices. **R. Crisp**, J. Zhang, J. Gao, A. Marshall, D. Kroupa, E. Miller, M.C. Beard, **J. Luther**
- ENFL **363.** Hierarchical nanomaterial electrodes for energy storage. **L. Mai**, X. Xu, L. Xu, Q. Wei
- ENFL **364.** Nonaqueous all-cobalt redox flow battery using 1,10-phenanthrolinecobalt(II) hexafluorophosphate as the active species. **Y. Li**, X. Xing
- ENFL **365.** Photons to formate: Solar driven conversion of CO₂ to solar fuels. **H. Pan**, Y. Zou, M.D. Heagy
- ENFL **366.** Ag nanoparticles modified photocatalytic for photocatalytic water splitting. **X. Zhang**
- ENFL **367.** CdS-mesoporous ZnS core-shell particles of Type I structure for efficient and stable photocatalytic hydrogen evolution under visible light. **Z. Yu**
- ENFL **368.** Investigation of the morphology evolution of nanoscale Cu₂S electrodes during electrochemical cycling via ex situ electron microscopy. **E. Jackson**, A.L. Prieto
- ENFL **369.** AFePO₄NO₃ (A = Li, Na): Nitrophosphate as a new family of cathode materials for alkali-metal-ion batteries. **H. Yaghoobnejad Asl**, A. Choudhury
- ENFL **370.** Spectroelectrochemical studies of charge transfer processes in stable nitroxyl radical-containing polymers. **B.K. Hughes**, W. Braunecker, J.C. Johnson, A. Ferguson, T. Gennett
- ENFL **371.** Molecular level insight into the lithiation mechanism of RuO₂ and the implication for its use as lithium-ion battery electrode material. **A. Hassan**, B.R. Ramachandran, C.D. Wick, A. Navulla, L. Meda
- ENFL **372.** Screening of lithium oxygen cathode 3D composite nanonetworks enabled by M13 phage directed synthesis. **L. Tadesse**, J. Ohmura, D. Oh, A.M. Belcher
- ENFL **373.** Design and synthesis of direct growth of nanosized nickel oxides on stainless steel substrates as anode in lithium ion battery. **L. Meda**, A. Navulla, **C. Arnold**
- ENFL **374.** Catalytically activated palladium@ platinum nanowires for accelerated hydrogen gas detection. **X. Li**, Y. Liu, J.C. Hemminger, R.M. Penner
- ENFL **375.** Steam-biogas reforming over a metal-foam-coated (Pd-Rh)/(CeZrO₂-Al₂O₃) catalyst compared with pellet type alumina-supported Rh, Ru and Ni catalysts. **P.S. Roy**, C.S. Park, A. Raju, K. Kim
- ENFL **376.** Water soluble charged nanoparticles featuring core-shell morphology for energy harvesting. **H.P. Rathnayake**, J. Ferguson, A. Braun
- ENFL **377.** Co-reaction of methanol and ethylene over MFI and CHA zeolitic catalysts. **Q. Zhu**
- ENFL **378.** Product distribution of polyoxymethylene dimethyl ethers from methanol and formaldehyde. **D. Liu**

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

L. Hu, Y. Lin, *Organizers*
V. Barone, *Organizer, Presiding*
G. Yu, *Presiding*

- 1:00 ENFL 379.** Graphene based supercapacitors for integrated energy storage. R.B. Kaner
- 1:40 ENFL 380.** New charge storage mechanism in graphene oxide based solid state capacitors. Q. Zhang, K. Scraftford, M. Li, Z. Cao, Z. Xia, P.M. Ajayan, B. Wei
- 2:20 ENFL 384.** Modified porous graphene and its use in electrode reaction study. Y. Zhu, K. Liu, Y. Chen
- 2:50 ENFL 382.** SnO₂ - graphene dual aerogels as high rate sodium lithium ion battery anodes. Z. Li, D. Mitlin
- 3:10** Intermission.
- 3:25 ENFL 383.** Carbon nanomaterials in metal oxide based electrodes for supercapacitors. J. Liu, Y. Cheng, G. Lee, H. Zhang
- 4:05 ENFL 384.** Lithium battery applications of graphene materials. W. Ren, F. Li, H. Cheng
- 4:35 ENFL 385.** Lithium adsorption and diffusion in SnS₂ bulk, bilayer, monolayer, and nanoribbon: A computational investigation. K. Tu, Z. Chen

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry**Methane Activation**

Cosponsored by MPPG†
N. Kumar, J. J. Spivey, *Organizers, Presiding*

- 1:00 ENFL 386.** Continuous oxidation of methane to oxygenates under mild reaction conditions using ZSM-5 catalysts. J. Xu, R.D. Armstrong, S.J. Freakley, S.H. Taylor, G. Hutchings
- 1:40 ENFL 387.** Size- and support-dependent electronic and catalytic properties of size selected cluster catalysts on methanation of CO: A combined GIXAS, GISAXS and TPRx study. S. Lee, B. Lee, S. Seifert, R.E. Winans, S. Vajda
- 2:00 ENFL 388.** Structure-performance relationship in the design of Ru/TiO₂ catalyst for CO₂ methanation. A. Kim, C. Sanchez, C. Sassoey, D. Debecker
- 2:20 ENFL 389.** Carbon dioxide hydrogenation into methanol over promoted Cu/Zn-based catalysts. R.S. Monteiro, P. Coutinho, J. Miranda, C.J. Mota
- 2:40** Intermission.
- 2:50 ENFL 390.** Phase equilibria and characterization of cyclopentane - methane binary hydrates. P. Warrier, M. Khan, Z.T. Ward, Y. Yang, C.A. Koh
- 3:10 ENFL 391.** Gas hydrate phase equilibrium predictions for cyclopentane containing gas mixtures with optimized Kihara parameters. M.N. Khan, P. Warrier, C.J. Peters, C.A. Koh
- 3:30 ENFL 392.** Generation of chemicals from natural gas in a fuel cell. O.A. Marina, B. Kirby, C. Coyle, J. Frye, D. Edwards, L. Pederson, C. Freeman, J. Stevenson
- 3:50 ENFL 393.** Electrocatalytic reduction of CO₂ in water to CO+H₂ syngas mixtures. P. Kang, Z. Chen, A. Nayak, T.J. Meyer
- 4:10 ENFL 394.** On the route to commercialization of a CO₂ electrolyzer: Lessons learned from an industry effort to fight climate change. T.S. Matthews, M. Kaplun, Z. Liu, Q. Chen, R. Kutz, S. Luopa, K. Lewinski, R. Masel

TUESDAY EVENING**Energy and Materials**

Sponsored by POLY, Cosponsored by ENFL† and PMSE

WEDNESDAY MORNING**Section A**

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG†
Y. H. Hu, R. T. Koodali, N. Wu, *Organizers*
Y. H. Ng, Y. Wu, *Organizers, Presiding*

- 8:00** Introductory Remarks.
- 8:05 ENFL 395.** Engineered quantum dots for solar energy conversion. V.I. Klimov
- 8:45 ENFL 396.** Withdrawn.
- 9:05 ENFL 397.** Chemically modifying quantum dot surfaces to improve solar cell performance. A. Marshall, A.J. Nozik, M.C. Beard, J. Luther
- 9:25 ENFL 398.** Resolving carrier multiplication and charge transport in quantum dot solids with ultrafast transient photocurrent. A.F. Fidler, J. Gao, G. Chen, W. Koh, V.I. Klimov
- 9:45** Intermission.
- 10:00 ENFL 399.** Efficient harvesting of solar energy using quantum-dot luminescent solar concentrators. J.M. Pietryga, H. Li, T.A. Baker, J. Lim, H. McDaniel, V.I. Klimov
- 10:30 ENFL 400.** Field-effect transistors and light-emitting diodes with low-toxicity I-III-VI₂ quantum dots. H. McDaniel, S. Draguta, W. Bae, J. Lim, Y. Park, J.M. Pietryga, V.I. Klimov
- 10:50 ENFL 401.** Auger up-conversion in engineered heterostructured quantum dots for applications in solar energy conversion. N.S. Makarov, Q. Lin, K. Velizhanin, V.I. Klimov
- 11:10 ENFL 402.** Synthesis and analysis of CdTe quantum dot solar cells. K.M. McHenry, E. Kim, A.L. Asunskis, D.J. Asunskis
- 11:30 ENFL 403.** Highly ordered CdTe nanotube arrays for solar cells through patterned electrodeposition. W.P. Liyanage, M. Nath

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Li-ion
A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
J. Esbenschade, *Presiding*

- 8:00** Introductory Remarks.
- 8:05 ENFL 404.** All-solid-state polymer electrolyte with plastic crystal materials for secondary lithium-metal batteries. F. Ding
- 8:35 ENFL 405.** High-energy bulk-type all-solid-state lithium batteries using sulfide solid electrolyte. Y. Nam, D. Oh, K. Park, K. Lee, S. Lee, Y. Jung
- 9:05 ENFL 406.** Controllable uniform crystallization towards improved performance in glass-ceramic Li_{1-x}AlxGe_{2-x}(PO₃)₃ electrolyte membrane. A. Vyalkikh, V. Vizgalov, A. Sergeev, L.A. Trusov, E. Brendler, L.V. Yashina, D. M. Itkis
- 9:25 ENFL 407.** High ionic conductivity of flexible polymer-based electrolyte with low porosity. W. Zhao
- 9:45** Intermission.
- 9:55 ENFL 408.** High voltage cathodes for advanced lithium-ion batteries. J. Nanda, R.E. Ruther, S. Martha, H. Zhou
- 10:25 ENFL 409.** Investigation of atomic/molecular layer deposition coatings for Li-ion electrodes. C. Ban, D. Piper, Y. He, J. Travis, A.M. Wise, J. Weker, S. Son, J. Zhang, M. Toney, C. Wang, S. Lee, S.M. George

- 10:55 ENFL 410.** Iron borophosphates as novel cathode for alkali-ion battery. A. Choudhury, H. Yaghoobnejad Asl
- 11:15 ENFL 411.** Guiding principles for next-generation batteries from theoretical and experimental studies of LiMn₂O₄. M. Young, A. Holder, H. Dieter-Schnabel, S.M. George, C. Musgrave
- 11:35 ENFL 412.** Data-driven review of battery materials: Performance and resource considerations. L. Ghadbeigi, J. Harada, T. Sparks
- 11:55** Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

12th International Symposium on Heavy Oil Upgrading, Production & Characterization

Fouling and Asphaltenes
Cosponsored by MPPG†
J. J. Adams, C. Mesters, D. Mitlin, *Organizers*
J. F. Schabron, *Organizer, Presiding*

- 8:00 ENFL 413.** Thiophene mitigates high temperature fouling of metal surfaces in oil refining. D. Mitlin
- 8:45 ENFL 414.** Protocol for diagnosing and predicting petroleum fouling in upstream and downstream operations. J.J. Adams, J.F. Schabron
- 9:15 ENFL 415.** Influence of acid chemistry on bitumen viscosity. V. Gonzalez, A. de Klerk, S. Yang, V. Prasad
- 9:45 ENFL 416.** Cold flow behavior of waxy crude oil under elevated pressure. T. Wang, J. Xu, H. Zhao, L. Li, X. Guo
- 10:15** Intermission.
- 10:15 ENFL 417.** Asphaltenes diffusion into catalysts under hydroprocessing conditions. F. Gaulier, J. Barbier, B. Guichard, D. Espinat
- 10:45 ENFL 418.** Role of asphaltenes in oil and water emulsions. J.J. Adams, J.F. Schabron
- 11:15 ENFL 419.** Catalytic cracking of cold lake bitumen and Fischer-Tropsch wax mixtures: Coke suppression and viscosity analysis. X. Liu

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

V. Barone, L. Hu, *Organizers*
G. Yu, *Organizer, Presiding*
Y. Lin, *Presiding*

- 8:00 ENFL 420.** Efficient photocurrent generation in heterostructures of 2D layered materials. X. Duan
- 8:40 ENFL 421.** Hybrid layer materials for energy conversion and storage. Y.H. Hu
- 9:10 ENFL 422.** Engineering the catalysis at 2D materials for solar water splitting. L. Cao
- 9:40 ENFL 423.** Earth-abundant 2D materials as high performance electrocatalysts for photoelectrochemical energy conversion. S. Jin, Q. Ding
- 10:20** Intermission.
- 10:35 ENFL 424.** 2D structuring of photocatalytic bismuth-based metal oxides. T.T. Salguero, T. Pope, G. Neher, A. Bruning
- 11:05 ENFL 425.** Theoretical and computational studies of graphene-based materials for use as transparent conducting electrodes in solar cells. G.J. Martyna
- 11:25 ENFL 426.** Atomically thin transition metal disulfides on silicon for high performance water splitting photocathodes. S. Choi, K. Kwon, T. Kim, K. Hong, S. Lee, S. Kim, H. Jang

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry**CO₂ Conversion**

Cosponsored by MPPG†
N. Kumar, J. J. Spivey, *Organizers, Presiding*

- 8:00 ENFL 427.** Utilization of CO₂ as feedstock in C₁ chemistry. H. Dudder, L. Chew, M. Muhler
- 8:40 ENFL 428.** Kinetics of methanol synthesis from carbon dioxide and hydrogen. K. Kobl, L. Angelo, Y. Zimmermann, K. Parkhomenko, A. Roger
- 9:00 ENFL 429.** Dihydropteridine/pteridine as a 2H⁺/2e⁻ redox mediator for the catalytic reduction of CO₂ to methanol via hydride-proton transfer. C. Lim, Y. Kuo, A. Holder, J.T. Hynes, C. Musgrave
- 9:20 ENFL 430.** Catalysts for the CO₂ recycling into methanol. L. Angelo, K. Kobl, Y. Zimmermann, K. Parkhomenko, A. Roger
- 9:40 ENFL 431.** Liquid phase CO₂ hydrogenation to methanol and dimethyl ether using heterogeneous cascade catalysis. Y. Chen, S. Choi, L.T. Thompson
- 10:00** Intermission.
- 10:10 ENFL 432.** Catalysis for the conversion of CO and CO₂ to fuels and chemicals. A.T. Bell
- 10:50 ENFL 433.** Nanocomposite photocatalysts: Conversion of CO₂ to fuel. S. Hunyadi Murph, H. Sessions, Y. Kun, Y. Zhao
- 11:10 ENFL 434.** High efficient formate production by low temperature hydrogenation of amine captured CO₂ over Pd catalyst. H. Lin, J. Su
- 11:30 ENFL 435.** Modeling the HCOOH/CO₂ electrochemical couple: When details are key. S.N. Steinmann, C. Michel, P. Sautet

WEDNESDAY AFTERNOON**Section A**

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG†
Y. H. Hu, R. T. Koodali, Y. H. Ng, *Organizers*
N. Wu, Y. Wu, *Organizers, Presiding*

- 1:00** Introductory Remarks.
- 1:05 ENFL 436.** Efficiency limiting factors in light-driven H₂ generation using multicomponent semiconductor-metal colloidal nanorod heterostructures. T. Lian
- 1:35 ENFL 437.** Solar energy conversion and electrocatalysis using earth-abundant pyrite nanomaterials. S. Jin, M. Caban-Acoevado
- 2:05 ENFL 438.** Light-induced photoelectrochemical charging and discharging in metal oxide thin film. Y. Ng
- 2:35 ENFL 439.** Surface optimization strategy for photoelectrochemical H₂ production. T. Ogitsu, W. Choi, B. Wood
- 3:05** Intermission.
- 3:15 ENFL 440.** Highly efficient visible light photocatalytic production of H₂. Y.H. Hu, B. Han
- 3:45 ENFL 441.** Branched nanostructures for photoelectrochemical water splitting. Y. Mao
- 4:15 ENFL 442.** Designing a hybrid multifunctional material for CO₂ capture and photocatalytic conversion. L. Liu, Y. Li
- 4:45 ENFL 443.** Artificial photosystem I and II: Highly selective solar fuels and tandem photocatalysis. Y. Ding, I. Castellanos Beltran, V. Singh, P. Nagpal

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond**Li-ion**

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
D. Lu, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 444. Chemically integrated graphene/inorganic hybrid 2D materials as advanced energy storage electrodes. G. Yu

1:35 ENFL 445. Methods for fabrication of highly conductive Cu₂S nanoparticle electrode films through room-temperature processing. R.D. Robinson, O. Otelaja, D. Ha, T. Ly, H. Zhang

1:55 ENFL 446. MXene nanosheets as promising anode materials for nonlithium-ion batteries. Y. Xie, Y. Dall'Agnese, M. Naguib, Y. Gogotsi, M.W. Barsoum, H.L. Zhuang, P. Kent

2:15 ENFL 447. Iron fluoride based perovskite type cathode materials for Li/Na-ion batteries. T. Yi, W. Chen, L. Cheng, J. Lee, E. Chan, M. Doeff, K. Persson, J. Cabana

2:35 ENFL 448. Managing the volume fluctuation of iron pyrite cathode in lithium ion batteries using polyacrylonitrile. T. Yoder, J.E. Cloud, L. Cain, M. Tussing, X. Li, Y. Yang

2:55 ENFL 449. Controllably branched 3D electrodes as a test bed for investigating the effect of morphology on the performance of nanostructured V₂O₅ cathodes for Li ion batteries. E. Gillette, C. Liu, G. Rubloff, S. Lee

3:15 Intermission.

3:25 ENFL 450. Electrolyte additives and interfacial mechanisms for high-capacity lithium-ion cells. D. Abraham, I. Shkrob

3:55 ENFL 451. Electrolyte additives for high voltage LiNi_{0.8}Mn_{0.1}O₂ batteries. S. Delp, T.R. Jow

4:15 ENFL 452. Novel organophosphine oxide based redox shuttle additives for 4V lithium ion batteries. J. Huang, N. Azimi, Z. Zhang, L. Zhang

4:35 ENFL 453. Accelerating electrolyte discovery by high throughput screening. L. Cheng, R. Surendran Assary, X. Qu, A. Jain, S. Ong, N. Rajput, K. Persson, L.A. Curtiss

4:55 ENFL 454. Catholyte material development for nonaqueous redox flow batteries. J. Huang, L. Su, M.S. Ferrandon, F. Brushett, A.K. Burrell, L. Zhang

5:15 ENFL 455. Exploration of the effective location of surface oxygen defects in graphene-based electrocatalysts for the all-vanadium redox flow batteries. M. Park, J. Baek, J. Cho

5:35 Concluding Remarks.**Section C**

Colorado Convention Center
Mile High Ballroom 3C

12th International Symposium on Heavy Oil Upgrading, Production & Characterization**Characterization**

Cosponsored by MPPG†

C. Mesters, D. Mitlin, J. F. Schabron, *Organizers*
J. J. Adams, *Organizer, Presiding*

1:00 ENFL 456. Screening the adsorptive effect of metal oxides nanoparticles loaded activated carbons for sulfur compounds. T. Saleh, G.I. Danmaliki

1:30 ENFL 457. Modifications to a novel method for the isolation of interfacial material from Athabasca bitumen: Characterization by FT-ICR mass spectrometry. A.C. Clingenpeel, J.M. Jarvis, W.K. Robbins, R.P. Rodgers

2:00 ENFL 458. Study on transformation of dissolved organic matter in oilfield produced water during biodegradation using ultrahigh resolution mass spectrometry. Z. Min, D. Hao, Y. Hengye, S. Shanshan, Z. Zhongzhi

2:30 ENFL 459. Molecular reconstruction of vacuum residue from molecular distillation cuts and FT-ICR-MS. X.X. Ramirez, D.C. Palacio, J. Arenas, A. Guzman, J.E. Torres Macias, V. Kafarov

3:00 Intermission.

3:30 ENFL 460. Compositional model conversion of hydrocracking of vacuum gas oils using molecular reconstruction. X.X. Ramirez, J.E. Torres Macias, D.D. Perez

4:00 ENFL 461. Application of an in-line viscometer to study methane hydrate slurry properties. L. Chen, C.A. Koh

4:30 ENFL 462. Molecular characterization of dissolved organic matter in coal gasification waste water by negative ESI FT-ICR MS. Y. Li, D. Cui, C. Xu, Q. Shi

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

L. Hu, G. Yu, *Organizers*
Y. Lin, *Organizer, Presiding*
V. Barone, *Presiding*

1:00 ENFL 463. Predicting materials for solar energy conversion ab initio spectroscopy of heterogeneous interfaces. G.A. Galli

1:40 ENFL 464. Nanomechanics of bending 2D materials. T. Dumitrica

2:10 ENFL 465. Thermoelectricity layer by layer. M. Fornari

2:40 Intermission.

2:40 ENFL 466. Computational design of 2D nanomaterials toward carbon neutral energy. Z. Chen

3:10 ENFL 467. Materials cartography: Representing and mining material space using structural and electronic fingerprints. S. Curtarolo

3:40 ENFL 468. Interlayer commensurability and sliding in layered materials: The power of the registry index. O. Hod

4:10 ENFL 469. Electronic and adsorption properties of 2D materials by density functional theory calculations. V. Barone

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry**Syngas Chemistry**

Cosponsored by MPPG†

N. Kumar, J. J. Spivey, *Organizers, Presiding*

1:00 ENFL 470. Syngas to fuel and chemicals via FTS: Reaction network and structure-performance for catalyst development. Y. Sun, L. Zhong, T. Zhao

1:40 ENFL 471. Effect of support pretreatment on the performance of supported Fe Fischer-Tropsch catalysts. K. Keyvanloo, W. Hecker

2:00 ENFL 472. Fe-based Fischer Tropsch synthesis of biomass-derived syngas: Effect of synthesis method. K. Mai

2:20 ENFL 473. Experimental investigation of Fischer-Tropsch synthesis in a microchannel reactor. X. Ying, L. Zhang, H. Xu, Q. Luo, H. Zhu

2:40 ENFL 474. Kinetics of main reaction and deactivation by carbon of cobalt Fischer-Tropsch catalyst. K. Keyvanloo, W. Hecker, C.H. Bartholomew

3:00 Intermission.

3:10 ENFL 475. Supported iron catalyst for the direct conversion of synthesis gas to lower olefins. K. De Jong

3:50 ENFL 476. Direct dimethyl ether synthesis from synthesis gas: The influence of methanol dehydration on methanol synthesis reaction. F. Dadgar, R. Myrstad, P. Pfeifer, A. Holmen, H.J. Vevik

4:10 ENFL 477. Role of lanthanum oxide on cobalt-copper catalyst for the conversion of syngas to ethanol. Z. Wang, J.J. Spivey

4:30 ENFL 478. Gas phase selective oxidation of olefins from a model synthesis gas stream. S. Wiebe, S. Villano, A.M. Dean

Computational Pyrolysis & Upgrading of Bio-Oils**Reaction Engineering**

Sponsored by COMP, Cosponsored by ENFL† and MPPG

THURSDAY MORNING**Section A**

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG†

Y. H. Hu, N. Wu, Y. Wu, *Organizers*
R. T. Koodali, Y. H. Ng, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 479. Preparation of Cu-Sb-Se nanoparticles through a hot-injection route. D. Agocs, A.L. Prieto

8:25 ENFL 480. Spectroscopic and solution growth study of co-solvent effects on zinc oxysulfide buffer layers in earth abundant kesterite Cu₂ZnSnSe₄ solar cells. X. Steirer, R.L. Garris, J. Li, M. Reinisch, M.J. Dzara, P. Ndiome, K. Ramanathan, I. Repins, G. Teeter, C.L. Perkins

8:45 ENFL 481. Understanding the role of chemical treatments and device architecture on ink-based CdTe solar cells. R.W. Crisp, M.G. Panthani, D.V. Talapin, J.M. Luther

9:05 ENFL 482. Synthesis and characterization of mixed phase anatase TiO₂ and sodium-doped TiO₂(B) thin films by low pressure chemical vapour deposition (LPCVD). Y. Chimupala, G. Hyett, R. Simpson, R. Mitchell, R. Douthwaite, S.J. Milne, R.D. Brydson

9:25 ENFL 483. Tunable nanostructured contact for cSi solar cells. A.A. Dameron, W. Nemeth, V.A. LaSalvia, A.G. Norman, D.L. Young, P. Stradins

9:45 Intermission.

9:55 ENFL 484. Withdrawn.

10:15 ENFL 485. 1D hematite nanostructures for photoelectrochemical water splitting. D. Kim, J. Lee, H. Jang

10:35 ENFL 486. Enhanced photoelectrochemical water splitting on hematite thin film with ultrathin SiO₂ underlayer. M. Kang, Y. Kang

10:55 ENFL 487. Electrical characterization of nanoscale material interfaces ranging from single nanorods to functional solar cell devices using scanning Kelvin probe microscopy. S. Nanayakkara, R. Ihly, M. Law, J. Luther

11:15 ENFL 488. Systematic strategy to synthesize photoactive titanium metal-organic frameworks (MOFs). L. Zou, D. Feng, T. Liu, H. Zhou

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond**Li-ion**

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
D. Lu, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 489. Fundamental charge transfer processes in stable free-radical organic polymer systems. B.K. Hughes, T. Kemper, W. Braunecker, R. Larsen, D. Bobela, T. Gennett

8:25 ENFL 490. Close packing of radicals in the stable radical polymer, PTMA. D. Bobela, B.K. Hughes, W. Braunecker, R.E. Larsen, T. Kemper, T. Gennett

8:45 ENFL 491. In situ AFM nonindentation and morphology analysis of mechanically constrained microfabricated silicon anodes. C. Becker, K. Strawhecker

9:05 ENFL 492. Molecular structure and ion transport near electrode-electrolyte interfaces in lithium-ion batteries. V. Lordi, M. Ong, O. Verneris, A.C. Van Duin, E. Draeger, J. Pask

9:25 ENFL 493. Mitigating irreversible capacity losses from conducting carbon agents via surface modification. S. Son, D. Piper, J. Travis, Y. Lee, S.M. George, S. Lee, C. Ban

9:45 ENFL 494. Investigating improved capacity retention of AlPO₄-coated Cu₃Sb anodes for lithium-ion batteries. L.A. Kraynak, E. Jackson, A.L. Prieto

10:05 ENFL 495. Solvothermal route based in situ carbonization to Fe₃O₄@C as anode material for lithium ion battery. G. Chen, M. Zhou, H. Luo

10:25 Intermission.

10:25 ENFL 496. Lithium-ion battery performance of perfluoropolyether-based electrolytes. D. Wong, J.M. DeSimone, N.P. Balsara

10:45 ENFL 497. Spectroscopic investigations of liquid-phase chemistry for advanced battery technologies. J.L. Wheeler, J.M. Porter

11:05 ENFL 498. Computational studies of phosphorinated electrolytes for Li system. J.S. McNally, J.R. Klaehn, E.J. Dufek, H.W. Rollins, M.K. Harup

11:25 ENFL 499. Lithium ion solvation and diffusion in bulk organic electrolytes from first principles molecular dynamic. M. Ong, V. Lordi, E. Draeger, J. Pask

11:45 Concluding Remarks.**Section C**

Colorado Convention Center
Mile High Ballroom 3C

12th International Symposium on Heavy Oil Upgrading, Production & Characterization**Upgrading and Processing**

Cosponsored by MPPG†

J. J. Adams, C. Mesters, J. F. Schabron, *Organizers*
D. Mitlin, *Organizer, Presiding*

8:00 ENFL 500. Catalytic heavy crude oil upgrading using natural gas. H. Song, A. Guo, C. Wu, D. Zhang, Y. Luan, L. Zhao

8:30 ENFL 501. Visbreaking oils and bitumen at 300 °C. L. Yanez Jaramillo, A. de Klerk

9:00 ENFL 502. Low CO selectivity of copper-free ZnGaO catalysts used for dimethyl ether reforming to produce H₂. S. Zhou, M. Meng

9:30 Intermission.

9:45 ENFL 503. Electromembrane extraction of sulfur compounds from crude oils. B. Chabasha, I.M. Al-Zahrani, T. Maung

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.

† Cooperative Cosponsorship

- 10:15 ENFL 504.** Visbreaking of Fischer-Tropsch wax mixed with bitumen: Analysis of thermal behavior. **C. Melo Halmenschlagler, A. de Klerk**
- 10:45 ENFL 505.** Effect of hydrogenation and acidity properties of NiMo/Al₂O₃ catalysts on the hydrodemetallization. **T. Liu, Y. Zhou, Q. Wei, N. Wang, S. Ding, W. Zhou, L. Ju**

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

- Y. Lin, Organizer**
V. Barone, G. Yu, Organizers, Presiding
- 8:00 ENFL 506.** Can graphene appear greener to galvanization industry? **V. Gadhamshetty, V.K. Upadhyayula**
- 8:20 ENFL 507.** Synthesis, chemical functionalization and electronic devices of 2D atomic and molecular crystals. **X. Wang**
- 8:50 ENFL 508.** How we look at graphene and graphene oxide: A material, a chemical, a tool. **Y. Shao**
- 9:20 Intermission.**
- 9:30 ENFL 509.** Bulk graphene materials for energy applications. **Y. Chen**
- 10:00 ENFL 510.** Synthesis of 2D materials for energy applications. **S. Eichfeld, J.A. Robinson**
- 10:30 ENFL 511.** Synthesis and modification of holey graphene for energy storage. **Y. Lin, J. Kim, J.W. Connell**
- 11:00 ENFL 512.** NSF support of advanced materials for sustainable energy. **G.L. Rorrer**
- 11:30 Concluding Remarks.**

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry

Syngas Chemistry

Cosponsored by MPPG†

N. Kumar, J. J. Spivey, Organizers, Presiding

- 8:00 ENFL 513.** Reactor design and catalysts testing for hydrogen production by methanol steam reforming for fuel cells applications. **F. Vidal Vazquez**
- 8:20 ENFL 514.** O-functionalized CNT mediated CO hydrodeoxygenation and chain growth. **K. Mondal, S. Talapatra, M. Terrones, S. Pokhrel, C. Frizzel, B. Sumpter, V. Meunier, A. Elias**
- 8:40 ENFL 515.** Metal organic mediated synthesis of highly stable and active FTO catalysts. **V.P. Santos, T. Wezendonk, J. Delgado Jaén, A. Dugulan, A. Chojecski, S. Sina, A. Koeken, M. Ruitenbeek, T. Davidian, G. Meima, F. Kapteijn, M. Makkee, J. Gascon**
- 9:00 ENFL 516.** Citrate-nitrate auto-combustion synthesis of Co-Ce mixed bulk oxides with different cobalt content for the oxidation of CO. **Z. Lin, J. Liu, Z. Zhao, K. Cheng, C. Xu**
- 9:20 Intermission.**
- 9:30 ENFL 517.** Investigation of low temperature water-gas shift over MOF-assisted catalysts. **O. Kavakli, A.K. Avci**
- 9:50 ENFL 518.** Influence of coexisting metal oxide on the activity of copper catalyst for water-gas-shift reaction. **H. Yahiro, K. Sagata**
- 10:10 ENFL 519.** Homogeneous water-gas shift and production of methanol and ethanol from CO and H₂O without added H₂. **M.V. Mundschaue**
- 10:30 ENFL 520.** Effect of Cu dopant in zeolite on catalytic properties and deactivation in carbonylation of dimethyl ether. **S. Huang, X. Ma, H. Zhan, W. Huang**

ENVR

Division of Environmental Chemistry

Souhail Al-Abed, Program Chair

OTHER SYMPOSIA OF INTEREST:

- Applied Nanotechnology for Food & Agriculture** (see AGFD, Tue, Wed)
Fundamental Research in Colloids, Surfaces & Nanomaterials (see COLL, Sun)
Analytical Chemistry of Natural Resources: Environmental Analysis (see ANYL, Wed)
Ask Dr. Safety: EH&S Support of Nanotechnology R&D (see CHAS, Tue)
Basic Research in Colloids, Surfactants & Nanomaterials (see COLL, Sun, Wed, Thu)

SOCIAL EVENTS:

Reception, 6:00 PM: Tue

BUSINESS MEETINGS:

- ENVR Programs Planning Meeting, 2:00 PM: Sun**
ENVR Long Range Planning Committee Meeting, 3:00 PM: Sun
ENVR Division Executive Committee Meeting, 7:00 PM: Sun

SUNDAY MORNING

Section A

Colorado Convention Center
Room 703

Green Chemistry and the Environment

Cosponsored by CEI and MPPG

- S. O. Obare, Organizer**
A. M. Balu, R. Luque, Organizers, Presiding
- 8:30 Introductory Remarks.**
- 8:35 ENVR 1.** Aqueous chemistry in organic synthesis. **C. Len**
- 9:10 ENVR 2.** Deoxygenation and hydroisomerization of algae oils to hydrocarbon fuels. **J.S. Kruger, E.D. Christensen, R.L. McCormick, P.T. Pienkos**
- 9:30 ENVR 3.** Adipic acid production from lignin. **D.R. Vardon, M. Franden, C. Johnson, E. Karp, M. Guarnieri, J. Linger, M. Salm, T.J. Strathmann, G. Beckham, G.A. Ferguson**
- 9:50 ENVR 4.** Mechanism of lignin pyrolysis from model compound to actual lignin. **V. Custodis, P. Hemberger, J.A. Van Bokhoven**
- 10:10 Intermission.**
- 10:25 ENVR 5.** Use of green chemistry of chalcones synthesis. **E. Alarcón, N. Romero, H. Aguilar, J.L. Terán, A. Gómez Rivera, L.F. Roa, C. Lobato, A. Escobar**
- 10:45 ENVR 6.** Photochemical transformation of aliphatic-aromatic polyesters and its impacts to degradability. **M.A. Maurer-Jones, M. Zumstein, M. Sander, K.P. McNeill**
- 11:05 ENVR 7.** Transesterification of waste vegetable oil under simultaneous microwave and ultrasound Irradiations. **V. Gude, E. Martinez-Guerra**
- 11:25 ENVR 8.** Modified heterogeneous nickel catalysts for the production of chemicals and fuels from bioderived light olefins. **M. Menart, J. Hensley, R.M. Richards**
- 11:45 ENVR 9.** Overcoming production limitations of biosynthesis and tailoring rhamnolipid biosurfactant properties through chemical synthesis. **J.E. Pemberton, R. Palos Pacheco, C. Coss, R. Pölt**

Section B

Colorado Convention Center
Room 705

Assessing Toxicity of Environmental Contaminants

Cosponsored by AGRO, CEI and MPPG†

S. M. Uchimiya, B. Zhang, Organizers
X. Pan, J. Wang, Organizers, Presiding

8:00 Introductory Comments.

- 8:05 ENVR 10.** Measurement and evaluation of the rate of emission of semivolatile organic compounds from poly (vinyl chloride) sheets. **M. Noguchi, A. Yamasaki**
- 8:30 ENVR 11.** Environmental and human health risk assessment of amine emissions from post combustion power plants. **S. Manzoor, A. Korre, S. Durucan, A. Simperler**
- 8:55 ENVR 12.** Biological risk assessment of EDCs degradation by ozone. **L. Li, K. Yeung**
- 9:20 ENVR 13.** Assessing the uptake and effects of polycyclic aromatic hydrocarbons and their oxygenated derivatives on zebrafish using a metabolomics approach. **M.R. Elie, R.L. Tanguay**
- 9:45 ENVR 14.** Kinetic toxicity profile of haloacetonitriles, haloacetamides, and haloacetic acids. **Y. Yu, D. Reckhow**
- 10:10 Intermission.**
- 10:25 ENVR 15.** Toxicity of silica nanomaterials: Effects of porosity and surface chemistry, and correlations with in vitro and in vivo results. **S.E. Lehman, A. Wongrakpanich, A. Morris, A. Dodd, A.K. Salem, P.S. Thorne, V.H. Grassian, S.C. Larsen**
- 10:50 ENVR 16.** Inhibition of thyroid hormone sulfotransferase activity by brominated flame retardants in a human choriocarcinoma cell line, BeWo. **C. Leonetti, T. Neufeld, C. Butt, H.M. Stapleton**
- 11:15 ENVR 17.** Identifying disinfection by-products (DBPs) capable of endocrine disruption through binding to the androgen receptor. **B.E. Holmes, L. Smeester, R.C. Fry, H. Weinberg**
- 11:40 ENVR 18.** Resistance measurements for Ar/O₂ and H₂O plasma modified SnO₂ nanomaterials for enhanced gas sensing. **E.P. Stuckert, E.R. Fisher**

Section C

Colorado Convention Center
Room 707

Chemical Processes at Environmental Interfaces

Chemistry and Imaging at Air/Liquid(Solid) Interfaces of Atmospheric Systems

Cosponsored by COLL

- H. M. Ali, N. Kabengi, Organizers**
H. A. Al - Abadleh, R. Z. Hinrichs, Organizers, Presiding
- 8:00 Introductory Remarks.**
- 8:10 ENVR 19.** Role(s) of adsorbed water in the surface chemistry of oxide nanoparticles with atmospherically relevant molecules. **V.H. Grassian**
- 8:40 ENVR 20.** Effects of particle size, relative humidity, and sulfur dioxide on iron solubility in atmospheric particulate matter. **B.T. Cartledge, A.R. Marcotte, A.D. Anbar, P. Herckes, B. Majestic**
- 9:00 ENVR 21.** Complexation and dark degradation of catechol by iron(III): Bulk vs. surface chemistry. **H.A. Al - Abadleh**
- 9:20 ENVR 22.** Chemical imaging of atmospheric particles. **A. Laskin**
- 9:50 Intermission.**
- 10:10 ENVR 23.** Ozone initiated heterogeneous oxidation of atmospheric organics. **Y. Liu, C. Leng**
- 10:40 ENVR 24.** Reactive uptake of biogenic volatile organic compounds on mineral aerosol substrates and their subsequent heterogeneous ozonolysis. **R.Z. Hinrichs**
- 11:00 ENVR 25.** Cascade oxidation of atmospheric aerosol dicarboxylic acids by gas-phase OH-radicals. **S. Enami, M.R. Hoffmann, A.J. Colussi**

- 11:30 ENVR 26.** Atmospheric oxidation of benzene: Effect of temperature, pH, ionic strength, and oxygen content at the air-water interface. **A.A. Heath, L.C. Cormier, C.A. Leger, K.T. Valsaraj**
- 11:50 ENVR 27.** Elucidating the mechanisms of HONO formation from nitrate photochemistry on environmental surfaces. **J.D. Raff**

Section D

Colorado Convention Center
Room 709

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Cosponsored by AGRO and MPPG†

W. Arnold, Y. Chin, K. H. Wammer, Organizers, Presiding

8:30 Introductory Remarks.

- 8:30 ENVR 28.** Environmental photochemistry of alrenogest. **K.H. Wammer, K.C. Anderson, P.R. Erickson, S. Kliegman, K. McNeill, D. Martinovic-Weigelt, D.M. Cwiertny, E.P. Kolodziej**
- 8:50 ENVR 29.** Characterizing lampricide photoproduct formation under laboratory based and field based conditions. **M. McConville, C.K. Remucal**
- 9:10 ENVR 30.** Comparative triplet photochemistry of natural and treated effluent organic matter: Wavelength dependence of quantum yields for singlet oxygen and oxidizing triplets. **C.M. Sharpless, J. Laszakovitz**
- 9:30 ENVR 31.** Environmental photochemistry of bacitracin. **R. Lundeen, C. Chu, M. Sander, K. McNeill**
- 9:50 Intermission.**
- 10:05 ENVR 32.** Matrix effects in the photodegradation of 2,4,6-trinitrotoluene. **K.A. Thorn**
- 10:25 ENVR 33.** Does debromination dominate BDE-47 photodegradation in natural environments? **M.L. Wei-Haas, Y. Chin**
- 10:45 ENVR 34.** Insights into photochemical transformation pathways of triclosan and 2'-HO-BDE-28. **Y. Zhang, J. Chen, Q. Xie**
- 11:05 ENVR 35.** Distinct photolytic mechanisms and products for different dissociation and metal complexation species of ciprofloxacin. **X. Wei, J. Chen**

Section E

Colorado Convention Center
Room 711

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs

Cosponsored by MPPG†

D. L. Drogos, M. Urynowicz, Organizers, Presiding

8:00 Introductory Remarks.

- 8:10 ENVR 36.** Enhancing production of coalbed biogenic natural gas: History, status, and perspectives. **S. Jin, R.M. Flores**
- 8:30 ENVR 37.** Biogenic methane potential of Bowen Basin, Queensland coal preparation plant rejects. **S.K. Lane, H. Zheng, V. Rudolph, S. Golding, P.C. Gilcrease**
- 8:50 ENVR 38.** Impacts of natural gas developments on methanogenesis in deep aquifers in natural gas field. **T. Katayama, H. Yoshioka, S. Sakata, Y. Muramoto, J. Usami**
- 9:10 Intermission.**
- 9:30 ENVR 39.** Decarbonization of shallow unconventional biogenic gas: Bridging the gap between fossil fuels and renewable energy. **M. Urynowicz**
- 9:50 ENVR 40.** Subsurface bio-electrochemical conversion of carbon dioxide into methane by using indigenous microorganisms. **H. Maeda, M. Ikarashi, H. Kobayashi, N. Fukushima, K. Sato**
- 10:10 ENVR 41.** Impact of CO₂ injection into depleted oil field on the methanogenic activity and pathway. **H. Maeda, T. Wakayama, M. Ikarashi, D. Mayumi, S. Sakata, H. Tamaki, Y. Kamagata**
- 10:30 ENVR 42.** Stimulating effect of protein-rich matter on the biogenic recycling of CO₂ to CH₄. **J. Vilcaez**
- 10:50 Panel Discussion.**

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 703

Green Chemistry and the Environment

Cosponsored by CEI and MPPG

R. Luque, Organizer

A. M. Balu, S. O. Obare, Organizers, Presiding

1:30 Introductory Remarks.

1:35 ENVR 43. Green photoelectrochemical solar cell based on water redox. H. Zhang, H. Xu, H. Wang, J. Xuan

2:05 ENVR 44. Pd-reduced-graphene oxides with oxygen annealing for advanced direct formic acid fuel cells. D. Li, D. Leung, H. Xu, H. Wang, J. Xuan

2:25 ENVR 45. Simultaneous energy generation and organics removal from real pharmaceutical wastewater by packed bed-microbial fuel cell. Z.Z. Ismail, A.A. Habeeb

2:45 ENVR 46. Withdrawn.

3:05 Intermission.

3:20 ENVR 47. Binary hierarchical systems for green chemistry processes. R.R. Ozer, H.A. Al-Zubaidi, S.O. Obare

3:40 ENVR 48. Upcycling of packing-peanuts into carbon electrodes for electrochemical energy storage. V. Etacheri, C. Hong, V. Pol

4:00 ENVR 49. Facile microwave-induced rapid synthesis of triazepinone: An adduct of metformin and methylglyoxal. B. Dayal, R. Gohil, B. Garsondiya, S. Nirujogi, M.A. Lea

4:20 ENVR 50. Tyrosinase-catalyzed immobilization of catalase onto regenerated silk fibroins. P. Wang, G. Tang, L. Cui, Q. Wang, X. Fan

4:40 ENVR 51. Multipurpose application of Sacha inchi *Plukenetia volubilis* L plant: Panacea from the Andean region. B. Kumar, L. Cumbal, A. Debut

Section B

Colorado Convention Center
Room 705

Assessing Toxicity of Environmental Contaminants

Cosponsored by AGRO, CEI and MPPG†

S. M. Uchimiya, B. Zhang, Organizers
X. Pan, J. Wang, Organizers, Presiding

1:30 ENVR 52. Utilizing high-throughput bioassays associated with US EPA ToxCast Program to assess biological activity of environmental contaminants: A case study of chemical mixtures. B. Blackwell, A. Schroeder, G. Ankley, M. Lee, K. Jensen, K. Houck, R. Judson, D. Villeneuve

1:55 ENVR 53. Uptake and reproductive toxicity of the metal oxide nanoparticle ZnO in *Caenorhabditis elegans*. L.A. Bush

2:20 ENVR 54. Sublethal impacts of engineered and biogenic nanomaterials on social behavior of environmental bacteria. A. Mohanty, B. Cao

2:45 ENVR 55. New measuring method of nicotine in tobacco smoke to estimate personal exposure of secondhand smoke. M. Noguchi, A. Yamasaki

3:10 ENVR 56. Impacts of nanomaterials on bacterial growth, biofilm Formation, and microbial community function. Y. Liu, P. Ymele-Leki, M. Ramamoorthy

3:35 Intermission.

3:50 ENVR 57. Toxicity of binary and ternary mixtures of nickel, copper, zinc and cadmium to *Daphnia magna*. E. Traudt, J.F. Ranville, S. Smith, K. Ebeling, J. Meyer

4:15 ENVR 58. Simulated sunlight induces oxygen loss and decreases nanosheet size for graphene oxide in aqueous suspensions demonstrating zebrafish toxicity. J.N. Wheeler, M. Kim, W. Heideman, R.E. Peterson, J.A. Pedersen, R.J. Hamers

4:40 ENVR 59. Effect of *Daphnia magna* age on the variability of cadmium toxicity. S. Smith

5:05 ENVR 60. Metabolic pathways of polychlorinated biphenyls (PCBs) mediated by the active center of cytochrome P450s: A computational study with PCB-52 and PCB-77. Z. Fu, Y. Wang, Z. Wang, J. Chen

5:30 Concluding Remarks.

Section C

Colorado Convention Center
Room 707

Chemical Processes at Environmental Interfaces

Chemistry and Imaging at Air/Liquid(Solid) Interfaces of Atmospheric Systems

Cosponsored by COLL

H. A. Al - Abadleh, R. Z. Hinrichs, N. Kabengi, Organizers
H. M. Ali, Organizer, Presiding

1:30 ENVR 61. Photolysis of secondary organic aerosol material as a source of small oxygenated volatile organic compounds. K. Malecha, S.A. Nizkorodov

1:50 ENVR 62. Sunlight-driven synthesis and self-assembly of a model amphiphile at the air-water interface. R. Rapf, E. Griffith, V. Vaicida

2:10 ENVR 63. Effects of solutes on pollutant photolysis kinetics at ice surfaces. T.F. Kahan, P. Malley, J. Grossman

2:40 ENVR 64. Attenuated total reflection spectroscopy of frozen aqueous salt solutions and vapor-deposited ice. R.R. Michelsen, H. Marocco, K. Searles, R. Walker

3:00 Intermission.

3:20 ENVR 65. Effects of air pollution and climate change on allergenic protein containing aerosols in the anthropocene. C.J. Kampf, F. Liu, K. Reinmuth-Selzle, M. Shiraiwa, U. Pöschl

3:40 ENVR 66. In situ probing of environmental liquid surfaces and interfaces by time-of-flight secondary ion mass spectrometry. X. Yu

4:00 Discussion.

4:05 ENVR 67. Adsorption and self-assembly of alkylammonium surfactants at silica/water interfaces studied by interface-specific vibrational spectroscopy: Investigating pH and ionic strength conditions relevant to hydraulic fracturing. P. Hayes, L.L. Torres

4:35 ENVR 68. Characterization of quantum dot suspensions with SEC-ICP-MS. P. Laresse-Casanova, P. Payday

Section D

Colorado Convention Center
Room 709

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Cosponsored by AGRO and MPPG†

W. Arnold, Y. Chin, K. H. Wammer, Organizers, Presiding

1:30 ENVR 69. Insights into the (bio)transformation processes of benzotriazoles from compound-specific isotope analysis and transformation product identification. B. Rani, S. Spahr, S. Emma, J. Hollender, T.B. Hofstetter

1:50 ENVR 70. Establishing predictive relationships between specific bacterial 16S rRNA sequences and micropollutant biotransformation rates. D.E. Helbling, D. Johnson, T. Lee, A. Scheidegger, K. Fenner

2:10 ENVR 71. Experimental and computational evidence for reduction mechanisms of N-oxides by soluble Fe⁰ species. Y. Chen, H. Zhang

2:30 ENVR 72. Fate of urban micropollutants and their transformation products in black carbon amended stormwater bioinfiltration systems. B.A. Ulrich, E. Im, D. Werner, C.P. Higgins

2:50 Intermission.

3:05 ENVR 73. Withdrawn.

3:25 ENVR 74. Ozone degradation of cylindrospermopsin (cyanotoxin): Degradation mechanisms and toxicity assessments. S. Yan, A. Jia, S. Merel, S.A. Snyder, W. Song

3:45 ENVR 75. Doxycycline transformation during water disinfection with chlorine. N. Kennedy, O. Keen

4:05 ENVR 76. Electropexone treatment of the anti-inflammatory drug ibuprofen: operation parameters and degradation mechanism. X. Li, Y. Wang, G. Yu

Section E

Colorado Convention Center
Room 711

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs

Cosponsored by MPPG†

D. L. Drogos, M. Urynowicz, Organizers, Presiding

1:30 ENVR 77. Relationship between coal biodegradation, microbial methane generation, and redox conditions in coalbeds indicated by coupled water, gas, and microbial analyses. D. Ritter, E. Barnhart, H. Schweitzer, D. Vinson, J.C. McIntosh, M. Fields

1:50 ENVR 78. Molybdate, cobalt, and copper affect microorganisms associated with deep on subsurface coal by enhancing methane production and shifting the methanogenic community structure. B. Unal, M. Sanderson, V. Ryan Perry, K. Chin, K. Nusslein

2:10 ENVR 79. Enhanced production of biogenic coalbed methane from coals following chemical oxidation. Z. Huang, M.A. Urynowicz

2:30 ENVR 80. Use of a kinetic model to identify rate-limitations for biological methane production from coal. S.L. Papendick, S. Golding, V. Rudolph, P.C. Gilcrease

2:50 Intermission.

3:10 ENVR 81. Characterization of microbial communities of methanogenically productive and unproductive coals. L. Gallagher, A.W. Glossner, L.L. Landkamer, L.A. Figueroa, K.W. Mandernack

3:30 ENVR 82. Biodegradation pathways and organic intermediates in the conversion of coal geopolymers to methane. W.H. Orem, D.M. Akob, E. Barnhart, A. Clark, A. Cunningham, D. Dunlap, M. Fields, J.C. McIntosh, L. Ruppert, M. Varonka

3:50 ENVR 83. Molecular characterization of microbes and metagenome of an Indian coal bed for biotransformation of coal into methane and other valued products. D.N. Singh, A. Kumar, M.P. Sarbhai, A. Gupta, A.K. Tripathi

4:10 ENVR 84. Evolution of acetate metabolism in methanogenic Archaea. E. Barnhart, M. McClure, K. Johnson, S. Cleveland, K. Hunt, M. Fields

4:30 Panel Discussion.

4:50 Concluding Remarks.

MONDAY MORNING

Section A

Colorado Convention Center
Room 703

Green Chemistry and the Environment

Cosponsored by CEI

A. M. Balu, Organizer
R. Luque, S. O. Obare, Organizers, Presiding

8:30 Introductory Remarks.

8:35 ENVR 85. Sonochemical water treatment of dyeing waste water on carpet workshop. S. Sedaghat

8:55 ENVR 86. Morphology-dependent of alpha-MnO₂ for catalytic decomposition of ozone. J. Jia, P. Zhang

9:15 ENVR 87. Effect of initial pH on iron-oxidizing bacteria assisted pyrite oxidation system for mine tailings treatment. W. Ju, E. Jho, K. Nam

9:35 ENVR 88. Biotic and abiotic treatment methods for alkaline leachates from steel slags. S. Kim, K. Nam, E.G. Jho

9:55 ENVR 89. Environmental application of PEI based hydrogels in different morphology and sizes: Bulk, microgel, and cryogel. N. Sahiner, S. Demirci, M. Sahiner, H.A. Al-Lohedan, N. Aktas

10:15 Intermission.

10:30 ENVR 90. Effect of two-phase pre-treatment of rice straw on polyhydroxyalkanoates (PHAs) synthesis by *Cupriavidus necator*. J. Ahn, E.G. Jho, K. Nam

10:50 ENVR 91. Insights on the solubility of CO₂ in 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide from the microscopic point of view. L.T. Costa, T. Lourenço, D. Van Der Spoel

11:10 ENVR 92. Novel vapor-phase hydrolysis approach for preparing of nanosilica: Recycling of silicon tetrachloride. F. Yan, J. Jiang, M. Zhao

11:30 ENVR 93. Nitrous oxide emission from de-ammonification process. P.L. Noophan

11:50 ENVR 94. [Brim]Cl ionic liquid as a novel solvent and reaction medium for the preparation of keratin biodegradable thermoplastic. J. Yuan, Y. Yu, P. Wang, X. Fan, Q. Wang

12:10 ENVR 95. Metal occurrence in and potential recovery from municipal biosolids. K.S. Smith, P.L. Hageman, G.S. Plumlee, J.G. Crock, T.J. Yager, R.B. Brobst, S.C. Gebhard

Section B

Colorado Convention Center
Room 705

Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter

Cosponsored by MPPG

S. M. Lomnicki, Organizer, Presiding

8:00 ENVR 96. Exposure to combustion-derived particulate matter: an unrecognized risk factor in severity of respiratory viral infection in infants. S. Cormier, G. Lee, J. Saravia, D. You, B. Shrestha, S. Jaligama, V. Hebert, T.R. Dugas

8:30 ENVR 97. Withdrawn.

8:50 ENVR 98. Temporal-spatial variations, sources, and transport of PM_{2.5} and associated trace metals in the Yangtze River Delta (YRD), China. L. Ming, J. Li, G. Zhang, X. Li

9:10 ENVR 99. Spatial variation of rainwater chemistry in Ile-Ife, Osun State, Nigeria. A.A. Okoya

9:30 ENVR 100. Chemical speciated components of atmospheric organic aerosol in the St. Louis Region, U.S. Y. Zhang, B. Williams, R. Martinez, D. Mitro, M. Walker, C. Oxford, X. Zuo, D. Hagan, J. Turner, L. Du, D. Millet, M. Baasandorj, L. Hu, R. Weber, L. King

9:50 Intermission.

10:05 ENVR 101. Oxidant production from source-oriented particulate matter: hydrogen peroxide and hydroxyl radical. N.K. Richards-Henderson, J.G. Charrier, K.J. Bein, A.S. Wexler, C. Anastasio

10:25 ENVR 102. Formation of biologically persistent free radicals (BPF_R) via reaction of nano metal oxide with a selected component of broncho-alveolar lavage fluid (BALF). A.N. Dela Cruz, S.M. Lomnicki

10:45 ENVR 103. Effect of black carbon nanoparticles on epithelial cell proliferation. N. Beebe, A.M. Johansen

11:05 ENVR 104. Main contributors to the diesel exhaust and wood smoke particles toxicity. Do we know them? A. Kubátová, R. Cochran, K. Ondrušová, J. Rousová, A.I. Totlandsdal, J. Øvrevik, P.E. Schwarze, M. Låg

11:25 ENVR 105. Determination of atmospheric organosulfates using HILIC chromatography with MS detection. E.A. Stone, A. Hettiyadura, S. Kundu, Z. Baker, E. Geddes, K. Richards, T. Humphry

11:45 ENVR 106. Particulate matter containing environmentally persistent free radicals induce aryl hydrocarbon receptor-dependent cytokine production in human bronchial epithelial cells. V. Hebert, S. Cormier, R. Reed, W. Backes, T.R. Dugas

† Cooperative Cosponsorship

Section C

Colorado Convention Center
Room 707

Chemical Processes at Environmental Interfaces**Chemistry at Aqueous/Mineral(Solid) Interfaces**

Cosponsored by COLL

H. A. Al - Abadleh, H. M. Ali, R. Z. Hinrichs, *Organizers*
N. Kabengi, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ENVR 107. Structure, dynamics, and reactivity of the interface between aqueous solutions and mineral surfaces. D. Wesolowski, A.G. Stack, H. Wang

8:40 ENVR 108. Integrated approach to study surface reactions using spectroscopy and calorimetry. M. Chrysochoou, N. Kabengi

9:10 ENVR 109. Speciation dynamics of metal at biochar-soil interface: Effects of biochar and soil properties. R. Huang, Y. Tang

9:30 ENVR 110. Zinc interaction with struvite during and after mineralization from phosphorus-rich sources. A. Rouff, K. Juarez

9:50 Intermission.

10:10 ENVR 111. Adsorption of Cr(VI), Cd(II), and Pb(II) on nanomagnetite and maghemite-coated silica. C. Koretsky, M. Komarek, D. Alessi, K. Stephen, A. Troy

10:40 ENVR 112. DFT calculations in support of XANES and NMR studies of Cd and Pb on gibbsite and kaolinite. J.D. Kubicki, H. Watts, E. Powelleit, K.T. Mueller, N. Govind, P. ODay, M. Small

11:10 ENVR 113. Development of DFT methods to aid in NMR data interpretation for Cd(II) adsorbed to clay minerals. H.D. Watts, E.T. Powelleit, K.T. Mueller, J.D. Kubicki

11:30 ENVR 114. Exploring nano shape effects on reactivity in Keggin-type aluminum hydroxide clusters through DFT studies. K.W. Corum, S.E. Mason

11:50 ENVR 115. Surface chemistry enhanced microbial electrodes: Biofilm modeling and characterization. J.A. Cornejo, K. Artyushkova, C. Santoro, S. Babanova, L.K. Ista, A.J. Schuler, P.B. Antonov

Section D

Colorado Convention Center
Room 709

Hydraulic Fracturing Impacts on Water, Soil and Air Quality**Groundwater Impacts**

Cosponsored by MPPG†

R. Jackson, R. D. Vidic, *Organizers*
J. Blotvogel, T. Borch, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 116. Approaches for groundwater monitoring for shale gas impacts: Concepts and field examples. B. Parker, J. Chery, A. Cahill

8:35 ENVR 117. Controls on methane occurrences in aquifers in the footprint of Texas shale plays. J. Nicot, P. Mickler, T.E. Larson, M. Castro, Z. Hildenbrand, R. Darvari, K. Uhlman, R.C. Smyth, L. Bouvier, B.R. Scanlon

9:00 ENVR 118. Simulating mobility and degradation of chemical contaminants from unconventional gas development. C. Kanno, D. Edlin, T. Borrillo-Hutter, J.E. McCray

9:25 ENVR 119. Fate of hydraulic fracturing chemicals in agricultural topsoil. M. McLaughlin, T. Borch, J. Blotvogel

9:50 Intermission.

10:05 ENVR 120. Trace levels of diesel range organic compounds in shallow groundwater wells in northeastern Pennsylvania elevated near Marcellus shale gas wells. B. Drollette, K. Schreglmann, N. Warner, T.H. Darrah, M.P. O'Connor, O. Karatum, R. Nelson, M. Elsner, C.M. Reddy, A. Vengosh, R. Jackson, D.L. Plata

10:30 ENVR 121. Toxicity and fate of the chemicals of matrix acidization, an unconventional oil stimulation technique. K. Abdullah, J. Taylor, I. Suffet

10:55 ENVR 122. Fate and transport of four organic compounds frequently used in hydraulic fracturing fluids in laboratory columns containing aquifer sediments. J.D. Rogers, S.G. Osborn, J.N. Ryan

11:20 ENVR 123. WII4HF: A conceptual model for computing water impact index for hydraulic fracturing. R. Kandiah, K. Nedunuri, X. Wei, N. Zhang, M.G. Smith

Section E

Colorado Convention Center
Room 711

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment**Use of Mass Spectrometry and Other Methods to Characterize NOM in Diverse Environments**

Cosponsored by ANYL and MPPG

G. Aiken, K. Cawley, *Organizers*
J. A. Korak, F. L. Rosario, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 124. From molecular analyses to remote sensing: Characterization of dissolved organic matter in the Gulf of Maine. G. Aiken, X. Cao, J. Mao, K. Schmidt-Rohr, R. Spencer, S. Belanger, W. Balch, T. Huntington

8:35 ENVR 125. Ultrahigh resolution mass spectrometry study of sea spray aerosol water soluble and water insoluble organic matter composition. A.S. Wozniak, A.S. Willoughby, S.D. McElhenie, P.K. Quinn, D.J. Coffman, P. Hatcher

9:00 ENVR 126. Using Fourier transform ion cyclotron resonance mass spectrometry to identify potential disinfection byproduct precursors in leaf litter leachate. G. McKee, C.C. Rhoades, T. Borch

9:25 ENVR 127. Meta-metabolomics as a systems-level tool for examining shifts in organic matter composition driven by environmental change. C.M. Boot

9:50 ENVR 128. Halogenated moieties incorporated into humic acid as a result of oxidation of tetrahalobisphenol A and their characterization using a TMAH-pyrolysis-GC/MS. R. Kodama, T. Miyamoto, Q. Zhu, M. Igarashi, M. Fukushima

10:15 Intermission.

10:30 ENVR 129. Antarctic ice-locked reservoirs of organic matter: Probing the bulk and molecular level chemical nature of organic matter by fluorescence spectroscopy and mass spectrometry. J. D'Andrilli, C.M. Foreman, H.J. Smith

10:55 ENVR 130. Transformations in autochthonous DOM: An Antarctic supraglacial case study. H.J. Smith, M.L. Wei-Haas, M. SanClements, J. D'Andrilli, C.M. Foreman, Y. Chin, D. McKnight

11:20 ENVR 131. Patterns in DOC absorbance with photodegradation and microbial processing in tundra watersheds in the Kolyma River Basin. M. Behnke, J. Schade, K. Whittinghill, N. Zimov

11:45 ENVR 132. DOC variability and characteristics in alpine watersheds. K. Dee, J.F. Ranville, K. Walton-Day, K.S. Smith

MONDAY AFTERNOON**Section A**

Colorado Convention Center
Room 703

Dispersion of Nanoparticles and its Implication for Interfacial, Biological and Environmental Processes**Interface and Transport**

N. B. Saleh, B. Xing, *Organizers*
B. Pan, P. J. Vikesland, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 133. Interaction between graphene oxide and minerals in aqueous phase. J. Zhao, Z. Wang, B. Xing

2:10 ENVR 134. Natural organic matter's influence on pollutant toxicity: An interface point of view. R.D. Williams, C.L. Schneider, L.M. Ojwang, R.L. Cook

2:45 ENVR 135. Effect of extracellular polymeric substances on the fate and transformation of engineered nanomaterials. A.S. Adeleye, A.A. Keller

3:05 ENVR 136. Measuring iron particle formation in seawater through advances in spICP-MS. B.T. Cartledge, E.K. Cutler, K.E. Whitworth, B. Majestic

3:25 Intermission.

3:45 ENVR 137. Heteroaggregation of carboxylated multiwalled carbon nanotubes (COOH-MWCNTs) and kaolinite in aquatic systems and their cotransport behavior in porous media. T. Wang, P. Coogan, Q. Li

4:05 ENVR 138. Promoted dispersion of cerium oxide nanoparticles from Fe²⁺-induced redox reactions at the nanoparticle surface. Y. Jun, J.R. Ray, X. Liu, C.W. Neil, Q. Li

4:25 ENVR 139. Elucidating critical roles of light and electron acceptors during aqueous colloidal C₆₀(nC₆₀) formation. J. Wu, A. Montoya, W. Li, J. Fortner

4:45 ENVR 140. Controlled evaluation of copper-based nanomaterial dissolution kinetics. R.D. Kent, P.J. Vikesland

Section B

Colorado Convention Center
Room 705

Chemistry in the Marine Boundary Layer

Cosponsored by MPPG

J. Donaldson, *Organizer*
B. D'Anna, *Organizer, Presiding*

1:30 ENVR 141. Ocean-atmosphere interaction and marine multiphase chemistry. H. Herrmann, M. van Pinxteren, D. van Pinxteren, K. Müller, W. Fomba, P. Brüner

1:55 ENVR 142. Impact of biological activity in the sea surface microlayer on sea spray aerosol and cold cloud formation. J.Y. Aller, P. Alpert, W.P. Kilthau, D. Bothe, T.W. Wilson, B. Murray, D.A. Knopf

2:15 ENVR 143. Sea spray organic matter and virus-induced plankton dynamic. M. Facchini, C.D. O'Dowd, R. Danovaro

2:35 ENVR 144. Surface-atmosphere exchange of ammonia in the summertime Canadian Arctic marine boundary layer. G. Wentworth, J. Murphy, J. Tremblay, J. Gagnon, J. Côté, I. Courchesne

2:55 Intermission.

3:05 ENVR 145. Bringing the ocean into the laboratory for detailed studies on sea spray aerosols. K.A. Prather

3:30 ENVR 146. Impact of air-sea exchanges on the Mediterranean marine boundary layer composition. N. Marchand, J. Pey, H.L. Dewitt, B. Temime-Roussel, S. Hellebust, A. Mème, B. Rmili, B. Charrière, R. Sempéré, S. Mas, D. Parin, J. Cerro, N. Perez, C. Rose, A. Schwier, M. Elser, S. Szidat, A.S. Prévôt, K. Sellegri, B. D'Anna

3:50 ENVR 147. Size-resolved sea spray aerosol particles studied by vibrational sum frequency generation. F. Geiger

4:10 Intermission.

4:20 ENVR 148. Sunlight-driven photochemical halogenation of dissolved organic matter in seawater: A natural abiotic source of organobromine and organiodine. J.J. Pignatello, J. Méndez-Díaz, K. Shimabuku, J. Ma, Z.O. Enumah, W. Mitch, M.C. Dodd

4:45 ENVR 149. Simulation of the photochemical heterogeneous activation of halogens (Cl and Br) from salt pans and salt aerosol in chamber experiments. C. Zetzsch

5:05 ENVR 150. On the reaction of CH₃O₂ radicals with OH radicals and its impact on the MBL. C. Fittschen

5:25 ENVR 151. Impact of organosulfur compounds at the marine/urban interface in a decreasing SO₂ world. V. Perraud, S. Meinardi, D.R. Blake, J. Horne, M. Dawson, A. Martinez, D. Dabduj, J. Kalinowski, R.B. Gerber, B.J. Finlayson Pitts

Section C

Colorado Convention Center
Room 707

Solutions to Metals Contamination of Water

Cosponsored by MPPG†

S. Ahuja, J. W. Finley, J. N. Seiber, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 152. Notable solutions to water contamination. S. Ahuja

2:00 ENVR 153. Arsenic removal technology for drinking water for developing countries. S. Chaudhari, T. Banerji

2:25 ENVR 154. Quantification of arsenic and uranium in unregulated water sources on the Navajo and Hopi reservations. J. Credo, E.R. Peaches, T. Rock, S.B. Garcia, J.C. Ingram

2:50 ENVR 155. Feasibility study of iron oxide nanoparticles prepared by different synthetic methods for arsenic removal. N.I. Gonzalez Pech, C. Avendano, G. Escalera, A. Bohliou, V.L. Colvin

3:15 Intermission.

3:30 ENVR 156. Influence of acid-base properties of zinc oxide nanomaterials on their arsenic uptake capacity. E. Rukundo, A. Applebitt

3:55 ENVR 157. Extraction, recovery, and identification of inorganic contaminants from water. R.E. Del Sesto, A. Newsham, M. Jones, B.H. Barton, A.T. Koppisch, D. Fox

4:20 ENVR 158. Optimizing the treatment performance of graphene oxide-based hydrogels. T.A. Duster, L.F. Greenlee

4:45 ENVR 159. Removal of heavy metals with steel furnace slag. B. Mercado-Borrayo, R. Contreras, A. Sánchez, X. Font, R. Schouwenaars, R. Ramirez-Zamora

Section D

Colorado Convention Center
Room 709

Hydraulic Fracturing Impacts on Water, Soil and Air Quality**Surface Water Impacts/Fluid Chemistry**

Cosponsored by MPPG†

J. Blotvogel, T. Borch, *Organizers*
R. Jackson, R. D. Vidic, *Organizers, Presiding*

1:30 ENVR 160. Water quality challenges associated with energy resource extraction from Marcellus Shale. R.D. Vidic

2:00 ENVR 161. Appropriation of fresh water for shale gas development in Pennsylvania's Marcellus Shale. J. Saier, E. Barth-Natilan

2:25 ENVR 162. Transformation kinetics and pathways of hydraulic fracturing biocides under downhole conditions: Focus on glutaraldehyde. G. Kahrilas, J. Blotvogel, T. Borch

2:50 ENVR 163. Exploring the potential for rare earth elements as geochemical fingerprints of salinity sources. A. Karamalidis, C.W. Noack, D.A. Dzombak

3:15 Intermission.

3:25 ENVR 164. Analysis of hydraulic fracturing flowback and produced waters using accurate mass: Identification of ethoxylated surfactants. E. Thurman, I. Ferrer, J. Blotvogel, T. Borch

3:55 ENVR 165. Endocrine disrupting activity of hydraulic fracturing chemicals and health outcomes following prenatal exposure in mice. C. Kassois, C. Lin, D.E. Tillitt, S.C. Nagel

4:20 ENVR 166. Contaminant mobilization via reactions between Marcellus shale and synthetic fracturing fluids. W.D. Burgos, T. Tasket

4:45 ENVR 167. Ultrahigh resolution mass spectrometry of hydraulic fracturing produced waters. L. Jenna, M. Gonsior, P. Schmitt-Kopplin, J. Batista

5:10 ENVR 168. Molecular-level characterization of water-soluble organic species from eagle ford shale oil by ultrahigh resolution ft-icr mass spectrometry. A.M. McKenna, D.C. Podgorski, H. Chen, L.C. Krajewski, Y. Corilo

Section E

Colorado Convention Center
Room 711

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment**Extraction Techniques to Isolate NOM and Characterization of Pyrogenic Organic Matter (Biomass Burning)**

Cosponsored by ANYL and MPPG

J. A. Korak, F. L. Rosario, *Organizers*
G. Aiken, K. Cawley, *Organizers, Presiding*

1:30 ENVR 169. Solid phase extraction of organic matter, past to present: A review of isolation mechanisms from XAD to today's sorbents. E.M. Thurman, I. Ferrer

2:00 ENVR 170. Characterization of soil organic matter (SOM) using online supercritical fluid extraction (SCFE) techniques coupled with liquid chromatography-ultrahigh resolution mass spectrometry (LC-UHR MS). K.M. Roscioli, Y. Shen, R. Zhao, T. Fillmore, N. Tolic, M. Tfaily, B. Anderson, N.J. Hess, L. Paša-Tolić, E.W. Robinson

2:25 ENVR 171. New solvent methods for molecular characterization of SOM by high resolution spectrometry. M.M. Tfaily, R. Chu, N. Tolic, K.M. Roscioli, L. Paša-Tolić, E.W. Robinson, N.J. Hess

2:50 ENVR 172. Effects of chemical treatments on soil organic matter composition identified by DRIFT, NMR and py-MBMS characterization. F.J. Calderón, A.J. Margenot, K.A. Magrini, R.J. Evans

3:15 Intermission.

3:30 ENVR 173. Structural interrogation of dissolved organic matter and pyrogenic black carbon and molecular characterization by ultrahigh resolution FT-ICR mass spectrometry. A.M. McKenna, D.C. Podgorski, Y. Corilo, W.T. Cooper, D.F. Smith, N.K. Kaiser

3:55 ENVR 174. Speciation of organics in aged atmospheric particles from a biomass burning event: Relationship to light absorption and comparison to humic acids. R.A. Di Lorenzo, K.J. Jobst, X. Ortiz, C.J. Young

4:20 ENVR 175. Comparative analysis of wood stove smoke. V.M. Porden

4:45 ENVR 176. Characterization and concentration of water soluble organic matter (WSOM) and inorganic constituents from wildfire impacted stream bank material. K. Cawley, A.K. Hohner, P. Omur-Ozbek, R. Summers, F.L. Rosario

MONDAY EVENING**Section A**

Colorado Convention Center
Halls C/D

Sci-Mix

S. R. Al-Abed, *Organizer*

8:00 - 10:00

ENVR 177. Profile of metal bioaccumulation in selected invertebrates from the eastern and western shores of the Susquehanna River near Hummels Wharf Pennsylvania. A. Pritzlaff, C.P. Hallen, C. Venn

ENVR 178. Organic matter and nitrogen removal within field-scale constructed wetlands: Reduction performance and microbial identification studies. T. Yeh
203, 210, 336, 351, 360, 362-363, 366, 370-371, 374, 377, 379, 381, 383, 386, 388-389, 394, 396, 400-401, 403, 407, 414-415, 417, 419, 422, 430-431, 438, 443, 446-447, 450-451, 454, 460. See subsequent listings.

TUESDAY MORNING**Section A**

Colorado Convention Center
Mile High Ballroom 4D

Dispersion of Nanoparticles and its Implication for Interfacial, Biological and Environmental Processes**Sorption and Dispersion**

B. Pan, N. B. Saleh, P. J. Vikesland, *Organizers*
B. Xing, *Organizer, Presiding*
R. L. Cook, *Presiding*

8:00 ENVR 179. Toward a mechanistic understanding of the effect of natural organic matter coatings on nanoparticle aggregation. G.V. Lowry, S. Louie, E.R. Spielman-Sun, R.D. Tilton

8:35 ENVR 180. Coadsorption, desorption hysteresis, and sorption thermodynamics of sulfamethoxazole and carbamazepine on graphene oxide and graphite. B. Pan, C. Wang, H. Li, B. Xing

9:10 ENVR 181. Arsenic adsorption in highly dispersed conductive TiO₂-CNT nanosystems: Enhanced sorption behavior due to mass transport, electro-sorption, and adsorbent dispersion. H. Liu, K. Zuo, C.D. Vecitis

9:30 ENVR 182. Role of air bubbles overlooked in the adsorption of perfluorooctane sulfonate on carbon nanotubes. S. Deng, P. Meng, B. Xing

9:50 Intermission.

10:10 ENVR 183. Influence of humic acid on the dispersion and transport of nTiO₂ particles in water-saturated porous media. Y. Wu, T. Cheng

10:30 ENVR 184. Surface engineering magnetic nanoparticles for aqueous applications: Design and characterization of tailored organic bilayer. W. Li, C.H. Hinton, S. Lee, J. Wu, Y. Jiang, J.D. Fortner

10:50 ENVR 185. Disruption of quorum sensing by adsorption of acyl-homoserine lactone to engineered nanomaterials. K.B. Gregory, J.M. Vanbriesen, E. McGivney

11:10 ENVR 186. Synthesis and characterization of anion exchange resin coated SWCNTs for dissolved organic content removal. J.C. Poler, B. Johnson, Y.J. Baik, R. Furst

Section B

Colorado Convention Center
Room 705

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Cosponsored by AGRO, ANYL and MPPG

D. Alvarez, *Organizer*
T. L. Jones-Lepp, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 187. New environmental monitoring framework for contaminants of emerging concern (CECs). K.A. Maruya, N.G. Dodder, A.C. Mehinto

8:55 ENVR 188. Microplastics emerging contaminants: a new source of toxic compounds. L.M. Rios Mendoza, E. Soto

9:15 ENVR 189. Naphthenic acid analysis using differential mobility spectrometry coupled with accurate mass time of flight mass spectrometry. P. Winkler, L. Campbell, T. Sakuma, A. Schreiber, K. Peru, J. Headley

9:35 ENVR 190. Quantification and risk assessment of emerging organic contaminants in Ikpa River basin, Niger Delta, Nigeria. N.O. Ofiong, E. Inam, J. Essien, S. Kang, G. Udofia, B. Antia, S. Kang, P. Yang

9:55 Intermission.

10:15 ENVR 191. Using a novel photo-micro-reactor to remove benzoylcegonine in wastewater treatment: Uncovering phototransformation products and the reaction pathways with advanced mass spectrometry tools. S.D. Richardson, K.H. Cochran, M. Vaccaro, D. Russo, D. Spasiano, R. Marotta, R. Andreozzi, N.M. Reis, G. Li Puma

10:35 ENVR 192. Novel methods for sampling perfluorinated acids in the atmosphere. J.J. MacInnis, T.C. Vandenboer, C. Young

10:55 ENVR 193. Adsorption and desorption of pharmaceuticals by bluegill exposed at constant concentrations in a flow-through aquatic exposure system. J. Zhao, E.T. Furlong, D.W. Kolpin, E.A. Schwab, D.J. Feiterek, K.L. Bird, H. Schoenfuss, G. Ying

11:15 ENVR 194. Presence of UV filters (sunscreens) in marine surface waters of bays within the Virgin Islands National Park. D. Alvarez, T. Bargar

11:35 ENVR 195. Using 5-hydroxyindoleacetic acid as an anthropogenic population biomarker in wastewater treatment plant influent. D.A. Burgard, H. Fryhle, M.C. Pellman

Section C

Colorado Convention Center
Room 707

Solutions to Metals Contamination of Water

Cosponsored by MPPG†

S. Ahuja, J. W. Finley, J. N. Seiber, *Organizers, Presiding*

8:30 ENVR 196. Immobilization of mercury by stabilized iron sulfide nanoparticles: Reaction mechanisms and effects of stabilizer. D. Zhao, Y. Gong, Y. Liu, Z. Xiong

8:55 ENVR 197. Solar UV photooxidation as pretreatment for stripping voltammetric trace metal analysis in river water. G. Flechsig, G. Woldemichael

9:20 ENVR 198. Lignin-coated magnetic nanoparticles for mercury adsorption. L. Peña Duque, N. Robitaille Brown

9:45 ENVR 199. Mercury uptake by oysters in the New York Harbor indicates early success of novel approach to water restoration. E. Park

10:10 Intermission.

10:25 ENVR 200. Binding of inorganic mercury in surface water to DOM and alum flocs: How much removal can we get? F.A. Diaz, L.E. Katz, D.F. Lawler

10:50 ENVR 201. Utilization of fruit juice with high vitamin C content for the remediation of wastewater contaminated with chromium (VI). Y.S. Mendoza, J.R. Pinzón

11:15 ENVR 202. Efficient and robust removal of chromium using engineered metal-reducing biofilms. Y. Ding, B. Cao

11:40 ENVR 203. Adsorption of Cs, Sr, and Co by mesoporous materials. K. Guo, F.X. Han, Z. Arslan, H. Yu

Section D

Colorado Convention Center
Room 709

Hydraulic Fracturing Impacts on Water, Soil and Air Quality**Air & Water Quality**

Cosponsored by MPPG†

R. Jackson, R. D. Vidic, *Organizers*
J. Blotvogel, T. Borch, *Organizers, Presiding*

8:00 ENVR 204. Characterizing air quality impacts of oil and gas development in the Bakken formation region. J.L. Collett, A. Evanoski-Cole, A. Prenni, D. Day, A. Sullivan, Y. Li, B.C. Sive, Y. Zhou, J. Hand, K. Gebhart, M. Schurman, B. Schichtel

8:30 ENVR 205. Observations of acyl peroxy nitrates (PANs) during the Front Range Air Pollution and Photochemistry Experiment (FRAPPE) field campaign. J. Zaragoza, E.V. Fischer, E.E. McDuffie, W.P. Dubé, S.S. Brown, D.K. Farmer, F.M. Flocke

8:55 ENVR 206. Locating, quantifying, and attributing methane emissions from fossil-fuel extraction. E. Kort, M. Smith, A. Gvakharia, C. Sweeney, A. Karion, J. Peischl, T.B. Ryerson, C. Frankenberg, M. Dubey

9:20 Intermission.

9:35 ENVR 207. Influence of salinity, concentration, and redox on the biodegradability of organic additives in hydraulic fracturing fluids. P. Mouser

10:05 ENVR 208. Disinfection by-products formed during the treatment of produced waters at wastewater treatment plants. M.L. Hladik, M. Focazio

10:30 ENVR 209. Produced water exposure from hydraulic fracturing alters bacterial response to biocides. A. Vikram, D. Lipus, K. Bibby

10:55 ENVR 210. Anaerobic biodegradation of polypropylene glycols within hydraulic fracturing fluid. K.M. Heyob, J. Blotvogel, T. Borch, P.J. Mouser

11:20 ENVR 211. Feasibility of reusing brine recovered from the produced for drilling mud formulation. N. Cely

Section E

Colorado Convention Center
Room 711

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment**NMR and Photochemical Analysis of NOM**

Cosponsored by ANYL and MPPG

J. A. Korak, F. L. Rosario, *Organizers*
G. Aiken, K. Cawley, *Organizers, Presiding*

8:00 ENVR 212. Combined mass spectrometry - NMR spectroscopy approach for characterizing organic phosphorus in treatment of wetlands. W.T. Cooper, L. Skiba, C. Stulz, S. Newman

8:30 ENVR 213. New forms of dissolved organic nitrogen identified by multibond 2D NMR spectroscopy. X. Cao, M.R. Mulholland, P.W. Bernhardt, J. Helms, J. Mao, K. Schmidt-Rohr, Z. Zhou

8:55 ENVR 214. Composition and structure of natural organic matter isolated by reverse osmosis and ultrafiltration. Y. Ran, W. Huang, X. Cao, J. Mao

9:20 Intermission.

9:35 ENVR 215. Further insights on the chemical structure of humic substances (HS) and chromophoric dissolved organic matter (CDOM) in relation to their optical/chemical properties. R. Del Vecchio, T. Schendorf, N.V. Blough

10:00 ENVR 216. pH effects on DOM photodegradation using semi-continuous fluorescence excitation emission matrices. S. Timko, M. Gonsior, W.J. Cooper

10:25 ENVR 217. Temperature dependence of the photochemical formation of hydroxyl radical from dissolved organic matter. G. McKay, F.L. Rosario

10:50 ENVR 218. Comparing triplet reaction mechanisms for DOM characterization. A. Maizel, W. Kamp, C.K. Remucal

11:15 ENVR 219. Dynamic light scattering and zeta potential investigation of fulvic and humic acid reversible self-assembly in low electrolytic conductivity solutions. M.J. Wells, M.R. Eshfahani, H.A. Stretz

11:40 ENVR 220. Assessment of novel natural organic matter characterization tools: Application to the drinking water industry. Y. Park, A. Stoddart, M. Brophy, W. Krkosek, G.A. Gagnon

TUESDAY AFTERNOON**Section A**

Colorado Convention Center
Room 703

Dispersion of Nanoparticles and its Implication for Interfacial, Biological and Environmental Processes**Benefit and Risk**

B. Pan, P. J. Vikesland, B. Xing, *Organizers*
N. B. Saleh, *Organizer, Presiding*
Z. Zhang, *Presiding*

1:30 ENVR 221. Interactions between plants and rare earth oxide nanoparticles.

Z. Zhang, Y. Ma, P. Zhang, X. He, Y. Zhao

† Cooperative Cosponsorship

2:05 ENVR 222. Bioaccumulation of ionic silver and silver nanoparticles within freshwater crayfish using inductively coupled plasma optical emission spectroscopy. **S.W. Brittle**, D.P. Foose, M.T. Ruis, M.T. Amato, S.A. Paluri, N.H. Lam, B. Buttigieg, Z.E. Gagnon, I.E. Pavel Sizemore

2:25 ENVR 223. Bioavailability of fullerene in the presence of environmentally relevant matrices: Effects of humic acid and fetal bovine serum (FBS) on the lipid accumulation and cellular uptake. **Y. Ha**, H. Liljestrand, L.E. Katz, J. Maynard

2:45 ENVR 224. Interaction strength of supported lipid bilayers with the underlying substrate influences the disruptive effect of engineered nanoparticles. **N. Yousefi**, A. Wargenau, N. Tufenkji

3:05 Intermission.

3:25 ENVR 225. Application of carbon nanotube yarn as a filter media to treat nitroaromatic-contaminated water. **S.R. Kanel**, B. Doane, H. Misak, S. Mall, S.W. Brittle, I.E. Pavel Sizemore, T. Ebrahimian, D. Kempisty, M.N. Goltz

3:45 ENVR 226. Engineered carbon nanoparticle tracers: Groundwater transport and implications for the migration of environmental nanoparticles. **C.N. King**, W.E. Sanford, Y.V. Li

4:05 ENVR 227. Probing photosensitization by functionalized carbon nanotubes in aquatic environments. **C. Chen**, R.G. Zepf

4:25 ENVR 228. Modification of zero-valent iron nanoparticles and its application for the decoloration of malachite green. **X. Wang**, J. He, L. Le

4:45 Concluding Remarks.

Section B

Colorado Convention Center
Room 705

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Cosponsored by AGRO, ANYL and MPPG

T. L. Jones-Lepp, *Organizer*
D. Alvarez, *Organizer, Presiding*

1:30 ENVR 229. Spatial and temporal variability of excitation emission matrix (EEM) fluorescence spectra in a wastewater effluent impacted river. **M.J. Wells**, G.A. Mullins, K.Y. Bell, A.K. Da Silva, E.M. Navarrete

1:50 ENVR 230. Application of field portable PLOT-cryo-adsorption headspace sampling apparatus for detection of diesel fuel in soil. **S. Bukovsky-Reyes**, T. Bruno, M. Harries

2:10 ENVR 231. Analysis of complex environmental samples by 2D-GC combined with high-resolution mass spectrometry. **A. Dane**, M. Ubukata, R.B. Cody

2:30 ENVR 232. Detection, quantification, and partitioning property estimation of bioaccumulative pollutants in aquatic environments using GCxGC-ENCI-TOFMS and GCxGC-ECD. **J.S. Arey**, S. Samanipour, P. Dimitriou-Christidis, D. Nabi, J. Gros

2:50 Intermission.

3:10 ENVR 233. Determination of perchlorate in polar ice cores down to sub-ng L⁻¹ level using ion chromatography-tandem mass spectrometry. **K.M. Peterson**, J. Cole-Dai, D. Brandis, T. Cox, S. Splett

3:30 ENVR 234. Periodic table of elements for the water heavy metal monitoring on paper. **M. Li**, R. Cao, A. Nilghaz, L. Guan, W. Shen

3:50 ENVR 235. Hydroxyl radical generation on graphite and modified graphite surfaces for AOPs: An EPR investigation. **M.A. Morsy**, A.M. Kawde, M.A. Daous, T.A. Saleh

4:10 ENVR 236. Identifying trace environmental contaminant in CO₂ capture solvents from coal-fired power plants using ICP-MS and high resolution time-of-flight mass spectrometry (TOF-MS). **J.G. Thompson**, Q. Huang, K. Liu

4:30 Concluding Remarks.

Section C

Colorado Convention Center
Room 707

Solutions to Metals Contamination of Water

Cosponsored by MPPG†

S. Ahuja, J. W. Finley, J. N. Seiber, *Organizers, Presiding*

1:30 ENVR 237. Efficient and versatile carbon-based nanocomposite for the adsorption of heavy metal ions from aqueous environments. **A.B. Dichiara**, M.R. Webber, R.E. Rogers

1:55 ENVR 238. Effects of the presence of oxyanions during birnessite synthesis on birnessite particle sizes and application for removal of lead. **Q. Wang**, X. Liao, M. Zhu

2:20 ENVR 239. Engineered superparamagnetic iron oxide nanoparticles for uranyl separation in water. **W. Li**, S. Lee, C.H. Hinton, J. Wu, J.D. Fortner

2:45 ENVR 240. Cr(VI) removal using magnetite-non oxidative graphene composite as a new sorbent: A comparative study with magnetite-graphene oxide and magnetite-reduced graphene oxide. **M. Zheng**, Y. Yoon, W. Park, W. Yang, J. Kang

3:10 Intermission.

3:25 ENVR 241. Double-stranded DNA encased single-walled carbon nanotubes for optical sensing of cupric ions. **B. Ergul**, W. Zhao

3:50 ENVR 242. Speciation behavior of transition and rare earth metal binding by monorhamnolipids. **R. Eismn**, R.M. Maier, J.E. Pemberton

4:15 ENVR 243. Water purification through graphene oxide-insoluble salt composite membranes. **D. Wang**, W. Zhao

4:40 Concluding Remarks.

Section D

Colorado Convention Center
Room 709

Hydraulic Fracturing Impacts on Water, Soil and Air Quality

Treatment and Regulations

Cosponsored by MPPG†

J. Blotvogel, T. Borch, *Organizers*
R. Jackson, R. D. Vidic, *Organizers, Presiding*

1:30 ENVR 244. Origin of radioactivity in Marcellus Shale flowback water and potential concerns with radioactivity in wastes generated by unconventional gas industry. **T. Zhang**, R.D. Vidic

1:55 ENVR 245. Advanced treatment for water-recycling: Characterization and pretreatment of the particulate foulants for microfiltration in flowback and produced water from Marcellus shale gas play. **B. Xiong**, M. Kumar, A.L. Zydney

2:20 ENVR 246. Composition and associated hazards of well stimulation fluids used in California (USA). **W. Stringfellow**, T. McKone, W. Sandelin, R. Maddalena, M. Heberger, C. Varadharajan, P. Jordan, J. Domen, H. Cooley, M. Reagan, R. Tinnacher, M. Camarillo, J. Houseworth, J. Birkholzer

2:50 ENVR 247. Identifying gaps in hydraulic fracturing wastewater management practices across four North American basins. **D.S. Alessi**, C.A. Notte, D. Thompson, S. Kletke, J. Brisbois, D.M. Allen, J. Gehman, G.G. Goss

3:15 ENVR 248. Characterization and analysis of liquid waste from Marcellus Shale gas development. **J. Shih**, J. Sakers, S.C. Anisfeld, J. Chu, L. Muehlenbachs, S. Olmstead, **A. Krupnick**

3:40 Intermission.

3:55 ENVR 249. Perspectives on hydraulic fracturing in Atlantic Canada: Overview of recent regulatory activities and social license to operate with an environmental context. **G.A. Gagnon**, W. Krkosek, B. Trueman, L. Anderson

4:20 ENVR 250. Examining memorandums of understanding as a policy solution for hydraulic fracturing in Colorado. **S. Zilliox**, A. Shaffer, J.S. Rolston

4:45 ENVR 251. Managing the risks of shale gas development using innovative legal and regulatory approaches. **S. Olmstead**, N. Richardson

5:10 Concluding Remarks.

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 703

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Cosponsored by CEI and MPPG†

T. Y. Cath, K. Linden, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 252. Chemicals used for matrix acidization, an unconventional oil stimulation technique. **K. Abdullah**, M. Stenstrom, I. Suffet

8:30 ENVR 253. Water supply and unconventional energy development in the Denver-Julesburg basin: A case study in the South Platte watershed. **E. Walker**, A. Anderson, C. Barry, T.S. Hogue

8:55 ENVR 254. Feasibility of thermal technologies for reuse of oil and gas exploration and production wastewaters. **V. Gadhamshetty**, V. Gude

9:20 ENVR 255. Mechanically strong aerogel fabrics for oil capture and recovery. **O. Karatum**, S.A. Steiner III, D.L. Plata

9:45 ENVR 256. Application of AMD for produced water reuse: Equilibrium and kinetics of solid precipitation and solid waste management. **C. He**, R.D. Vidic

10:10 Intermission.

10:10 ENVR 257. Comparing electrocoagulation, dissolved air flotation, and traditional coagulation/flocculation as pretreatment for hydraulic fracturing wastewater. **K. Sitterley**, J. Rosenblum, K. Linden

10:35 ENVR 258. Removal mechanisms of boron during aluminum electrocoagulation of hydraulic fracturing flowback water. **S. Chellam**, M. Sari

11:00 ENVR 259. Coupling magnetic Pickering emulsions to membrane filtration for non-fouling oil/water separations. **D. Jassby**

11:25 ENVR 260. Engineered osmosis technology for desalination of oil and gas exploration wastewaters: Progressive assessment of membrane performance and process sustainability. **B.D. Coday**, T.Y. Cath

Section B

Colorado Convention Center
Room 705

Surface Physicochemical Processes in Engineered and Natural Systems

Cosponsored by AGRO and MPPG†

H. J. Zhang, *Organizer*
J. M. Cerrato, H. Liu, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 261. Multifunctional nanostructured composite materials for highly active reductive catalysis water treatment applications. **J. Liu**, X. Chen, Y. Wang, P. Wang, C.J. Werth, **T.J. Strathmann**

9:15 ENVR 262. Photocatalytic reductive treatment of hexavalent chromium using barium doped TiO₂. **M. Chen**, W. Wang, Y. Yin, H. Liu

9:35 ENVR 263. Transformation of hexavalent chromium via redox pathways in drinking water: Implications on Cr(VI) control and treatment. **H. Liu**, M. Chebeir, H. Sohn

9:55 ENVR 264. Hexavalent chromium removal by electrocoagulation in drinking water system. **C. Pan**, D. Giammar, M. Marni, J.G. Catalanò

10:15 ENVR 265. Effects of water hardness and humic substances on Cr(VI) removal from aqueous systems using pyrite as the reducing agent. **C. Kantar**, M.S. Bulbul

10:35 Intermission.

10:50 ENVR 266. Impact of hematite nanoparticle (no-Fe₂O₃) morphology and size on photocatalytic potential as exemplified by reduction of chromate. **A.W. Lounsbury**, J. Yamani, N. Billmyer, J.B. Zimmerman

11:10 ENVR 267. Functionalization of boron-doped diamond electrodes for the minimization of perchlorate formation during electrochemical advanced oxidation processes. **B.P. Chaplin**, W. Jawando, P. Gayen

11:30 ENVR 268. One-pot electrospinning/Fabrication of Pd-carbon nanofiber catalysts for contaminant hydrogenation. **T. Ye**, D. Shuai

11:50 ENVR 269. Visible-light-responsive graphitic carbon nitride for photocatalytic degradation of persistent waterborne contaminants. **Q. Zheng**, D. Shuai, N. Bensalah

Section C

Colorado Convention Center
Room 707

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment

Cosponsored by AGRO

D. Shuai, *Organizer*
B. P. Chaplin, W. Zhang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 ENVR 270. Green algae cultivation and engineering of its fatty acid synthase. **M.D. Burkart**

9:20 ENVR 271. Using a pH-stat to understand how the N source affects the concentration of inorganic carbon in microalgae culture. **B. Nguyen**, B.E. Rittmann

9:40 ENVR 272. Using carbon dioxide to maintain the abundance of the oleaginous microalgae *Scenedesmus dimorphus* in mixed-culture growth reactors. **M.J. Giannetto**, A. Retotar, H. Rismani Yazdi, J. Peccia

10:00 Intermission.

10:20 ENVR 273. Energy efficient urban wastewater treatment using *Galdieria sulphuraria*. **T. Selvaratnam**, N. Nagamany, L. Peter

10:40 ENVR 274. Novel shortcut nitrogen removal process by algal-bacterial consortia in a sequencing batch photobioreactor (SBPR). **M. Wang**, H. Yang, S. Ergas, P. van der Steen

11:00 ENVR 275. Role of filamentous cyanobacteria in granular biofilms containing microalgae and bacteria. **K. Stauch-White**, C. Kuo-Dahab, K. Millerstedt, C. Park, C. Butler

11:20 ENVR 276. Light and COD effects on the performance of photosynthetic microbial desalination cells. **B. Kokabian**, V. Gude

11:40 ENVR 277. Passive membrane photobioreactor for the isolated cultivation of algal resource utilizing selectivity (ICARUS) using wastewater as a feed stock. **I. Drexler**, M. Pickett, M. Heintz, D. Yeh

Section D

Colorado Convention Center
Room 709

Trace Materials in Air, Soil, and Water

Cosponsored by MPPG†

A. Rihana, *Organizer*
M. A. Benvenuto, K. R. Evans, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 278. Flame retardants in Chicago's atmosphere and sediment of the Chicago Sanitary and Ship Canal. **A. Peverly**, M. Venier, Y. Ma, Z. Rodenburg, K.C. Hornbuckle, R.A. Hites

8:55 ENVR 279. Are pink salt, blue salt, and other "healthy" salts worth their price? Their analysis by energy dispersive X-ray fluorescence spectrometry. **S. Maurice**, C. Roberts, C. Kashat, M.A. Benvenuto, E. Roberts-Kirchoff

9:15 ENVR 280. New insights into mercury speciation in freshwaters using mercury-thiourea complex ion chromatography with ICP-MS detection. **T.H. Huang**, O.A. Todd, R.J. Hudson

9:35 ENVR 281. Single extraction methodology for amino sugars as biomarkers in environmental matrices. T.C. Vandenboer, R. Hems, R. Di Lorenzo, S. Ziegler, C. Young
9:55 Intermission.

10:10 ENVR 282. Molecular sensing at graphene grain boundaries. P. Kral

10:30 ENVR 283. Iron analysis in aging water pipes using cloud point extraction method. Z. Li, A. Rihana, K.C. Lanigan

10:50 ENVR 284. Analyzing the correlation of volatile organic compounds with ozone formation in the Houston-Galveston-Brazoria area Using CAMx. M. Shahriar, A. Kadiyala, R.R. Kommalapati, Z. Huque

11:10 ENVR 285. Fate of oxyhalide disinfection by-products in hypochlorite solution storage tanks. A. Breytus, S. Prabakar, A.P. Kruzic

11:30 Concluding Remarks.

Section E

Colorado Convention Center
Room 711

Environmental Implications of Nano: Release from Consumer Products and Advances in Nanometrology

C. P. Higgins, J. F. Ranville, *Organizers*
R. B. Reed, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 286. Tracking nanomaterials through the laundry wash cycle: Release, dissolution, and complexation. D. Mitrano, B. Nowack

8:25 ENVR 287. Prospecting silicon dioxide in foods: Occurrence, characterization, and toxicity. Y. Yang, J. Faust, J. Schoepf, K. Hristovski, R.L. Tanguay, D.G. Capco, P. Herckes, P.K. Westerhoff

8:45 ENVR 288. Characterization of nanosilica release from a weathered nanosilica/polyurethane coating. L. Sung, S. Huang, Y. Cheng, D. Stanley, S. Rabb, P. Krommenhoek, L. Yu, T. Nguyen

9:05 ENVR 289. Evaluation of nanoparticle release from polymer nanocomposites loaded with fluorescent quantum dots. K. Pillai, P. Gray, C. Tien, R. Bleher, L. Sung, T.V. Duncan

9:25 ENVR 290. Influence of loading on the degradation and release of carbon nanotubes from polymer nanocomposites. H. Fairbrother, R. Lankone, D.G. Goodwin, E.J. Bouwer, J.F. Ranville, J. Wang

9:45 ENVR 291. Evaluation of silver nanoparticle-impregnated fabrics across their life cycle. R.B. Reed, J.F. Ranville, R.L. Tanguay, J.E. Hutchison, P.K. Westerhoff, T. Zaikova

10:05 Intermission.

10:20 ENVR 292. Engineered nanoparticles in the environment: From theory to practice. A.P. Gondikas, F. Von Der Kammer, R.B. Reed, R. Kaegi, T. Hofmann

10:40 ENVR 293. Single particle ICP-MS (SP-ICP-MS) for the detection of metal-based nanoparticles in environmental matrices. C. Stephan

11:00 ENVR 294. Development of novel methodology to quantify silver release from polymer nanocomposites. A. Barber, R. Lankone, J. Wang, H. Fairbrother, P.K. Westerhoff, J.F. Ranville

11:20 ENVR 295. Improvements in the detection and characterization of silica nanomaterials using spICP-MS. M.D. Montano, B. Majestic, J.F. Ranville

11:40 ENVR 296. Measuring nanocarbon fluxes by tracing stable isotope labelled nanomaterials. T.D. Berry, T.R. Filley

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by COLL, Cosponsored by CATL and ENVR

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 703

Water Sustainability in Oil and Gas

Exploration: Treatment Issues

Cosponsored by CEI and MPPG†

T. Y. Cath, K. Linden, *Organizers, Presiding*

1:30 ENVR 297. Removal of radium from shale gas wastewater using cation exchange resin. Y. Bi, H. Zhang, K.F. Hayes, B. Ellis

1:55 ENVR 298. Fate of radium in wastewater produced during unconventional gas extraction during carbonate precipitation reactions. Y. Li, R.D. Vidic

2:20 ENVR 299. Fate of NORM in flowback water and waste management strategies during water reuse for hydraulic fracturing in Marcellus Shale. T. Zhang, R.D. Vidic

2:45 ENVR 300. Biological treatment of flowback water from a hydraulically fractured well. J. Rosenblum, K. Sitterley, I. Morrissey, K. Linden

3:10 Intermission.

3:30 ENVR 301. Anammox biocathode for sustainable microbial desalination of brackish waters. B. Kokabian, V. Gude

3:55 ENVR 302. Microbial mats as a biological treatment approach for produced water from hydraulic fracturing. B. Akyon, E. Stachler, N. Wei, K. Bibby

4:20 ENVR 303. Microbial capacitive desalination for organic and salt removal and energy production from unconventional natural gas produced water. C. Forrestal, A. Haeger, L. Dankovich, Z. Ren

4:45 ENVR 304. Biological active filtration treatment of O&G flowback and produced waters. T.Y. Cath, D.E. Freedman, S.M. Riley

5:10 Concluding Remarks.

Section B

Colorado Convention Center
Room 705

Surface Physicochemical Processes in Engineered and Natural Systems

Cosponsored by AGRO and MPPG†

H. J. Zhang, *Organizer*

J. M. Cerrato, H. Liu, *Organizers, Presiding*

1:30 ENVR 305. Interactions and reactions of organic compounds at interfaces between water and pyrogenic carbonaceous materials. J.J. Pignatello

2:10 ENVR 306. Oxidative reactivity of MnO₂ in mixtures with Fe⁰ oxides and/or natural organic matter (NOM). H. Zhang, S. Taujale

2:30 ENVR 307. Oxidative degradation of trinitrotoluene by mixed metal oxide nanoparticles in water. G.S. Harbison, Y. Kye, M.A. Langell, M. Kumbier

2:50 ENVR 308. Adsorption and photocatalysis of ciprofloxacin using alumina-titania particles synthesized via sol-gel process. C. Dozier, L.E. Katz, H. Liljestrand

3:10 ENVR 309. Mechanistic comparison of isomeric oxorhenium(V) complexes coordinated with a oxazoline-phenolate ligand for highly active perchlorate reduction in water. J. Liu, D. Wu, S.Y. Kimura, J.R. Shapley, M.M. Abu-Omar, C.J. Werth, T.J. Strathmann

3:30 Intermission.

3:45 ENVR 310. Post-pyrolysis air oxidation of biochars: A simple and effective method for enhancing adsorption of ionizable organic compounds. F. Xiao, J.J. Pignatello

4:05 ENVR 311. Photoenhanced chlorination of hydroxylated fullerene (fullerol) in water. J. Wu, L. Alemany, D.N. Benoit, W. Li, J. Fortner

4:25 ENVR 312. Insight into anti-scaling mechanisms of phosphonates and organic polymers for the control of barium sulfate scales. C. He, R.D. Vidic

4:45 ENVR 313. Mesoporous silica supported bimetallic Pd/Fe nanocomposites for enhanced reductive dechlorination of tetrachloroethylene. R. Doong, C. Lee

Section C

Colorado Convention Center
Room 707

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment

Cosponsored by AGRO

B. P. Chaplin, *Organizer*

D. Shuai, W. Zhang, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 ENVR 314. Applications of polymer-coated magnetic nanoparticles for algal biomass harvesting. W. Zhang, S. Ge, M. Agbakpe

2:00 ENVR 315. Fluorescein induced spectral conversion for the growth of *Chlorella vulgaris*. Y. Orduz, J.R. Pinzón

2:20 ENVR 316. Direct visualization of nutrient consumption within microbial communities using NanoSIMS. C.R. Anderson, J.K. Cole, J.J. Moran, J.M. Mobberley, M. Hess, S.R. Lindemann, L. Paša-Tolić

2:40 ENVR 317. Photogeneration of reactive oxygen species (ROS) by extracellular organic matter (EOM) in *Chlamydomonas reinhardtii* photobioreactor cultures. R. Tenorio, T.J. Strathmann

3:00 Intermission.

3:20 ENVR 318. Predicting microalgae hydrothermal liquefaction biocrude oil yield and properties from microalgae biochemical composition. S. Leow, J.R. Witter, D.R. Vardon, B.K. Sharma, J.S. Guest, T.J. Strathmann

3:40 ENVR 319. Coupling fluid dynamics with kinetic modeling to quantify the effects of photosynthetic bioreactor design and operation on yield performance. R. Manavi, S. Yamamoto, J.W. Lewis, J. Ducoste, F. De Los Reyes, R. Ranjithan

4:00 ENVR 320. Life cycle-optimization framework for photosynthetic biorefineries. R. Manavi, A. Karam, C. McMillan, J.W. Lewis, F. De Los Reyes, J. Ducoste, R. Ranjithan

4:20 ENVR 321. Environmental and economic performance analysis of three techniques for breaking microalgae cell wall in the biodiesel production process. M. Colotta, R. Lee, A. Ramos, P. Champagne, P.G. Jessop, W. Mabee

Section D

Colorado Convention Center
Room 709

Trace Materials in Air, Soil, and Water

Cosponsored by MPPG†

K. R. Evans, *Organizer*

M. A. Benvenuto, A. Rihana, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 322. Elemental characterization of PM_{2.5} and PM₁₀ emitted from light duty vehicles in the Washburn Tunnel of Houston, Texas: Release of rhodium, palladium, and platinum. S. Chellam, A. Bozlaker, N. Spada, M. Fraser

1:55 ENVR 323. Synthesis of a series of highly multi-dentate podand ligands as possible water remediation agents. C. Kashat, M.A. Benvenuto

2:15 ENVR 324. Metal concentrations and soluble iron speciation in fine particulate matter from light rail activity in the Denver-Metropolitan area. B.T. Cartledge, B. Majestic

2:35 ENVR 325. Nontoxic, air stable quantum dots for low level metal detection in water. H. Meyelemans, L. Cambrea

2:55 Intermission.

3:10 ENVR 326. Stable isotopes of lead and strontium as tracers of sources of airborne particulate matter in Kyrgyzstan. N. Dewan, B.J. Majestic, M.E. Ketterer, J.P. Miller-Schulze, M.M. Shafer, J.J. Schauer, P.A. Solomon, M. Artamonova, B.B. Chen, S.A. Imashev, G.R. Carmichael

3:30 ENVR 327. Monitoring metal contamination from artisanal and small-scale gold mining (ASGM) communities in Ecuador Part I: Mercury emissions to air. A.M. Kiefer, C.S. Seney

3:50 ENVR 328. Monitoring metal contamination from artisanal and small-scale gold mining (ASGM) communities in Ecuador Part II: Analysis of water, soil, and tailings. C.S. Seney, A.M. Kiefer, J.D. Mims

4:10 ENVR 329. New diffusive gradients in a thin film technique for measuring nitrate using ion exchange resin. J. Huang, W. Bennett, P. Teasdale, D. Welsh

4:30 ENVR 330. Modeling TCE concentration in groundwater using MATLAB. A. Rihana, Y. Pang, Y. Gao

4:50 Concluding Remarks.

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by COLL, Cosponsored by CATL and ENVR

WEDNESDAY EVENING

Section A

Colorado Convention Center
Hall C

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Cosponsored by MPPG

D. Alvarez, T. L. Jones-Lepp, *Organizers*

6:00 - 8:00

ENVR 331. Quantitation and identification of PPCP in environmental samples using accurate mass MS/MS technology. C. Borton, R. Kern, A. Schreiber

ENVR 332. Contaminants of emerging concern in effluent dominated coastal waterways in southern California. K.A. Maruya, N.G. Dodder, T. Anumol, S. Shane, W. Lao, A. Sengupta, J. Drewes

Section A

Colorado Convention Center
Hall C

Assessing Toxicity of Environmental Contaminants

Cosponsored by MPPG†

S. M. Uchimiya, J. Wang, *Organizers*

X. Pan, B. Zhang, *Organizers*

6:00 - 8:00

ENVR 333. Influences of environmental conditions on the aquatic toxicity of silver nanoparticles to *Daphnia magna*. R.M. Sofield, A. Nieman, M. Abernathy, A. Gibson

ENVR 334. Hydrogen peroxide production in the presence of soot and biological electron donors. D. Hinz, J. Barnes, A.M. Johansen

Section A

Colorado Convention Center
Hall C

Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment

Cosponsored by MPPG†

M. F. Benedetti, *Organizer*

H. Henry, J. F. Ranville, *Organizers*

6:00 - 8:00

ENVR 335. Remediation of soil polluted area in Ondo State, Nigeria. A.E. Folunso

ENVR 336. Phytoremediation on heavy metal contaminants in sewage river sediment. X. Mao, F.X. Han, K. Guo

ENVR 337. Relative impact of temperature, groundwater chemistry, and groundwater hydrology on inorganic nitrogen processing and nitrogen cycle functional genes in sediments of a groundwater flow-through lake. D.L. Stoliker, D.A. Reper, R.L. Smith, B. Song, C.H. Conaway, D.R. LeBlanc, T.D. McCobb, S. Hyun, D. Koh, H. Moon, K. Ha, D.B. Kent

† Cooperative Cosponsorship

Section A

Colorado Convention Center
Hall C

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs

Cosponsored by MPPG†

D. L. Drogos, M. Urynowicz, *Organizers*,
Presiding

6:00 - 8:00

ENVR **338**. Impacts of microbial community diversity on the occurrence and quantity of crude oil biodegradation and microbial methanogenesis. J. Shelton, D.M. Akob, J.C. McIntosh, J.E. McCray

Section A

Colorado Convention Center
Hall C

Chemical Processes at Environmental Interfaces

H. A. Al - Abadleh, H. M. Ali, R. Z. Hinrichs,
N. Kabengi, *Organizers*, *Presiding*

6:00 - 8:00

ENVR **339**. Adsorptive removal of taste and odor compounds onto granular mesoporous carbon (GMC). S. Kim, Y. Kim, H. Choi
ENVR **340**. Au nanostar-enabled multifunctional reverse osmosis membranes for reduced mineral scaling, organic-, and bio-fouling. J. Ray, S. Tadeipalli, S.Z. Nergiz, K. Liu, L. You, Y. Tang, S. Singamaneni, Y. Jun

Section A

Colorado Convention Center
Hall C

Chemistry in the Marine Boundary Layer

Cosponsored by MPPG

B. DAnna, J. Donaldson, *Organizers*

6:00 - 8:00

ENVR **341**. Ocean organics vs. inorganics: The contributions to suppressed ClNO₂ yield from the ocean surface following N₂O₅ uptake. O.S. Ryder, N. Campbell, T.H. Bertram
ENVR **342**. On the role of dimethyl sulfide and marine biogenic volatile organic compounds in sea spray aerosol growth post production. N.R. Campbell, M.J. Kim, M. Zorab, T.H. Bertram

Section A

Colorado Convention Center
Hall C

Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter

Cosponsored by MPPG

S. M. Lomnicki, *Organizer*

6:00 - 8:00

ENVR **343**. Using the chemical mass balance for the changes of source apportionment at the heating time of three period in Tianjin, China. W. Hong, X. Bi, Y. Feng, J. Wu, K. Chen
ENVR **344**. Comparative study of PM_{2.5} vertical characteristics between heavy pollution weather and clean weather in Tianjin, China. W. Hong, S. Han, Y. Zhang, J. Wang, Y. Feng

Section A

Colorado Convention Center
Hall C

Environmental Chemistry: Pedagogical Models and Practices

Cosponsored by CHED, MPPG† and YCC

K. C. Lanigan, E. Roberts-Kirchhoff, *Organizers*

6:00 - 8:00

ENVR **345**. Paper spectrometers: The intersection of environmental chemistry and engineering. A. Kahl

Section A

Colorado Convention Center
Hall C

Environmental Implications of Nano: Release from Consumer Products and Advances in Nanometrology

C. P. Higgins, J. F. Ranville, R. B. Reed,
Organizers, *Presiding*

6:00 - 8:00

ENVR **346**. Role of CO₂ in the equimolar C₂H₂-CO₂ reaction to synthesize carbon nanotubes: Environmental and mechanistic implications. W. Shi, Y. Peng, D.L. Plata
ENVR **347**. Detection of single walled carbon nanotubes using microsecond single particle ICP-MS. J. Wang, R. Lankone, H. Fairbrother, C.P. Higgins, J.F. Ranville
ENVR **348**. Aggregation and stabilization of multiwalled carbon nanotubes in aquatic system: Influence of carboxymethyl cellulose, starch, and humic acid. W. Liu, X. Zhao, D. Zhao
ENVR **349**. Theoretical and experimental studying of sedimentation of TiO₂ nanoparticles in aqueous solutions. J. Lu, D. Liu, H. Liu, X. Yang, F. Cui
ENVR **350**. Dissolved organic matter adsorption to titanium dioxide nanoparticles: Effect of molecular weight fractions and the interaction mechanisms. X. Yang, T. Jiang, F. Cui
ENVR **351**. Comparative study of Fe(II)-GAC for bromate or perchlorate removal. H. Xu
ENVR **352**. Challenges in the differentiation of nanoparticles when analyzing complex sample matrices using spICP-MS. E. Gray, J.F. Ranville, A. Bednar, C.P. Higgins
ENVR **353**. Titanium dioxide nanoparticles induces mitochondrial dysregulation and loss of liver functions. V. Natarajan, C. Wilson, S.L. Hayward, S. Kidambi
ENVR **354**. Isotopically-labeled core-shell-shell Ag₁₀₀@Au@Ag₁₀₀ nanoparticles to ion and particle bioavailability. R.C. Merrifield, J. Lead
ENVR **355**. Asymmetric flow field flow fractionation online with Single particle - inductively coupled plasma mass spectrometry: Detection and quantification of silver nanoparticles in aqueous samples. K. Huynh, E. Siska, E. Heithmar

Section A
Colorado Convention Center
Hall C

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters
Cosponsored by AGRO and MPPG†
W. Arnold, Y. Chin, K. H. Wammer, *Organizers*

6:00 - 8:00

ENVR **356**. Polychromatic method to determine the wavelength dependence of singlet oxygen quantum yields for natural and effluent organic matter. J.R. Laszakovits

Section A
Colorado Convention Center
Hall C

General Posters
S. R. Al-Abed, *Organizer*

6:00 - 8:00

ENVR **357**. Electrolytic disinfection of water contaminated with *E. coli* by treatment with an alternating current using stainless steel and copper electrodes: Role of hydroxyl radicals and hydrogen peroxide formation. N. Barashkov, T. Sakhno, I. Irgibayeva
ENVR **358**. Hydrooligomerization of acetylene from electrocracking gas over Ni/CNFs catalyst. A.S. Ismail
ENVR **359**. Removal of micropollutants from surface water and groundwater by portable water filtering system designed for rural communities in underdeveloped countries. S. Jeong, K. Koo, Y. Jeong

ENVR **360**. Functional forms of the unburned carbon present in coal fly ashes: Role of surface oxygen species in the formation of organic fluorine forms on the carbon surface. N. Tsubouchi, Y. Ohtsuka
ENVR **361**. Development of a sheathless particle classifier with an electrometer to measure the particles from automobile. H. Yamada, H. Okuda
ENVR **362**. Behavior of mercury in coal combustion residue contaminated sediments. T.R. Gofstein, A. Heyes
ENVR **363**. Compared fluorescence characterization of salt marsh pore water using PARAFAC analysis. J. Bowen, W.J. De Bruyn, C.D. Clark
ENVR **364**. Analysis of diazepam, diphenhydramine, carbamazepine and metabolites drugs in fish from grocery markets by gas chromatography - mass spectrometry (GC-MS) using SIM mode. M. Arafat, C. Stowe, D. Johnson, M.J. Mezziani, M. Mottaleb
ENVR **365**. Withdrawn.
ENVR **366**. Trace metals in trout species collected from high altitude Colorado lakes. M. Spedale
ENVR **367**. Study on the adsorption of ammonia Nitrogen on zeolite modified by ultrasonic and sodium. W. Qun, Y. Zhichao, G. Mingkun, C. Bin, X. He, C. Shuang
ENVR **368**. GCMS identification and quantification of the lipids produced via esterification to FAMEs in *Neochloris minuta* (UTEX 776) algae induced by nitrogen deprivation. D.G. Giarikos, R. Razeghifard, M. Margupuram, C. Chialfair
ENVR **369**. Enhanced reductive degradation of *p*-chloronitrobenzene in a coupled bioelectrode-UASB system. L. Zhu, X. Xu, K. Gao, J. Jin
ENVR **370**. Race for the gold metal: A novel approach for reclaiming specialty metals from industrial waste and processing streams. M.P. O'Connor, D.L. Plata
ENVR **371**. Spectroscopic and microscopic investigation of soil mineral and natural organic matter-treated silver nanoparticles. S.R. Kanel, B.A. Manning, S.W. Brittle, I.E. Pavel Sizemore, D. Felker, D. Kempisty, M.N. Goltz
ENVR **372**. Assessment of clay minerals selectivity for adsorption of humic acid fraction. M.E. ElSayed, M.M. Khalaf, J.A. Rice
ENVR **373**. Quantitative analysis of single-particle mass spectra acquired in Northfield, MN. A. Janes, D.S. Gross
ENVR **374**. Airborne metal concentrations during and after pollution restrictions in Shenzhen. N. Dewan, B. Majestic, Y. Wang, Z. Yuan-Xun
ENVR **375**. Photoluminescence quenching of graphene oxide by enzymatic reaction for optical sensing of pesticides. T. Kang, S. Jeon, H. Kim, J. Kim
ENVR **376**. Combining Fenton's oxidation and biodegradation to degrade decabromodiphenyl ether in soil. C. Lin, C. Yang, Y. Chang
ENVR **377**. Assessment and spatial variation analysis of water quality in Grand Bay national estuarine research reserve. J. McComb, C.C. Thomas, Z. Arslan, F.X. Han
ENVR **378**. Groundwork for the development of a model for determining atmospheric mercury in the arid West using leaves. D.W. Lehmpuhl, L.M. Bartolo, K.A. Wager
ENVR **379**. Photochemical inactivation of *E. faecalis* in the presence of organic matter. S. Mostafa, M. Rubinato, F.L. Rosario, K. Linden
ENVR **380**. Disinfection by-products as endocrine active substances. B.E. Holmes, L. Smeester, R.C. Fry, H. Weinberg
ENVR **381**. Dissolved organic carbon (DOC) release following drought: influence of DOC source and drought severity on drinking water treatment. J. Ritson, N. Graham, M. Templeton, J. Clark, C. Freeman
ENVR **382**. Synthesis and characterization of nanocomposites of Au@Ag@rGO and their use in degradation of organic dyes. E. Mejia-Ospino, R. Cabanzo, S.E. Castellanos

ENVR **383**. Enhanced air-cathode microbial fuel cell (MFC) performance with oxygen supply from an externally connected algal bioreactor (ABR). R. Kakarla, B. Min
ENVR **384**. Microbial electrosynthesis of high-value products from volatile fatty acids present in anaerobic digestion effluent. S. Kondaveeti, B. Min
ENVR **385**. Reduced polyoxometalates initiate HO formation from aqueous ozone. B. Solomon, J. Ferry
ENVR **386**. Quantitative analysis of atmospheric aerosol with atomic force microscopy. W. Kong, L. Hawkins
ENVR **387**. Halide ions as tracers for human wastewater inputs to an agricultural watershed. A. Thayer, C. Spiess
ENVR **388**. Reductive remediation of trichloroethylene (TCE) solution by granulated nano zero-valent iron (nZVI). Y. Shih, C. Su, C. Chen, C. Chen, C. Dong
ENVR **389**. Photolysis and UV/H₂O₂ advanced oxidation processes of bisphenol-s in water. M. Mbewe, R. Bell, J. Jin, P.A. Ruiz-Haas
ENVR **390**. Exploring the relevant parameter space in shale rock geochemistry: Organic transformations at temperature and pressure. A. Sumner, B. Drollette, D.L. Plata
ENVR **391**. Silver nanoparticle adsorption to corundum surfaces as a function of solution pH and time. J. Purvis, K. O'Neil, S.W. Brittle, I.E. Pavel Sizemore, S.R. Higgins
ENVR **392**. Toxic effects of multiwall carbon nanotubes to *Pseudomonas aeruginosa* and its predator *Tetrahymena thermophila*. M. Mortimer, E. Orias, E. Petersen, B.A. Buchholz, P. Holden
ENVR **393**. Photolysis and toxicity of the organic UV filter chemical octylmethoxycinnamate and its photoproducts. C.A. Berg, L. MacManus-Spencer, M.G. Paulick
ENVR **394**. Heterogeneous photochemistry of nitrate chemisorbed on TiO₂ as a function of relative humidity. D.M. Lesko, H.D. Swomley, J.G. Navea
ENVR **395**. Improvement of antislintering of Ca-based sorbents by thermally treated vermiculite. J. Meng, H. Li, B. Meng, J. Li, L. Shan, Y. Yu, Y. Min, D. Xu
ENVR **396**. Experiment on CO₂ capturing capacity of attapulgite modified CaO-based sorbent in calcination/carbonation cycle. L. Shan, H. Li, J. Meng, B. Meng, J. Li, Y. Yu, Y. Min, D. Xu
ENVR **397**. Metal oxide modified limestone for CO₂ adsorption. J. Li, H. Li, B. Meng, Y. Yu, Y. Min, D. Xu
ENVR **398**. Enhancement of CO₂ sequestration of limestone with carbon additives. B. Meng, H. Li, W. Yang, J. Li, Y. Yu, Y. Min, D. Xu
ENVR **399**. Virucidal activity of a multilevel antimicrobial air filter. W. Han, Q. Chang, Y. Lai, Y. Li, Y. Yang, C. Wu, K.L. Yeung, C. Chao, Z. Yang
ENVR **400**. Design, synthesis, and characterization of isoprene hydroperoxides. E. Lozano, V. Kumar, A. Abdelhamid, A. Hasson, S. Maitra
ENVR **401**. Exploring the environmental controls on the degradation of oil by marine fungi. C.M. Poutasse, R. Simister, H.K. White
ENVR **402**. Exposure to engineered nanomaterials in various consumer products. B. Lee, G. Yu, M. Kim, H. Kim
ENVR **403**. Reactivity of an epoxy coating with free and combined chlorine in drinking water service lines. E.F. Peltier, Z.A. Breault, R.F. Lane, S.J. Randtke, R.E. Carter, C.D. Adams
ENVR **404**. Oxidation of surface-adsorbed anthracene on a quartz fiber substrate. J. Bilek, R. Cochran, H. Jeong, E.I. Kozliak, A. Kubatova
ENVR **405**. Effect of relative humidity on HCl formation from the reaction of H₂SO₄, HNO₃ and with NaCl. K. Newhouse, B. Fong, H.M. Ali
ENVR **406**. Resistance of synthetic organic aerosol chromophores to photobleaching under oxidative conditions. A. Lemire, L. Hawkins

- ENVR 407.** Degradation of diclofenac in water with TAML activators and hydrogen peroxide. **M.R. Mills, A.V. Cheng, A.D. Ryabov, T.J. Collins**
- ENVR 408.** Limonene reactivity on mineral surfaces and the impact of relative humidity and adsorbed nitric acid. **A. Staniec, R.Z. Hinrichs**
- ENVR 409.** Quantifying the solar energy absorbed by nitrophenols adsorbed on atmospheric aerosol substrates. **J. Trivedi, R.Z. Hinrichs**
- ENVR 410.** Investigating the reversibility of self-assembled humic acid structures. **G. Chilom, M.M. Khalaf, J.A. Rice**
- ENVR 411.** Withdrawn.
- ENVR 412.** Use of chlorate, nitrate, and perchlorate to promote crude oil mineralization in salt marsh sediments. **M. Brundrett, J. Horita, T.A. Anderson, D. Reible, J. Pardue, A. Jackson**
- ENVR 413.** Influence of stabilizer size and chelation strength on iron nanoparticle oxidation. **N. Rentz, L.F. Greenlee**
- ENVR 414.** Online monitoring of ambient fungal spore concentrations in the harbour region of Cork, Ireland. **D.J. O'Connor, D.A. Healy, J.R. Sodeau**
- ENVR 415.** Quantum mechanical calculations of nitric acid chemisorbed on several crystalline structures of TiO_2 anatase. **M.J. Lueckheide, J.G. Navea**
- ENVR 416.** Simultaneous removal of SO_2 and NO_x from combustion flue gas in a discharge plasma reactor. **L. Qi, Y. Zhang**
- ENVR 417.** Array-based detection of carcinogens and carcinogen metabolites in urine. **L. Gareau, N. Serio, L. Prignano, M. Levine**
- ENVR 418.** Arsenic release mechanism in the shallow and deep aquifer in Chiayi County, Taiwan. **C. Lee, Y. Lin, S. Wang**
- ENVR 419.** Effect of photochemical weathering on the composition and spectroscopic properties of crude oil. **O.C. Stewart, C.M. Sharpless, C.M. Reddy, B. Swarthout, C. Aeppli**
- ENVR 420.** Use of LIBS to detect CO_2 leaks from geological storage based on mineral carbonate interactions in groundwater. **J. Jain, H. Edenborn, C. Goueguel, C. Carson, D. McIntyre**
- ENVR 421.** Examining the desorption of oil from persistent surface residual oil balls (SRBs). **S.L. Lyons, H.K. White**
- ENVR 422.** Comparative evaluation of the dissolution of fly ash from different source regions under atmospherically relevant conditions. **J.R. Borgatta, A. Paskavitz, J.G. Navea**
- ENVR 423.** Colorimetric evaluation of the cation exchange of aluminum with iron in humic acids. **J.R. Borgatta, J.G. Navea**
- ENVR 424.** Electrochemical dechlorination of TCE in the presence of natural organic matter, metal ions and nitrates in a simulated karst aquifer. **N. Fallahpour, X. Mao, L. Rajic, A. Alshawabkeh, S. Yuan**
- ENVR 425.** Electrochemical degradation of chlorobenzene in groundwater using Pd-catalytic electro-Fenton's reaction. **R. Nazari, A. Ciblak**
- ENVR 426.** New spectroscopic method for characterizing the nutritional quality of fruit resources available to wildlife in a Western New York habitat. **S.B. Smith, M. Bida, S. Schroeder, G. Wink, T.E. Pagano**
- ENVR 427.** Extraction and separation of contaminants in water systems. **M. Jones, B. Caldwell, A. Newsham, B.H. Barton, R.E. Del Sesto, A.T. Koppisch, S. Iyer**
- ENVR 428.** Measuring the emission efficiency and nicotine delivery of electronic cigarette. **G. Wink, R.J. Robinson, A.G. DeFrancesco, S.B. Smith, T.E. Pagano**
- ENVR 429.** Microbe-metal interactions along a produced water impacted stream system. **J. Klings, D.M. Akob**
- ENVR 430.** Airborne antibiotic resistant genes upwind and downwind of poultry concentrated animal feeding operation. **H.M. Sanchez, J.A. Jay**
- ENVR 431.** Withdrawn.
- ENVR 432.** Direct synthesis of $\text{V}_2\text{O}_5\text{-WO}_3\text{-TiO}_2$ nanoparticles with enhanced low-temperature activity for $\text{NH}_3\text{-SCR}$. **K. Cheng, Z. Zhao, J. Liu**
- ENVR 433.** Enantioselective disposition of 2,2',3,5',6-hexachlorobiphenyl (PCB 95) and its metabolites in mouse dams dosed during pregnancy. **I. Korwel, C. Barnhart, K. Truong, P. Lein, H.J. Lehmler**
- ENVR 434.** Withdrawn.
- ENVR 435.** Use of flue gas desulfurization (FGD) gypsum as a heavy metal stabilizer in contaminated soils. **N.H. Koralegedara, S.R. Al-Abed, D.D. Dionysiou**
- ENVR 436.** Trace metal emissions from the combustion of fecal char briquettes and a comparison to other solid fuels. **M.J. Price, W.M. Champion, B.J. Ward, B.T. Cartledge, B. Majestic, L.D. Montoya**
- ENVR 437.** Hexadecyl trimethyl ammonium bromide dispersed nano zero-valent iron for discoloration of methyl orange. **X. Wang, P. Wang, L. Le**
- ENVR 438.** Wireless glucose sensor utilizing magnetic nanoparticles embedded hydrogel. **J. Park, C. Zhang, P.V. Braun, R.A. Siegel, B. Ziaie**
- ENVR 439.** Fecal and urinary elimination kinetics of cephalosporin and lincosamide antibiotics in dairy cows following intramammary infusion: Application of SPE clean-up and UPLC-MS/MS quantification approach. **P. Ray, K.F. Knowlton, C. Shang, K. Xia**
- ENVR 440.** New insights into the function of potassium carbonate species and the superiority of base metals to noble metals in the polytitanate nanobelt supported LNT catalysts. **Y. Zhang, M. Meng**
- ENVR 441.** Effects of filtration on the detection, quantification, and characterization of engineered nanoparticles in water samples using single particle inductively coupled plasma mass spectrometry. **E. Siska, K. Huynh, E.M. Heithmar**
- ENVR 442.** Analysis of water and soil of La Encantada fall in Anasco, Puerto Rico. **K. Matias**
- ENVR 443.** Effects of speciation on mercury co-selection for antibiotic resistance genes in fresh and brackish water microcosms. **C.M. Echeverria Palencia, S. Hafeznezhad, C. Maramba Jones, A. Zimmer-Faust, V. Thulsiraj, S. Mahendra, J.A. Jay**
- ENVR 444.** Withdrawn.
- ENVR 445.** Developing tailored bioactive silica-gels for pollutant removal and biodegradation. **J.K. Sakkos, A. Ish Am Radian, B.R. Mutlu, L.P. Wackett, A. Aksan**
- Section A**
Colorado Convention Center
Hall C
- Green Chemistry and the Environment**
A. M. Balu, R. Luque, S. O. Obare, Organizers
- 6:00 - 8:00**
- ENVR 446.** Multi-electron transfer process for the degradation of toxic organophosphorus contaminants. **S. Santos, S.O. Obare**
- ENVR 447.** Superoxide radical as a green reagent and an ultimate solution of environmental problems. **U. Stoin, Y. Sasson**
- ENVR 448.** Development of low density solvent DLLME-GC/MS method for quantitation of tetrabromobisphenol-A from dust. **J.E. Owens, C. Barrett, D.A. Orban, S.E. Seebeck, L. Lowe**
- ENVR 449.** Glow in the dark: Luminescent metal organic frameworks (MOFs) grown from cotton fibers. **R.R. Ozer, J.P. Hinestroza**
- Section A**
Colorado Convention Center
Hall C
- Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment**
Cosponsored by ANYL and MPPG
- G. Aiken, K. Cawley, J. A. Korak, F. L. Rosario, Organizers**
- 6:00 - 8:00**
- ENVR 450.** Evaluating the treatability and reactivity of wildfire-impacted DOM using leachates from burned sediments. **A.K. Hohner, K. Cawley, P. Omur-Ozbek, R. Summers, F.L. Rosario-Ortiz**
- ENVR 451.** Photochemical processing of wastewater impacted streams. **C. Glover, F.L. Rosario**
- ENVR 452.** Development of a novel microscope spectrofluorometer for individual bioparticle characterization. **B.E. Swanson, J.A. Huffman, D.R. Huffman**
- ENVR 453.** Evaluation of total petroleum hydrocarbon analysis specificity. **D.A. Gratson**
- Section A**
Colorado Convention Center
Hall C
- Solutions to Metals Contamination of Water**
Cosponsored by MPPG†
- S. Ahuja, J. W. Finley, J. N. Seiber, Organizers**
- 6:00 - 8:00**
- ENVR 454.** Novel method for measuring arsenic in water using nanostructured surface. **N. Mosquera, W. Marimon Bolivar, L. Yate, E. Coy, E. Gonzalez**
- ENVR 455.** Biosurfactants as a tool for metal removal from waste effluents. **D. Hogan, J.E. Pemberton, R.M. Maier**
- ENVR 456.** Chitosan-grafted carbon for the sequestration of heavy metals in aqueous solution. **A.A. Okoya**
- Section A**
Colorado Convention Center
Hall C
- Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use**
Cosponsored by AGRO and MPPG†
- I. C. Escobar, J. Hestekin, Organizers**
- 6:00 - 8:00**
- ENVR 457.** Pilot-scale study on the removal of nutritional elements in agricultural runoff by iron-modified biochar. **T. Chi, J. Zuo, F. Liu**
- ENVR 458.** Kinetics of hydroxyl radical reactions with chloramines in support of recycling wastewater. **K. Couch, S.P. Mezyk, K.P. Ishida**
- ENVR 459.** Sulfate radical remediation of pharmaceuticals in DOM containing wastewater. **T. Reutershan, S.P. Mezyk**
- Section A**
Colorado Convention Center
Hall C
- Water Sustainability in Oil and Gas Exploration: Treatment Issues**
Cosponsored by CEI and MPPG†
- T. Y. Cath, K. Linden, Organizers**
- 6:00 - 8:00**
- ENVR 460.** Evaluation of forward osmosis membranes in long-term oil and gas wastewater treatment stud. **L. Bell, T.Y. Cath, B.D. Coday**
- THURSDAY MORNING**
- Section A**
Colorado Convention Center
Room 703
- Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment**
Cosponsored by MPPG†
- M. F. Benedetti, Organizer**
H. Henry, J. F. Ranville, Organizers, Presiding
- 8:00** Introductory Remarks.
- 8:05 ENVR 461.** Toxicity implications of sulfate radical based oxidative treatment for groundwater remediation. **W. Li, D.L. Sedlak, D. Schlenk, H. Liu**
- 8:25 ENVR 462.** Methods for simulating the restoration and recovery of acid mine drainage-impacted stream sediment. **J. Williamson, J.F. Ranville, M.R. Pastorinho, J. Meyer, W.H. Clements**
- 8:45 ENVR 463.** Diffusive gradient in thin film (DGT) passive samplers for monitoring metals in contaminated sediments: Contribution of metal sulfide nanoparticles. **A. Pham, D. Manley, C. Johnson, H. Hsu-Kim**
- 9:05 ENVR 464.** Biogeochemical processes controlling trace elements in the Grand Bay National Estuarine Reserve in the northern Gulf of Mexico. **J. McComb, F.X. Han, C. Rogers, C.C. Thomas, Z. Arslan, A. Ardeshir, P. Tchounwou**
- 9:25 ENVR 465.** Stable oxygen isotope enrichment during biotic and abiotic reduction of selenate. **A. Schellenger, L. Xia, D. Jaisi, P. Laresse-Casanova**
- 9:45 ENVR 466.** In situ immobilization of uranium in Hanford sediments with the amendment of phosphate. **Z. Pan, D. Giammar, V. Mehta, L. Troyer, J.G. Catalano, Z. Wang**
- 10:05** Intermission.
- 10:20 ENVR 467.** D. Magna metal toxicity in a mining impacted stream: Comparing results in simulated and field-collected waters. **K. Ebeling**
- 10:40 ENVR 468.** Comparing the partition and sorption behavior to agricultural soils of Bisphenol A (BPA) and BPA alternatives: BPS and BPAF. **Y. Choi, L.S. Lee**
- 11:00 ENVR 469.** Perfluoroalkyl acids inhibit TCE dechlorination by repressing *Dehalococcoides* growth. **T.S. Weathers, K. Harding, L. Alvarez-Cohen, C.P. Higgins, J.O. Sharp**
- 11:20 ENVR 470.** Enantioselective biotransformation of chiral PCBs in aquatic to riparian food webs. **C.M. Lee, V.D. Dang, D. Delach, K. Mitra**
- 11:40 ENVR 471.** Compound specific isotope analysis of aromatics and chlorinated aromatics at a fine vertical resolution across the groundwater – surface water sediment interface. **E. Passeport, R. Landis, K. Chu, G. Lacrampe-Couloume, E. Lutz, E.E. Mack, B. Sherwood Lollar, K. West**
- Section B**
Colorado Convention Center
Room 705
- Surface Physicochemical Processes in Engineered and Natural Systems**
Cosponsored by AGRO and MPPG†
- H. J. Zhang, Organizer**
J. M. Cerrato, H. Liu, Organizers, Presiding
- 8:30 ENVR 472.** Fe(II)-catalyzed recrystallization of hematite and goethite revisited. **M. Scherer, A.J. Friedrich, R.M. Handler, M. Helgeson, K. Rosso, C. Johnson**
- 9:10 ENVR 473.** Interfacial processes affecting the mobility of metals from abandoned uranium mine wastes. **S. Avasarala, J. Blake, K. Artyushkova, M. Ali, A. Breatly, C. Shuey, P. Robinson, E. Escheverria, F. Escheverria, C. Hirani, J.M. Cerrato**
- 9:30 ENVR 474.** Identification of Mackinawite surface products formed upon reaction with carbon tetrachloride. **Y. Lan, E.C. Butler**
- 9:50 ENVR 475.** Acoustically enhanced sediment remediation: Characterization of diffusion and pore flow in porous media. **Z. Wei, J.J. Lenhart, L. Weavers**
- 10:10 ENVR 476.** Characterizing the reactivity of naturally occurring reducing materials with agarose-bound powder disk electrodes. **M.J. Bradley, R. Meuwissen, P.G. Tratnyek**
- 10:30** Intermission.

- 10:45 ENVR 477.** Mechanisms of fluoride removal: Adsorption and co-precipitation with aluminum hydroxide in the presence and absence of NOM. L.E. Katz, D.F. Lawler, K. Alfredo, M. Stehouwer, C. Ernst
- 11:05 ENVR 478.** Heterogeneous nature of permanganate oxidation reactions. X. Xia, A.T. Stone
- 11:25 ENVR 479.** Efficacy of CaCO₃ and CaSO₄ scaling resistance of polyethylene glycol hydrophilically-modified reverse osmosis membranes in the presence of humic acid. J. Ray, W. Wong, Y. Jun
- 11:45 ENVR 480.** Radioluminescent/photocatalytic composite materials for pursuing fixed-bed heterogeneous advanced oxidation using X-rays. F. Li, E.L. Cates
- 12:05** Concluding Remarks.

Section C

Colorado Convention Center
Room 707

Environmental Chemistry: Pedagogical Models and Practices

Cosponsored by CHED, MPPG† and YCC

K. C. Lanigan, E. Roberts-Kirchhoff, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 481. Environmentally-themed chemistry activities and experiments focused on water quality for a range of instructional levels. K.C. Lanigan, E. Roberts-Kirchhoff

8:25 ENVR 482. Engaging undergraduates: Investigating local environmental issues at the intersection of science and society. S.L. Scribner, J. Hamming-Buhl

8:45 ENVR 483. Using environmental chemistry to teach analytical chemistry. K.H. Weaver, D.J. Eves

9:05 ENVR 484. Integrating environmental and sustainability challenges into a capstone chemistry course. K. Miller, B. Murugavel

9:25 ENVR 485. Chemistry lab water quality analysis in an integrated thematic learning community. W.J. Donovan, E.R. Wheland, A. Bilia, G.A. Smith, T.A. Wagler

9:45 Intermission.

10:00 ENVR 486. Using climate change context to engage students in general chemistry. D.B. King, J.E. Lewis, K. Anderson, D.E. Latch, S. Suthemer, G.H. Webster, C.H. Middlecamp, R.S. Moog

10:20 ENVR 487. Using models of growth in the Amazon to bring an environmental chemistry topic into the general chemistry class. M.A. Benvenuto, D. Archey

10:40 ENVR 488. Teaching environmental toxicology by cooperative learning methods: Capstone travel course on the environment of Thailand. L.J. Berliner

11:00 ENVR 489. Benefits of working in an environmental water-testing laboratory: How applying what you learn prepares you for the real world. D.J. Eves, J.T. Redd, K.H. Weaver, N.S. Werner, M. Valentine, S. Potter, D. Callison

11:20 ENVR 490. Southern Utah University internship: A working model of peer mentorship. J.T. Redd, K.H. Weaver

11:40 Concluding Remarks.

Section D

Colorado Convention Center
Room 709

Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use

Cosponsored by AGRO and MPPG†

I. C. Escobar, J. Hestekin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 491. Recycling wastewater: Quantitative removal of antibiotic activity in waters using advanced oxidation processes. S.P. Mezyk, S.C. Otto

8:30 ENVR 492. A few options for energy and water autarky in water-power systems. V. Gude

8:55 ENVR 493. Water reuse: Right technology for you. V. Frenkel

9:20 Intermission.

9:35 ENVR 494. Reactivity of chlorine atoms with antibiotics under wastewater treatment conditions. C.A. Rice, S.P. Mezyk

10:00 ENVR 495. Feasibility of integrated bioelectrochemical/membrane technologies for wastewater reuse in power plants. V. Gadhamshetty, N. Shrestha

10:25 ENVR 496. Smart event detection system for online water quality monitoring and wastewater source control. T. Li, S. Zhang, H. Zhao

10:50 ENVR 497. Adsorption mechanism of phosphorus removal in agricultural runoff by iron-modified biochar. T. Chi, J. Zuo, F. Liu

11:15 ENVR 498. Phosphorus speciation in anaerobic digestion of biosolids for efficient phosphorous recovery. C.F. Gutierrez, K. Kinney, L.E. Katz

FLUO

Division of Fluorine Chemistry

V. Petrov, *Program Chair*

SUNDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Silverton Ballroom 1

ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur

Cosponsored by WCC

D. A. Dixon, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 FLUO 1. Green metrics for the assessment of selective direct fluorination processes. G. Sandford

9:00 FLUO 2. Preparation and structure of 1,2,3,4,5,6,-hexafluorocyclohexane stereoisomers. D. O'Hagan

9:30 FLUO 3. Probe solute association via the water proton NMR signal. Y. Feng, M. Taraban, Y.B. Yu

10:00 Intermission.

10:20 FLUO 4. Recent progress in the synthesis of aryl triflones. N. Shibata

10:50 FLUO 5. Use of 1,3-dipolar cycloadditions for the preparation of SF₆-substituted heterocycles. W.R. Dolbier, S.E. Lopez, A. Mitani

11:20 FLUO 6. Influence of fluorination on alcohol hydrogen bonding and lipophilicity properties. B.J. Linclau

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Silverton Ballroom 1

ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur

Cosponsored by WCC

D. A. Dixon, *Organizer*

D. O'Hagan, G. Sandford, *Presiding*

1:30 Introductory Remarks.

1:50 FLUO 7. AgF-mediated fluorinative cross-coupling of two olefins. B. Gao, Y. Zhao, J. Hu

2:20 FLUO 8. Our recent studies in fluoroalkylation chemistry. S.G. Prakash

2:50 FLUO 9. New frontier in fluorine chemistry. K. Mikami

3:20 FLUO 10. Reagents and catalysts for fluorination and perfluoroalkylation reactions. A. Togni

3:50 FLUO 11. Computational studies of fluorine containing molecules: Lewis acidities and radical reaction mechanisms. D.A. Dixon

4:20 FLUO 12. Award Address (ACS Award for Creative Work in Fluorine Chemistry sponsored by the Juhua Group Technology Center (China)). Expanding the range of 18F-tags for PET applications. V. Gouverneur

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

V. Petrov, *Organizer*

8:00 - 10:00

FLUO 13. Solvation/desolvation and crystal structures of monovalent metal salts of the superweak anion B₁₀F₁₂²⁻. E.V. Bukovsky, D. Peryshkov, T.C. Folsom, S.H. Strauss

FLUO 14. Spectral characterization of steroids following fluorination by selectfluor. H. Hakk, S. Svendsen

FLUO 15. Expansion of polyaromatic π systems via fluoroannulation reactions. K. Rippey, I.V. Kuvychno, T. Clikeman, E.V. Bukovsky, O. Boltalina, S.H. Strauss, Y. Chen

FLUO 16. Acid cation salts of the superweak anion B₁₀F₁₂²⁻. W.M. Jones, E.V. Bukovsky, M. Malischewski, D.V. Peryshkov, K. Seppelt, S.H. Strauss

FLUO 17. Withdrawn.

FLUO 18. Self-assembly of novel fluorosurfactants with polyoxometalates (POMs) as polar component in acetonitrile/water solution. B. Zhang

FLUO 19. Biological applications of trifluoromethylfullerene. K.P. Castro, A. Mitchell, J.M. Sloan, S.A. Rolfe, A.J. Fleming, A. Ferguson, J. Blackburn, S.H. Strauss, O.V. Boltalina

FLUO 20. Molecular design of fluorine-containing fullerene electron acceptor materials for organic photovoltaics. N. DeWeerd, L. San, S.H. Strauss, O.V. Boltalina

FLUO 21. Synthesis, structural features, and dielectric properties of coordination polymers based on poly(azolate) ligands. A. Cimino, A. Maspero, S. Galli, C. Giacobbe, G. Palmisano, C. Yang, S. Tekarli, M. Omari

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Cripple Creek Ballroom 2

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe

Cosponsored by INOR

D. A. Dixon, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 FLUO 22. Our excursions into iodine chemistry. S.G. Prakash

9:10 FLUO 23. Iodocarbon molecules and materials. N.S. Goroff

9:50 Intermission.

10:10 FLUO 24. Organohypervalent iodine chemistry. V.V. Zhankin

10:50 FLUO 25. Iodine driven self-assembly processes. G.P. Resnati, P. Metrangolo, G. Terraneo, G. Cavallo

11:30 FLUO 26. Recent progress in the chemistry of iodine fluorides, oxofluorides, and oxides. R. Haiges, K.O. Christe

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Cripple Creek Ballroom 2

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe

Cosponsored by INOR

D. A. Dixon, *Organizer*

R. M. Haiges, *Presiding*

1:30 FLUO 27. Iodine serving fluorine. A. Togni

2:10 FLUO 28. Formation, characterization, and uses of 3D metallacages via coordination directed self-assembly. P.J. Stang

2:50 Intermission.

3:10 FLUO 29. Role of iodine in the chemical oxygen iodine laser. W. McDermott

3:50 FLUO 30. Computational studies of iodo compounds. D.A. Dixon

GEOC

Division of Geochemistry

S. Kerisit, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Analytical Chemistry of Natural Resources: Environmental Analysis (see ANYL, Wed)
Analytical Chemistry of Natural Resources: Instrumentation and Methods (see ANYL, Wed)

BUSINESS MEETINGS:

GEOC Executive Meeting, 6:30 PM: Sun
GEOC Business Meeting, 5:30 PM: Tue

SUNDAY MORNING

Section A

Colorado Convention Center
Room 710

Understanding the Geochemical Interactions of Organic Compounds in the Subsurface

Cosponsored by MPPG†

J. Blotvogel, V. Glezakou, A. Karamalidis, *Organizers, Presiding*

8:00 GEOC 1. Structure-dependent interactions between feldspars and organic compounds: Implications for geologic carbon sequestration. Y. Jun, Y. Yang, Y. Min

8:30 GEOC 2. Determination of binding geometry, local water structure and topological at FeOOH surfaces. E.J. Bylaska, Y. Chen, J. Wear

9:00 GEOC 3. Effects of organic ligands on scCO₂ saturated brine-biotite interactions: Implications for organic-rich geologic CO₂ sequestration. L. Zhang, Y. Jun

9:20 GEOC 4. Effects of carboxylic acid ligands on plagioclase dissolution under conditions relevant to geologic sequestration. Y. Min, Y. Jun, J.D. Kubicki

9:40 Intermission.

10:00 GEOC 5. NMR and computational molecular dynamics investigation of mineral-NOM interactions at atmospheric and elevated pressures. R.J. Kirkpatrick, G.M. Bowers, A.O. Yazaydin, B. Ferguson, D.W. Hoyt, S. Burton, T. Varga, V. Reddy

10:30 GEOC 6. Molecular-scale Interactions of Ca²⁺, NOM, H₂O, and smectites in Ca-NOM-H₂O and Ca-Smectite-NOM-H₂O systems: Roles of pH history, NOM activity, H₂O activity, and ionic strength. G.M. Bowers, B. Ferguson, H.E. Argersinger, T. Johnson, V. Reddy, R.J. Kirkpatrick, B. Arey

11:00 GEOC 7. Chemical controls of the micro-structure of NOM-smectite composite materials. **B. Ferguson**, H. Argersinger, R.J. Kirkpatrick, B. Arey, G.M. Bowers

11:20 GEOC 8. Water - supercritical CO₂ partitioning of selected organic compounds: Comparison of in-situ batch reactor experiments and model predictions. **A. Burant**, C.J. Thompson, G.V. Lowry, A. Karamalidis

11:50 GEOC 9. Measurement of organic partitioning coefficients in water-supercritical CO₂ systems by simultaneous in situ UV and near-infrared spectroscopies. **C.J. Thompson**, D. Bryce, H. Shao, K. Cantrell, J.S. Loring, B.P. McGrail

Section B

Colorado Convention Center
Room 712

Coupled Cycling of Biogeochemical Critical Elements and Contaminants

Metals/Contaminants: Field-scale

J. R. Bargar, B. Gu, M. Keiluweit, H. Lin, *Organizers, Presiding*

8:05 Introductory Remarks.

8:10 GEOC 10. Carbon and contaminants in the critical zone. **J.D. Chorover**

8:40 GEOC 11. Influence of natural organic matter on uranium mobility in the upper Colorado River Basin. **J.R. Bargar**, N. Janot, D.Q. Pham, M.E. Jones, S.E. Bone, J. Lezama-Pacheco, S.E. Fendorf, K. Williams, P.E. Long

9:00 GEOC 12. Uranium immobilization in acidic wetlands by natural organic matter and plant roots. **D. Li**, D. Kaplan, J. Seaman, P. Jaffe, K. Scheckel, C.U. Segre

9:20 GEOC 13. Assessment of tellurium in semi-arid mine tailings at Delamar, Nevada: Implications for human and ecosystem health. **N.A. Knight**, S.M. Hayes

9:40 GEOC 14. To migration, reduction, and redox rate scaling in Fe(II)-containing sediments from a natural redox transition zone at Hanford site. **C. Liu**, Y. Liu, R. Kukkadapu, J. McKinley, J. Zachara

10:10 Intermission.

10:30 GEOC 15. Fate of U and As in biostimulated mine tailings sediments. **T. Borch**, L.D. Troyer, K. Campbell, J. Stone, J. Lezama-Pacheco, J.R. Bargar

11:00 GEOC 16. Characterization of effluent and stormwater metal sources and influence on bioavailability in developed streams. **H. Luan**, T.M. Vadas

11:20 GEOC 17. Speciation and mobility of U, As, and co-occurring constituents at abandoned mine waste sites in the Southwest, USA. **J. Blake**, S. Avasarala, K. Artushkova, M. Ali, A. Bready, C. Shuey, P. Robinson, S. Billi, F. Escheverria, E. Escheverria, C. Hirani, J.M. Cerrato

11:40 GEOC 18. Silica availability in the volcanic Klamath Basin and its effect on bioavailability of phosphorus in Upper Klamath Lake, Oregon. **N.S. Simon**, K. Conko, T. Robertson, A. Vinci, K. Fischer

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 710

Understanding the Geochemical Interactions of Organic Compounds in the Subsurface

Cosponsored by MPPG†

J. Blotvogel, V. Glezakou, A. Karamalidis, *Organizers, Presiding*

1:15 GEOC 19. Understanding soil organic matter: Mineral interactions with large-scale molecular dynamics simulation of biopolymer-mineral interfaces. **A. Andersen**, N. Washon, P. Reardon, S. Chacon, M. Kleber

1:45 GEOC 20. Adsorption of light hydrocarbons and carbon dioxide confined in nanoporous synthetic sandstone rocks and shale. **G. Rother**, L. Vitek

2:15 GEOC 21. CH₄ and CO₂ interactions with model clay minerals. **M. Lee**, B.P. McGrail, H. Schaefer, V. Glezakou

2:35 GEOC 22. Use of LC-QTOF mass spectrometry in characterization of produced water for organic compounds: Application to geologic carbon storage and unconventional gas exploration. **V. Mishra**, A. Karamalidis, **J. Jain**, S. Hedges, A. Hakala

2:55 GEOC 23. Autoclave experiments to investigate possible interactions between black shales and stimulation fluid during unconventional gas production. **A. Vieth-Hillebrand**, F.D. Wilke, J. Erzinger, B. Horsfield

3:25 Intermission.

3:45 GEOC 24. Partitioning and reactivity of trace organics in unconventional oil and gas plays. **G.V. Lowry**, A. Burant, N. Edwards, A. Karamalidis

4:15 GEOC 25. How stable are hydraulic fracturing fluid chemicals deep below the Earth's surface? **T. Borch**, G. Kahrilas, E.M. Thurman, I. Ferrer, J. Blotvogel

4:45 GEOC 26. Minerals can be catalysts for organic reactions in hydrothermal environments. **H.E. Hartnett**, J. Shipp, Z. Yang, L. Williams, I.R. Gould, E. Shock

5:15 GEOC 27. Chromatographic fractionation and structural diversity of tetraporphyrins isolated from natural petroleum seeps by FT-ICR MS. **A.M. McKenna**, J.C. Putman, S.M. Rowland, D.L. Valentine, M.Y. Kellermann, C. Aepli, C.M. Reddy, R.P. Rodgers

5:35 GEOC 28. Computer simulation of the ascent, liquid-gas repartitioning, and dissolution of oil hydrocarbons in the deep water column during the Deepwater Horizon disaster. **J.S. Arey**, J. Gros, S. Soccolofsky, C.M. Reddy

Section B

Colorado Convention Center
Room 712

Coupled Cycling of Biogeochemical Critical Elements and Contaminants

Metals/Contaminants: Molecular-scale

J. R. Bargar, B. Gu, M. Keiluweit, H. Lin, *Organizers, Presiding*

1:15 GEOC 29. Viral influence on subsurface biogeochemical cycling and contaminant mobility. **D. Pan**, Z. Tan, J. Nolan, K. Williams, M.J. Robbins, N. Kanani-Zadeh, Y. Li, K.A. Weber

1:45 GEOC 30. Behavior of antimony(V) under Fe(III)- and sulfate-reducing conditions. **C.R. Johnson**, D. Antonopoulos, M. Boyanov, T. Flynn, K.M. Kemner, J. Koval, E.J. O'Loughlin

2:05 GEOC 31. Complex roles of cysteine in methylmercury production by *G. sulfurreducens* PCA. **H. Lin**, X. LU, L. Liang, B. Gu

2:25 GEOC 32. Differentiating kinetic and thermodynamic controls of microbial uranium reduction in the presence of iron oxides. **K.M. Belli**, T.J. DiChristina, P. Van Cappellen, M. Taillefer

2:45 GEOC 33. From plant materials to biochars: Speciation and transformation of sulfur and potassium during biofuel production. **S. Cheah**, N. Laroco, J. Olstad

3:05 Intermission.

3:25 GEOC 34. Coupled cycling of biogeochemically important elements (iron, sulphur, carbon) and toxic metal(oid)s (As, Pb, Cu, Zn, Cd, Ni, U, Th) in pelagic redox-clines of acidic pit lakes. **J. Sánchez-España**

3:55 GEOC 35. Rates and mechanisms of uranyl oxyhydroxide mineral dissolution. **E. Reinoso-Maset**, W. Um, J.D. Chorover, C. Steefel, P. O'Day

4:15 GEOC 36. Elucidating the role of monomeric U(IV) in uranium ore deposit genesis. **A. Bhattacharyya**, K. Campbell, S. Weyer, T. Borch

4:35 GEOC 37. Rapid mobilization of noncrystalline U(IV) coupled with FeS oxidation. **Y. Bi**, M. Stylo, R. Bernier-Latmani, K.F. Hayes

4:55 GEOC 38. Structural study of Sb(V) adsorption on hematite(1-102) surface. **C. Qiu**, F. Majis, P.J. Eng, J. Stubbs, T. Trainor

5:15 GEOC 39. Modelling Eu(III) speciation in a Eu(III)/PAHA/ α Al₂O₃ ternary system. **M.F. Benedetti**, J. Noémie, P. Reiller

MONDAY MORNING

Section A

Colorado Convention Center
Room 710

Geochemistry and Reactive Transport in Nano-Pore Geomaterials

Cosponsored by MPPG†

L. J. Criscenti, Y. Wang, H. Yoon, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 GEOC 40. Non-Darcian flow, imaging, and coupled constitutive behavior of heterogeneous shale. **T. Dewers**, J. Heath, H. Yoon

8:50 GEOC 41. Chemical and mechanical alterations of Portland Cement by aqueous CO₂ and SO₄²⁻ under geologic CO₂ sequestration relevant conditions. **Q. Li**, Y. Lim, Y. Jun

9:10 GEOC 42. Role of advanced reactive surface area characterization in improving predictions of mineral reaction rates in subsurface porous media. **L.E. Beckingham**, S. Zhang, E. Mitnick, D. Cole, L. Yang, L. Anovitz, J. Sheets, A. Swift, T. Kneafsey, G. Landrot, S. Mito, Z. Xue, C. Steefel, D. DePaolo, J. Ajo-Franklin, M. Voltolini

9:30 GEOC 43. Adsorption-enhanced mass transport in carbon nanotube. **S. Riewchotiskakul**, I. Akkutlu, K. Bui

9:50 GEOC 44. Characterization of shale pore topology and chemistry using combined TEM and FIB-SEM. **H. Yoon**, T. Dewers

10:10 Intermission.

10:30 GEOC 45. Neutron investigation of hydrocarbon and water in low-permeability geomaterials. **M. Ding**, M. Hart, R.P. Hjelm, Y. Wang, L. Daemen, Y. Wang, C. Jove-Colon

11:00 GEOC 46. CO₂ hydrate dissolution in pore space of marine sediments. **D. Kyung**, T. Kwon, W. Lee

11:20 GEOC 47. Nanopore wall effect on surface tension of methane. **K. Bui**, I. Akkutlu

11:40 GEOC 48. Understanding radionuclide interactions with layered materials: The effect of nanopore confinement. **Y. Wang**

Section B

Colorado Convention Center
Room 712

Coupled Cycling of Biogeochemical Critical Elements and Contaminants

Fundamental Redox/Elemental Cycling

J. R. Bargar, B. Gu, M. Keiluweit, H. Lin, *Organizers, Presiding*

8:00 GEOC 49. Properties and reactivity of Fe-organic matter associations. **D.L. Sparks**

8:30 GEOC 50. Temperature effects on carbon sequestration by iron oxide coated mineral surfaces. **E. Daugherty**, T. Borch

8:50 GEOC 51. Source of Mn(III)-L in the surface waters of the Saguenay Fjord, Quebec, Canada. **V.E. Oldham**, M. Jones, A. Mucci, B.M. Tebo, G.W. Luther

9:10 GEOC 52. Episodic anoxia drives geochemical formation of reactive oxygen species in coastal environments. **S.A. Murphy**, S. Meng, B.R. Solomon, T.J. Shaw, J.L. Ferry

9:30 GEOC 53. Timescales of soil redox oscillations and the role of iron in the critical zone. **A. Thompson**, B. Ginn, C. Meile, J. Wilmoth, D. Baeellos

10:00 Intermission.

10:20 GEOC 54. Biogeochemical cycling of Fe and S: Where are the electrons going and who is moving them? **K.M. Kemner**, E.J. O'Loughlin, M. Boyanov, D. Antonopoulos, B. Mishra, T. Flynn, D. Latta, M. Scherer, M. Kwon, T.J. Dichristina, K. Skinner

10:50 GEOC 55. Denitrification, reductive diffusion, and rate scaling in natural redox transition zone sediments. **Y. Liu**, S. Yan, C. Liu, L. Shi, J. Shang, H. Shan, J. Zachara, J. Fredrickson, D. Kennedy, C. Resch, C.J. Thompson, S. Fansler

11:10 GEOC 56. Evidence for the coupling of nitrogen and iron redox transformations in marine sediments. **N. Kiriazis**, J. Beckler, M. Taillefer

11:30 GEOC 57. Removal and behavior of metal contaminants during passive co-treatment of synthetic acid mine drainage and synthetic municipal wastewater. **P. Smyntek**, J. Bandstra, R.C. Wagner, W. Stronsnider, C. Marcollo

11:50 GEOC 58. Copper removal by bio-adsorption: A biotechnology approach. **D.F. Rodrigues**

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 3C

2015 Geochemistry Division Medal Symposium

D. B. Kent, *Organizer*

S. E. Fendorf, M. Hochella, *Presiding*

1:15 Introductory Remarks.

1:30 GEOC 59. Incidental nanomaterials in the environment, and why it is critical that we pay attention. **M. Hochella**, J. Dale, R. French, C. Johnson, B. Kim, Y. Yang

2:10 GEOC 60. Combined impact of (bio) chemical and physical processes in defining metal dynamics within soils. **S. Fendorf**, D. Hausladen, S. Ying

2:50 GEOC 61. Energetics of CO₂ confinement: Amorphous carbonates, layered double hydroxides, and metal organic frameworks. **A. Navrotsky**

3:30 Intermission.

3:50 GEOC 62. Geochemical reaction kinetics using nanometer-sized metal-hydroxide and -oxide ions. **W.H. Casey**

4:30 GEOC 63. Kinetics and mechanisms of geochemical processes: It's about interfaces and scale. **D.L. Sparks**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

S. N. Kerisit, *Organizer*

8:00 - 10:00

GEOC 64. Distribution and quantity of iodine with relationship to aquifer formations in northwestern Oklahoma brine waters. **J.R. Wickham**, C. Hoffman, A. Anderson, R. Fenton, D. Edlin

GEOC 65. Distribution of uranium and uranyl minerals near and within hyalite opal. **T.L. Spano**, T.A. Olds, A.M. Burd, J. Kovacs, P.C. Burns

GEOC 66. Seasonal changes in temperature and vadose zone gases due to microbial activity at a crude oil-contaminated site. **E. Warren**, J. Trost, N. Sitota, B. Bekins

GEOC 67. Using geochemical analysis to identify local vs. exotic sources of glacial clasts, Friis Hills, Antarctica. **J. Wrage**, C. Jacobs, A. Lewis, B. Saini-Eidukat

GEOC 68. Toward quantification of Mo and Re speciation in natural anoxic waters: Reverse phase ion pair chromatographic separation of oxythiomolybdate and oxythioperhenate mixtures. **E. Stong**, N. Young, L. Groskreutz, A. Chappaz, T.P. Vorlicek

GEOC 69. Abiotic addition of sulfide to dissolved organic matter. **B.A. Poulin**, J.N. Ryan, A. Stubbins, G. Aiken

[†] Cooperative Cosponsorship

- 70.** Reactive surfaces of altered clay minerals and their effect on the retention of metal(loid)s by clays. **C.A. Legrand**, M. Schindler, M. Hochella
- 71.** Disequilibrium of mineral phases in confined pore spaces in silica-rich coatings. **J. Caplette**, M. Schindler, M. Hochella
- 72.** Numerical simulation of groundwater flow and solute transport: A case study for Manati-Vega Baja limestone karst aquifer, Puerto Rico. **B. Maihemuti**
- 73.** Speciation of arsenic in water at Bakyrchik gold mine, Kazakhstan. **A. Seitkan**, S. Redfern
- 74.** Environmental factors affect production of methylmercury by *Geobacter bemedjensis*. **X. Lu**, H. Lin, B. Gu
- 75.** Thermodynamic studies of uranyl minerals: Enthalpies of formation of metatorbernite, metazeunerite, metaankoleite, metastudite, and metaschoepite. **E. Dzik**, P.C. Burns
- 76.** Copper sorption and lability from iron oxide and organic matter coprecipitates. **F. Koeningmark**, T.M. Vadas
- 77.** Redistribution of solid phase arsenic in aquaculture pond sediments. **S. Hafeznezami**, T. Lin, J.A. Jay
- 78.** Effect of exposure time on Cu(II) adsorption and retention to iron oxyhydroxide nanoparticles. **A.V. Torossian**, J.A. Jacobs, C.S. Kim
- 79.** Dark production of superoxide and hydrogen peroxide during oxidation of reduced dissolved organic matter in natural waters. **R. Marsico**, T. Rand, K. Roe, D.L. Macalady, B. Voelker

TUESDAY MORNING

Section A

Colorado Convention Center
Room 710

Iron Oxides: Formation, Structure, Reactivity and Applications

Formation and Transformation

Cosponsored by MPPG†

T. Borch, W. D. Burgos, Y. Hu, M. Zhu, *Organizers, Presiding*

- 8:00** **80.** Initial mechanisms of iron oxyhydroxide precipitation: Results from molecular spectroscopy and MD simulations. **G. Waychunas**, M. Zhu, H. Zhang, C. Frandsen, J.D. Kubicki, B. Puls
- 8:30** **81.** Mineral formation by cluster self-assembly: Schwertmannite as a partially crystallized nanomineral. **F.M. Michel**, H.E. King
- 9:00** **82.** Size-dependent solubility, stability, and nucleation of ferrihydrite. **T. Hiemstra**
- 9:20** **83.** Interactions among aqueous ions, quartz, and Fe (hydr)oxide polymers during heterogeneous Fe hydroxide nucleation and growth. **C. Dai**, Y. Hu
- 9:40** **84.** Nucleation and growth of synthetic chrysotile nanotubes: Insights into the structure of proto-serpentine. **A. Fernandez-Martinez**, R. Lafay, G. Montes-Hernandez, A. Auzende, A. Poulain
- 10:00** Intermission.
- 10:15** **85.** Fe(III) (hydr)oxide nucleation, and growth: Influences of local saturation changes, structural matches, and hydrophilicity. **Y. Jun**, Y. Hu, J.R. Ray, C.W. Neil, B. Lee
- 10:45** **86.** Natural organic matter impacts on heterogeneous iron(III) (hydr)oxide nucleation, growth, and composition in the presence of arsenate. **C.W. Neil**, B. Lee, Y. Jun
- 11:05** **87.** Thermodynamics of mixing of spinel solid solutions with magnetite end-member Part I: Mixing of normal and inverse spinels. **S. Sahu**, K. Lilova, B. Huang, B.F. Woodfield, A. Navrotsky

- 11:25** **88.** Thermodynamics of mixing of spinel solid solutions with magnetite (Fe₃O₄) end-member Part II: Mixing of two inverse spinels. **K. Lilova**, S.K. Sahu, C. Pearce, K. Rosso, A. Navrotsky
- 11:45** **89.** Nucleation and growth of (Fe,Cr)(OH)₃ nanoparticles: Implications for aqueous Cr removal. **C. Dai**, Y. Hu

Section B

Colorado Convention Center
Room 712

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Cosponsored by COLL

S. E. Mason, *Organizer*
A. Ilgen, S. Lee, *Organizers, Presiding*

8:05 Introductory Remarks.

- 8:10** **90.** Janus, striped and coarse-grained particles. **R. Hernandez**
- 8:40** **91.** Molecular simulation analysis of nanoparticle-biomolecule interactions: challenges and developments. **Q. Cui**
- 9:00** **92.** DFT-MD simulations of the quartz (101)-water interface as a function of pH, ionic strength, salt type and temperature: Implications for dissolution mechanisms. **J.D. Kubicki**, M. DelloStritto, J.O. Soto, M. Fedkin, L. Vitek, A.A. Chialvo, D. Wesolowski, O. Krouth, M. Predota, F. Bellucci, P. Fenter, F. Geiger, S.A. Saslow, A. Bandura
- 9:30** **93.** Structure of water at the quartz(101) surface: Effect of ions and pH. **M. DelloStritto**, J.D. Kubicki, J.O. Soto
- 9:50** Intermission.
- 10:10** **94.** Measure of absolute surface potential at the water-silica nanoparticle interface: Specific ion effects and pH dependence. **M.A. Brown**
- 10:30** **95.** Second harmonic generation studies of aqueous R-cut α -quartz and fused silica interfaces. **F. Geiger**
- 10:50** **96.** Monitoring the influence of ions on acid-base chemistry at the silica/water interface at low and high salt concentration using nonlinear optical methods. **J. Gibbs-Davis**, A. Darlington, M. Azam
- 11:10** **97.** Surface energies for Pt catalysts comprising C, CO, methanol, and glycerol adsorbates in liquid water calculated using density functional theory and molecular dynamics. **C. Bodenschatz**, R. Getman
- 11:40** **98.** Structure dynamics and reactivity of water-saturated supercritical CO₂ and anorthite interface from ab initio molecular dynamics. **V. Glezakou**, M. Lee, B.P. McGrath, R. Rousseau

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient

Kinetics and Mechanisms of Aqueous Geochemical Processes

S. E. Fendorf, D. B. Kent, *Organizers*
G. W. Luther, K. Scheckel, *Presiding*

- 1:15** Introductory Remarks.
- 1:20** **99.** Kinetic competence in bacterial iron oxide reduction: A model system study with proteoliposomes. **J. Zachara**, Z. Wang, L. Shi, G. White, D. Richardson, J. Fredrickson
- 1:55** **100.** Oxygen flux modulates net rates of Fe reduction and Fe solid phase composition in redox dynamic soils. **J. Wilmoth**, A. Thompson
- 2:20** **101.** Reduction kinetics of polymeric (soluble) manganese (IV) oxide (MnO₂) by ferrous iron (Fe²⁺). **M. Siebecker**, G.W. Luther
- 2:40** **102.** Crystallite size effects on the structure and physicochemical properties of ferrihydrite. **X. Feng**, X. Wang, W. Li, M. Zhu, F. Liu, D.L. Sparks

- 3:00** **103.** Molecular-level explanation for humification in peats and soils based on ultrahigh resolution mass spectrometry. **P. Hatcher**, H. Chen, B. Hartman, N. DiDonato, D. Waggoner
- 3:20** Intermission.
- 3:35** **104.** Characterizing high affinity binding sites within bacterial cell envelopes and on bacterial EPS molecules. **J. Fein**, Q. Yu
- 4:00** **105.** Role of NOM complexation in Fe(II) stabilization. **T. Borch**, E. Daugherty, P.S. Nico, B. Gilbert
- 4:25** **106.** Behavior of nitrite with goethite and surface Fe(II)-goethite complexes. **C.J. Matocha**, P. Dhakal
- 4:45** **107.** In-situ Cu(II)-fulvic acid systems studied using complementary spectroscopic techniques. **C. Phillips**, J. Hamilton, D. Hilger, D. Peak
- 5:05** **108.** Adjunctive, disjunctive, and "interjunctive"? Influence of ligand structure on kinetic pathways of ligand exchange. **N.E. Boland**, A.T. Stone, T. Nelson, M. Harned, A. Wildman

Section B

Colorado Convention Center
Room 710

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Cosponsored by COLL

S. Lee, *Organizer*
A. Ilgen, S. E. Mason, *Organizers, Presiding*

- 1:30** **109.** Molecular dynamics simulations of cation adsorption at mica-water interfaces. **I.C. Bourg**
- 2:00** **110.** Adsorption properties of cesium ions to micaceous clay minerals. **M. Okumura**, H. Nakamura, M. Machida, S.N. Kerisit
- 2:20** **111.** New insights into thermal effects of K, Na, Ca, Mg, and Cs-exchanged montmorillonite by in situ USAXS/SAXS study. **S. Lee**, T.B. Fischer, M.R. Stokes, R.J. Klingler, J. Ilavsky, D.K. McCarty, M.O. Wigand, R.E. Winans
- 2:40** **112.** Deciphering populations of Cd surface complexes on gibbsite and kaolinite with combined experimental and computational methods. **P.A. O'Day**, M. Small, N. Govind, H.D. Watts, J.D. Kubicki, K.T. Mueller
- 3:00** **113.** Reactivity of Sb(V) and Pb(II) on environmentally active (1-102) surface of hematite and alumina. **S. Ramadugu**, S.E. Mason
- 3:20** Intermission.
- 3:40** **114.** Co-sorption of Fe(II) with As(III) and As(V) at the solid-water interface of aluminum oxide. **Y. Zhu**, E.J. Elzinga
- 4:10** **115.** Characterization of Ba²⁺ adsorption on oxide minerals: Combined effects of solution and surface properties in complex systems. **J. Han**, S. Chun, L.E. Katz
- 4:30** **116.** Enhanced phosphate sorption on metal-doped birnessite. **Y. Tang**, R. Huang, B. Fields, M. Zhu, S. Zhao
- 4:50** **117.** Microfluidic device to determine the rate of mineral weathering. **D. Ciceri**, A. Allanore

Section C

Colorado Convention Center
Room 710

Iron Oxides: Formation, Structure, Reactivity and Applications

Formation and Transformation

Cosponsored by MPPG†

T. Borch, W. D. Burgos, Y. Hu, M. Zhu, *Organizers, Presiding*

- 1:20** **118.** Iron oxides in reactive systems. **A.M. Vmdedahl**, J.H. Strehlau, J.A. Solits, B.M. Toner, W. Arnold, **R. Penn**

- 1:50** **119.** Effect of solution and solid-phase conditions on the Fe(II)-accelerated transformation of ferrihydrite to lepidocrocite and goethite. **T.D. Waite**, D. Boland, R. Collins, C. Miller
- 2:20** **120.** Abiotic phase transformation of schwertmannite pelagic particles in acidic pit lakes: Influence on metal mobility. **J. Sánchez-España**, I. Yusta
- 2:40** **121.** Mineralogical changes in goethite during goethite-Fe(II) atom exchange: A microscopic and 55Fe-tracer study. **P. Joshi**, C. Gorski
- 3:00** **122.** Revisiting the α -Fe₂O₃ (0001) phase diagram using a surface specific GGA + Ud+p approach. **X. Huang**, S. Ramadugu, S.E. Mason
- 3:20** Intermission.
- 3:35** **123.** Dissolution, aggregation, surface chemistry, and biological effects of iron oxide nanomaterials. **V.H. Grassian**
- 4:05** **124.** Structure and thermodynamics of ferrihydrite from first principles. **M. Sassi**, K. Rosso
- 4:25** **125.** Withdrawn.
- 4:45** **126.** On the join between goethite and hematite: X-ray diffraction and FT-IR studies of "hydrohematite". **P.J. Heaney**, K.M. Peterson, F.T. Ling, J.E. Post
- 5:05** **127.** Technetium incorporation into goethite: An atomic-scale investigation. **F.N. Smith**

WEDNESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient

Kinetics and Mechanisms of Aqueous Geochemical Processes

S. E. Fendorf, D. B. Kent, *Organizers*
M. Hochella, A. L. Seyferth, *Presiding*

8:00 Introductory Remarks.

- 8:05** **128.** Determining chemical and microbial Fe(II) oxidation kinetics in situ: Iron oxidizing bacteria compete with chemical Fe(II) oxidation. **G.W. Luther**, C. Chan, D. Emerson
- 8:40** **129.** Mechanisms and kinetics of contaminant transformation by Mn(IV) oxides. **M.A. Ginder-Vogel**
- 9:05** **130.** Transformation of triclinic to hexagonal birnessite by common biological buffers. **F. Ling**, P. Heaney, X. Gao, J. Post
- 9:45** **131.** Co-sorption of aqueous Fe(II) and Mn(II) in anoxic aluminum-oxide suspensions. **E. Elzinga**, Y. Zhu
- 10:05** Intermission.
- 10:20** **132.** Iron mineral formation in an iron- and sulfide-rich early ocean model habitat. **E. Koeksoy**
- 10:40** **133.** Time resolved in situ spectroscopic studies of aqueous geochemical reactions. **D. Peak**
- 11:05** **134.** Novel synchrotron-based hard x-ray approaches to understanding controls on metal ion fate in subsurface and terrestrial environments. **K.M. Kemner**, M. Boyanov, B. Mishra, E.J. O'Loughlin, S.L. O'Brien, D. Sholto-Douglas, B. Lai, M. Balasubramanian, R. Gordon, S. Kelly, V. Bailey
- 11:30** **135.** Tackling rapid reaction kinetics at the mineral-water interface using quick-scanning X-ray absorption spectroscopy. **W. Li**, M. Siebecker, D.L. Sparks
- 11:50** **136.** Development of a rate law for arsenite oxidation by manganese oxides to assess the impact of the recycling of arsenic on microbial respiration processes. **S. Owings**, M. Taillefer

Section B

Colorado Convention Center
Room 712

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Cosponsored by COLL

A. Ilgen, *Organizer*

S. Lee, S. E. Mason, *Organizers, Presiding*

8:30 GEOC 137. Pathways and kinetics of Fe(II)-catalyzed redox recrystallization of Fe(III)-oxides. K. Rosso, V. Alexandrov, P. Zarzycki, S.N. Kerisit, M. Sassi

9:00 GEOC 138. Contribution of thiol structure on reduction kinetics of iron and manganese oxides. E.M. Eitel, M. Taillefert

9:20 GEOC 139. Iron electron transfer and atom exchange in clay minerals. D.E. Latta, W. Premaratne, K. Rosso, M. Scherer, A. Neumann

9:50 GEOC 140. Controls on the reactivity of clay structural Fe(II)/Fe(III) redox couple. A.G. Ilgen, D.R. Dunphy, J.N. Krueck, R.K. Kukkadapu, J.M. Cerrato, J.M. Argo, R.E. Washington

10:10 Intermission.

10:30 GEOC 141. Characterizing the dynamics of iron oxide aggregation and reactivity in aqueous systems. A.M. Vindedahl, J.H. Strehlau, W. Arnold, R. Penn

11:00 GEOC 142. Resolving conflicting effects of surfaces, ligands, and concentration on the evolution of reactive oxygen species during iron oxidation. S. Meng, B.R. Solomon, J.L. Ferry

11:20 GEOC 143. Effect of live *Acremonium strictum* KR21-2 fungus on the mobility of REEs during the biooxidation of Mn(II). Q. Yu, T. Ohnuki, K. Tanaka, N. Kozai, F. Sakamoto, Y. Tani

11:40 GEOC 144. Prebiotic role of fluoride minerals in the montmorillonite catalyzed synthesis of RNA. M.F. Aldersley, P.C. Joshi

Section C

Colorado Convention Center
Room 710

Iron Oxides: Formation, Structure, Reactivity and Applications**Biotic and Abiotic Redox Reactions**

Cosponsored by MPPG†

T. Borch, W. D. Burgos, Y. Hu, M. Zhu, *Organizers, Presiding*

8:00 GEOC 145. Speciation of particulate iron in marine geochemical gradients. B.M. Toner, P.J. Lam

8:30 GEOC 146. Iron oxide – aqueous Fe(II) standard reduction potential measurements: A mediated electrochemical study. R.A. Edwards, A.C. Costa, C.A. Gorski

8:50 GEOC 147. High spatial resolution analysis of biogeochemical iron cycling and iron mineral formation in freshwater sediments. C.L. Lockwood, T.K. Himpel, F. Schaedler, C. Schmidt, A. Kappler

9:10 GEOC 148. Effect of natural and engineered electron transfer in living cells on the reduction of iron oxides. K.K. Sand, M. TerAvest, C.M. Ajo Franklin, J. De Yoreo

9:30 GEOC 149. Harnessing community genomics to understand microbial iron and sulfur cycling in estuary sediments. B.J. Baker

10:00 Intermission.

10:15 GEOC 150. Biogeochemistry: Redox cycling of Fe(II) and Fe(III) in magnetite by Fe-metabolizing bacteria. J. Byrne, N. Klüglein, C. Pearce, E. Appel, A. Kappler

10:45 GEOC 151. Reactivity of bio-reduced iron-bearing phyllosilicates towards nitro-aromatic compounds. W.D. Burgos, F. Luan, C. Gorski

11:05 GEOC 152. Role of microbial communities in linking Fe (hydr)oxide transformation and nutrient cycling. M.A. Ginder-Vogel, E. Tomaszewski, J. Meija

11:25 GEOC 153. Characterization of redox potential and reactivity of sorbed Fe(II). D. Fan, A. Hinkle, R. Johnson, P.G. Tratnyak

11:45 GEOC 154. Evidence for the existence of soluble Fe(III) complexes in sedimentary environments. M. Taillefert, J. Beckler

WEDNESDAY AFTERNOON**Section A**

Colorado Convention Center
Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient**Structure and Bonding at the Mineral-water Interface**

S. E. Fendorf, D. B. Kent, *Organizers*

B. C. Bostick, M. A. Ginder-Vogel, *Presiding*

1:30 Introductory Remarks.

1:35 GEOC 155. Structural environments of ligands associated with amorphous ferric hydroxides, and their impact on goethite nucleation. S.C. Myneni, N. Crompton, J. Majzlan

2:10 GEOC 156. Silicate sorption on Fe oxyhydroxides: Identification of reaction sites from molecular spectroscopy, and reactive force field modeling of sorption/desorption processes. G. Waychunas, M. Kanematsu, J. Bolly, C.B. Keller, A. Wallace

2:35 GEOC 157. Alkaline earth metal ion sorption processes: From adsorption to precipitation. L.E. Katz, J. Choi, J. Han, L.J. Criscenti

3:00 GEOC 158. Ligand controlled chemical fate of CeO₂ nanoparticles in heterogeneous geochemical system. Y. Arai

3:20 Intermission.

3:35 GEOC 159. Adsorption and reaction at mineral/water interfaces: Relevance to natural products and agricultural chemicals. A.T. Stone

4:00 GEOC 160. Sulfate coordination environment in Schwesmannite. X. Wang, C. Gu, X. Feng, M. Zhu

4:20 GEOC 161. Identification and quantification of sulfate surface complexes on ferrihydrite. C. Gu, X. Wang, Z. Wang, M. Zhu

4:40 GEOC 162. Organo-mineral associations in agricultural soils: insights from multi-elemental STXM-NEXAFS analysis. C. Chen, J. Wang, J.J. Dynes, D.L. Sparks

5:00 GEOC 163. Ternary complexation of dissolved organic matter in kaolinite-Fe(III)-organic acid systems: An EXAFS spectroscopic study. J. Yang, D.L. Sparks, N. Bolan, R. Cornelia, W. Pan

5:20 GEOC 164. Macroscopic and microscopic investigation of adsorption and precipitation of Zn on γ-alumina as affected by As. Y. Wang, T. Fan, D. Zhou, W. Li, M. Zhu, D.L. Sparks

Section B

Colorado Convention Center
Room 710

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Cosponsored by COLL

S. E. Mason, *Organizer*

A. Ilgen, S. Lee, *Organizers, Presiding*

1:30 GEOC 165. Uncovering the local atomic structure of a hydrated amorphous magnesium carbonate: The computational chemistry and total scattering iterative methodology. C. White, N. Henson, L. Daemen, M. Hartl, K. Page

2:00 GEOC 166. How does the ionic strength control the nucleation of manganese oxide nanoparticles at quartz-water interfaces? H. Jung, Y. Jun

2:20 GEOC 167. In-situ observation of a single-layer gibbsite film at the muscovite (001)-water interface. S. Lee, M. Schmidt, T.T. Fister, N.C. Sturchio, K.L. Nagy, P. Fenter

2:40 GEOC 168. Mineralogical constraint of reverse weathering reactions. E.M. Saad, Y. Tang

3:00 Intermission.

3:20 GEOC 169. Role of citric acid in CaCO₃ crystallization. D.J. Tobler, J. Rodriguez Blanco, K. Dideriksen, N. Bovet, K.K. Sand, S.S. Stipp

3:40 GEOC 170. Role of borate ions in CaCO₃ crystallization. J. Rodriguez-Blanco, K. Dideriksen, D. Tobler, K. Sand, B. Vallina, L.G. Benning, S.S. Stipp

4:00 GEOC 171. Effect of varying cation:anion ratio on growth of sparingly-soluble minerals. J. Bracco, A.G. Stack, S.R. Higgins

4:20 GEOC 172. Impact of carbonate substitution on the interfacial kinetics and bulk stability of hydroxyapatite. L.N. Lammers

4:40 Concluding Remarks.

Section C

Colorado Convention Center
Room 710

Iron Oxides: Formation, Structure, Reactivity and Applications**Environmental Applications**

Cosponsored by MPPG†

T. Borch, W. D. Burgos, Y. Hu, M. Zhu, *Organizers, Presiding*

1:15 GEOC 173. Reactions of nanoscale zero-valent iron (nZVI) with heavy metals: Atomic resolution imaging and applications. W. Zhang, L. Ling

1:45 GEOC 174. Contaminant removal from water through oxidation-reduction and adsorption on iron oxides generated during electrocoagulation. D. Giammar, C. Pan, L. Wang, J.G. Catalano

2:15 GEOC 175. Interaction of Cr(III) and Cr(VI) with hematite studied by second harmonic generation. F. Geiger

2:35 GEOC 176. Sequestration of arsenate in zero-valent iron nanoparticles: Visualization of intraparticle reactions at Angstrom resolution. L. Ling, W. Zhang

2:55 GEOC 177. Redox reactions and oxidant degradation by Fe(II) and iron oxides in complex groundwater systems. J.H. Strehlau, B.M. Toner, W. Arnold, R. Penn

3:15 Intermission.

3:30 GEOC 178. Solute transport with pH variations through soil. S. Bryant, V. Prigobbe

4:00 GEOC 179. Immobilization of arsenate in soil and groundwater using starch-stabilized magnetite nanoparticles. D. Zhao, Q. Liang

4:30 GEOC 180. Withdrawn.

4:50 GEOC 181. Reactivity of various kinds of magnetite to adsorb heavy metals from contaminated wastewater. M. Usman, Z. Ajmal

5:10 GEOC 182. Density functional theory modeling of ferrihydrite nanoparticle charging and adsorption behavior. J.D. Kubicki, E. Cerkez, D.R. Strongin

THURSDAY MORNING**Section A**

Colorado Convention Center
Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient**Biogeochemical Processes in Soils and Sediments**

S. E. Fendorf, D. B. Kent, *Organizers*

A. Navrotsky, J. Stuckey, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC 183. Rhizosphere processes controlling metal speciation and bioavailability in soils. D.H. McNear

8:30 GEOC 184. Fate, transport, and cycling of hexavalent chromium in the soil environment. J. Fischel, D.L. Sparks

8:50 GEOC 185. Potential impacts of sea level rise on arsenic mobility and cycling. J.J. LeMonte, R. Tappero, D.L. Sparks

9:10 GEOC 186. Tracking the temporal dynamics of intracellular lead speciation in a model green alga by resonant X-ray emission spectroscopy. T. Stewart, J. Szielachetko, L. Sigg, R. Behra, M. Nachttegaal

9:30 GEOC 187. Impact of sea level rise on arsenic and chromium sorption in *Phragmites australis* root plaques. M. Fischel, D.L. Sparks

9:50 Intermission.

10:05 GEOC 188. Fate of arsenic at the soil-plant interface: Impacts of soil-incorporation of plant-available silicon on arsenic desorption, iron oxide plaque, and plant uptake. A.L. Seyfferth, R. Gill, E. Penido

10:30 GEOC 189. Root cell wall polysaccharides are involved in Cd hyperaccumulation in *Sedum alfredii*. T. Li, Q. Tao, X. yang, D.L. Sparks, Y. Liang

10:50 GEOC 190. Scaling up molecular reactions to ecosystem processes: Organic matter degradation controlled phosphorus cycling in the Chesapeake Bay. D. Jaisi, S. Joshi, R. Kukkadapu, D.L. Sparks

11:10 GEOC 191. Identification of biologically inert phosphorus pools in river waters: An application of phosphate oxygen isotope ratios of particulate P pools in East Creek, a Chesapeake Bay watershed. K. Bear, S.R. Joshi, D. Jaisi

11:30 GEOC 192. Using phosphorus distribution in soils and sediments to understand arsenic biogeochemistry. D.G. Strawn

11:50 GEOC 193. Using synchrotron-based techniques to elucidate the fate of militarily relevant metals in the environment. J. Seiter, B. Lafferty, R. Tappero, A. Bednar, A. Kennedy, S. Brasfield, M. Chappell

Section B

Colorado Convention Center
Room 712

Precipitation, Dissolution and Adsorption under Confinement**Mineral Dissolution and Precipitation**

A. Fernandez-Martinez, A. G. Stack, *Organizers, Presiding*

8:45 Introductory Remarks.

8:50 GEOC 194. Mineral precipitation in porous materials. A.G. Stack, A. Gordon, H. Wang, A. Fernandez-Martinez, L. Anovitz, K. Page

9:10 GEOC 195. Precipitates of Al(III), Sc(III), and La(III) at the muscovite-water interface. F. Geiger

9:30 GEOC 196. Nucleation and growth of barite (BaSO₄) observed in-situ in porous media using X-ray computed tomography. J. Godinho, A.G. Stack, M. Rivers

9:50 Intermission.

10:10 GEOC 197. Effects of reactivity and flow rate on dissolution of carbonates from the nano to the centimeter scale. L. Anovitz, C.A. Novack, T.R. Prisk, J. Ilavsky, J. Hammons, D.F. Milder, M.J. Wasbrough, D.L. Jacobson, D.S. Hussey

10:40 GEOC 198. Evolution of silica walls of nanopores filled of water and ions. D. Rébiscoul, J. Cambedouzo, M. Brossel

11:00 GEOC 199. In situ X-ray diffraction and infrared spectroscopic investigation of magnesite precipitation in interfacial water films. Q.R. Miller, J.P. Kaszuba, H.T. Schaefer, M.E. Bowden, C.J. Thompson, J.S. Loring

11:30 GEOC 200. Nanogeochemistry issues arising from borosilicate leaching experiments. S. Gin, P. Jollivet, F. Angélli, P. Frugier

THURSDAY AFTERNOON**Section A**

Colorado Convention Center
Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient**Biogeochemical Processes in Soils and Sediments**

S. E. Fendorf, D. B. Kent, *Organizers*

D. Giammar, D. H. McNear, *Presiding*

1:30 Introductory Remarks.

- 1:35 GEOC 201.** Environmental fate and transformation of engineered nanoparticles from consumer products. K. Scheckel, E. Lombi, E. Donner, R. Sekine, B. Miller, K. Vasiliev
- 2:00 GEOC 202.** Uranium(VI) uptake on iron oxide surfaces: The transition from adsorption to precipitation. D. Giammar, A. Singh, V. Mehta, L.D. Troyer, F. Maillot, J.G. Catalano
- 2:25 GEOC 203.** Chemistry of depleted uranium in military firing range soils. B. Lafferty, J. Seiter, A. Bednar, R. Tappero, F. Hill, M. Chappell
- 2:45 GEOC 204.** Kinetics-based approaches of predicting aqueous arsenic concentrations in soil and groundwater systems. B.C. Bostick, J. Sun, S. Chillrud, A. van Geen, B. Mailloux
- 3:10 GEOC 205.** Wetland hydrology dictates organic carbon reactivity controlling microbial arsenic release within the Mekong Delta. J. Stuckey, M. Schaefer, B. Kocar, S. Benner, S. Fendorf
- 3:30 GEOC 206.** Development and applications of stabilized nanoparticles for in situ immobilization of metals/metalloids in soil and groundwater. D. Zhao, X. Zhao, W. Xie, X. Wang, S. Tian
- 3:50 Intermission.**
- 4:05 GEOC 207.** Fe(III) affects arsenic mobilization and secondary mineral precipitate phase, morphology, and coverage during arsenopyrite oxidation. C.W. Neil, Y. Jun
- 4:25 GEOC 208.** Copper sequestration by black carbon in contaminated soil using STXM-C K-edge and Cu L-edge XANES spectroscopy. J. Yang, J. Liu, J. Wang, D.L. Sparks
- 4:45 GEOC 209.** Role of chlorite interlayers in Zn sequestration in smelter-affected soils. J. Hamilton, D. Peak
- 5:25 GEOC 211.** Modeling the impact of variable pH and dissolved salt concentration on sorption and transport of nickel, zinc, and lead in a quartz-sand aquifer. D.B. Kent, M. Kohler, G. Ng

Section B

Colorado Convention Center
Room 712

Precipitation, Dissolution and Adsorption under Confinement

Chemistry of Aqueous Solutions

A. Fernandez-Martinez, A. G. Stack, *Organizers, Presiding*

- 1:30 GEOC 212.** Adsorption and precipitation of Zn and Ni in nanoporous silica. J.M. Nelson, J.R. Bargar, G.E. Brown, K. Maher
- 1:50 GEOC 213.** Hydration-induced morphological evolution at glass-liquid interfaces. J. Ryan, P. Fiekie, S.N. Kerisit
- 2:10 GEOC 214.** Inhibition mechanism of DTPMP based on the analysis of barite nucleation and crystal growth using laser detection method and novel crystal growth model supported by cryo-TEM measurements. Z. Dai, F. Zhang, A.T. Kan, Z. Zhang, Y. Liu, L. Wang, F. Yan, N. Bhandari, V. Bolanos, M.B. Tomson
- 2:30 GEOC 215.** Inelastic neutron scattering techniques for the study of water confined in swelling clay minerals. M. Jimenez-Ruiz
- 3:00 Intermission.**
- 3:20 GEOC 216.** Aqueous geochemistry of water confined in clay and silica nanopores. I.C. Bourg
- 3:50 GEOC 217.** Structure, dynamics, and reactivity of geofluids in confined geometries. D. Cole, D.W. Hoyt, A. Kolesnikov, T. Liu, E. Mamontov, K.T. Mueller, S. Gautam, G. Rother, J. Sheets, A. Striolo, N. Washton, S. Welch
- 4:20 GEOC 218.** Confined pore spaces in mineral coatings of contaminated soils: Disequilibrium between abiotic and biotic processes and their environment. M. Schindler, M. Hochella
- 4:40 Concluding Remarks.**

HIST

Division of the History of Chemistry

S. C. Rasmussen, *Program Chair*

BUSINESS MEETINGS:

HIST Division Executive Committee Meeting, 5:00 PM: Sun

SUNDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Tower Court A

HIST Tutorial and General Papers

S. C. Rasmussen, *Organizer, Presiding*

- 1:00 HIST 1.** HIST Tutorial: Elemental sulfur – a natural (and unnatural) resource. M.E. Schott
- 1:40 HIST 2.** James Hyatt, chemist, scientist, and communicator: A man of his times. W.P. Palmer
- 2:10 HIST 3.** Inaccuracy of dates in accounts of the history of chemistry: A case of deliberate falsification? J. Gal
- 2:40 Intermission.**
- 2:55 HIST 4.** Rules, formulas, names: The lexical legacy of the 1892 Geneva Nomenclature Congress. E. Hepler-Smith
- 3:25 HIST 5.** NMR characterization of resin blocks from 13th century Java Sea Wreck. J.B. Lambert, A. Levy
- 3:55 HIST 6.** Investigation into the first isolation of carbonic acid. R.L. Hudson
- 4:25 HIST 7.** Foundation and influence of the Sydney School of Coordination Chemistry. A.T. Baker

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Tower Court A

Chemical Technology in Antiquity

Cosponsored by MPPG†

S. C. Rasmussen, *Organizer*
C. L. Heth, *Presiding*

- 8:25** Introductory Remarks.
- 8:30 HIST 8.** Pigments in antiquity: Colorful forerunners of every aspect of modern chemistry. M. Orna
- 9:15 HIST 9.** First artificial material: Ceramics from prehistory to the fall of Rome. N. Zumbulyadis
- 10:00 Intermission.**
- 10:15 HIST 10.** From honey wine to cultivation of the grape: An early history of fermented beverages. S.C. Rasmussen
- 11:00 HIST 11.** Metals of antiquity and their alloys. V.V. Mainz

MONDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Tower Court A

Chemical Technology in Antiquity

Cosponsored by MPPG†

S. C. Rasmussen, *Organizer, Presiding*

- 1:30 HIST 12.** The skin they were in: Leather and tanning in antiquity. C.L. Heth
- 2:00 HIST 13.** Modern chemistry of the ancient chemical processing of organic dyes and pigments. Z.C. Koren
- 2:45 HIST 14.** Scented oils and perfumes in antiquity. N. Balasubramanian
- 3:15 Intermission.**

- 3:30 HIST 15.** Soap production and use in antiquity. K.L. Konkol, S.C. Rasmussen
- 4:00 HIST 16.** Modern materials in antiquity: An early history of the art and technology of glass. S.C. Rasmussen

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

S. C. Rasmussen, *Organizer*

- 8:00 - 10:00**
- 11-12, 14.** See previous listings.

TUESDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Tower Court A

Modern Chemical Warfare: History, Chemistry, Toxicology, Morality

J. Gal, *Organizer*
J. A. Asper, *Presiding*

- 8:00** Introductory Remarks.
- 8:05 HIST 17.** Modern chemical warfare: A historical overview. J. Gal
- 8:35 HIST 18.** German chemists and chemical weapons: Fritz Haber and his legacy. S. Everts
- 9:05 HIST 19.** Chemical warfare and French chemists. P. Laszlo
- 9:35 Intermission.**
- 9:50 HIST 20.** American chemists and chemical warfare. T.T. Tidwell
- 10:20** "Haber: The Father of Chemical Warfare", a film by Daniel Ragussis.
- 11:00** Q&A with Daniel Ragussis.
- George C. Pimentel Award in Chemical Education: Symposium in Honor of I. Dwayne Eubanks**
- Sputnik to Smartphones: A Half-Century of Chemistry Education**
Sponsored by CHED, Cosponsored by HIST†

TUESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Tower Court A

Modern Chemical Warfare: History, Chemistry, Toxicology, Morality

J. Gal, *Organizer, Presiding*

- 1:00 HIST 21.** Chemical weapons: Clinical description and discussion of basic injuries. D. Gilmore
- 1:30 HIST 22.** Aiming chemical weapons at student engagement: Chemistry and war as a first year seminar. J.A. Asper
- 2:00 HIST 23.** Modern chemical warfare: A philatelic chronology. D. Rabinovich
- 2:30 HIST 24.** Chemical warfare: The American WWII aftermath. D.C. Neckers
- 3:00 Intermission.**
- 3:15 HIST 25.** Nerve agents: From inception to current concepts. S.W. Wiener
- 3:45 HIST 26.** Ethics of chemical weapons research. J.D. Kovac
- 4:15 HIST 27.** OPCW: Working for a world free of chemical weapons. D. Feakes, A. Kelle
- George C. Pimentel Award in Chemical Education: Symposium in Honor of I. Dwayne Eubanks**
- Sputnik to Smartphones: A Half-Century of Chemistry Education**
Sponsored by CHED, Cosponsored by HIST†

I&EC

Division of Industrial and Engineering Chemistry

P. Smith and M. Moore, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

- Nanostructured Porous Polymers: Synthesis, Properties and Applications**
(see PMSE, Sun, Mon)
- Drug Delivery and Drug Device Combination Product**
(see PMSE, Tue, Wed, Thu)
- Advances in Analytical Separations**
(see ANYL, Mon)
- 50th Anniversary of the NUCL Division**
(see NUCL, Tue, Wed)
- Glenn T. Seaborg Award: Symposium in Honor of Heino Nitsche**
(see NUCL, Sun, Mon)
- Chemical Angel Network: Chemists Investing in Chemical Companies**
(see PROF, Mon)

SOCIAL EVENTS:

Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

Business Meeting, 12:00 PM: Sun
Business Meeting, 6:30 PM: Mon

SUNDAY MORNING

Section A

Embassy Suites Denver-Downtown Convention Center
Crystal Ballroom A

ACS Award in Separations Science & Technology: Symposium in Honor of Richard D. Noble

D. L. Gin, *Organizer, Presiding*

- 8:30 I&EC 1.** Double salt ionic liquids with unique chemical environments for separations. R.D. Rogers, H. Wang, S.P. Kelley
- 9:05 I&EC 2.** Phase change ionic liquids for post-combustion CO₂ capture. J.F. Brennecke, S. Seo, L.D. Simoni, M.A. Stadtherr
- 9:40 I&EC 3.** Reverse osmosis membranes research-current development and future directions. N.N. Li, M. Tsai, J. Li
- 10:15 I&EC 4.** Materials and devices to enable low-energy-intensive gas separations. W. Koros
- 10:50 I&EC 5.** Improving distillation: Not an oxymoron. P. Wankat

Section B

Embassy Suites Denver-Downtown Convention Center
Crystal Ballroom B

Uranium in Seawater

The Chemistry

Cosponsored by CEI and MPPG†

P. F. Britt, *Organizer*
R. D. Rogers, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:05 I&EC 6.** Uranium and U. C.H. Middlecamp

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

8:25 I&EC 7. Design and synthesis of pyridine-based and amidoxime-based ligands for uranium adsorption. **C. Zhang, S. Dai**

8:45 I&EC 8. Polymer-supported amines and aminophosphonates as uranyl-selective extractants. **S. Alexandratos, R.C. Sellin, M. Florent, X. Zhu**

9:05 I&EC 9. Complexation of glutarimidedioxime with V(V), a major competing ion for the extraction of U(VI) from seawater. **C. Leggett, L. Rao**

9:25 Intermission.

9:45 I&EC 10. Accelerating extraction of uranium from seawater through high-performance computational science: Challenges and advances. **D.A. Penchoff, D.M. Jenkins, G.K. Schweitzer, R.J. Harrison**

10:05 I&EC 11. Development of bifunctional chelators for selective extraction of uranium from seawater. **C.W. Abney, J.C. Gihlula, W. Lin**

10:25 I&EC 12. Density functional theory methods to predict ligands pKa's, and stability constants for uranyl complexes. **V. Bryantsev, N. Mehio**

10:45 I&EC 13. Combinatorial peptid screening to discover new ligands for uranyl binding. **B. Parker, A. Knight, S. Vukovic, M.B. Francis, J. Arnold**

11:05 I&EC 14. Determination of formation constants for Uranyl(VI) complexes in aqueous solution by spectroscopic techniques. **R.D. Hancock**

11:25 I&EC 15. Nanofiber chitin mats for coextraction of value added metals from seawater: Improving the economics of uranium recovery. **R.D. Rogers, S.P. Kelley, G. Gurau, J.L. Shamshina**

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

ACS Award in Separations Science & Technology: Symposium in Honor of Richard D. Noble

D. L. Gin, Organizer, Presiding

2:00 I&EC 16. Award Address (ACS Award in Separations Science & Technology). Recent advances in the design of functional room-temperature ionic liquid-based materials for selective gas separations. **D.L. Gin, Y. Kohno, M.G. Cowan, W.M. McDanel, Z.V. Singh, Z. Shi, R.D. Noble**

2:35 I&EC 17. Influence of propane on CO₂/CH₄ and N₂/CH₄ separations in CHA zeolite membranes. **J.L. Falconer, H.H. Funke, R.D. Noble, T. Wu, M. Diaz, R. Zhou**

3:10 I&EC 18. Properties of membrane materials for solar fuels generators. **C.A. Koval**

3:45 I&EC 19. Ionic polyimides: New dimensions in the design of polymer materials for membrane separations. **J. Bara, J.D. Roveda, M. Shannon, D. Wallace**

4:20 I&EC 20. Composite Pd alloy membranes for high temperature hydrogen production with CO₂ capture. **J.D. Way, H. Abu El Hawa, S.N. Paglieri, S. Lundin, N. Patki**

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.

Section B

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom B

Uranium in Seawater

The Sorbents

Cosponsored by CEI and MPPG‡

R. D. Rogers, Organizer

P. F. Britt, Organizer, Presiding

1:00 I&EC 21. Improvements of radiation grafting of selective ligands onto polymeric substrates to produce high-capacity adsorbents for harvesting uranium from seawater. **T.C. Dietz, C. Tomaszewski, M.A. Adel-Hadadi, A. Barkatt, M. Al-Sheikhly**

1:20 I&EC 22. Advanced fiber adsorbents for recovery of uranium from seawater prepared via controlled radical polymerization. **S. Brown, S. Chatterjee, J.C. Johnson, L. Kuo, G.A. Gill, T. Saito**

1:40 I&EC 23. Fibrous adsorbents prepared by SI-ATRP for the recovery of uranium from seawater. **S. Brown, L. Kuo, S. Chatterjee, J.C. Johnson, Y. Yue, G.A. Gill, T. Saito, S. Dai**

2:00 I&EC 24. Preparation of uranium adsorbents by radiation-induced graft polymerization. **C. Janke, S. Das, R. Mayes, C. Tsouris, S. Dai**

2:20 I&EC 25. Nanofiber adsorbents for uranium extraction from seawater. **S. Xie, X. Liu, B. Zhang, H. Ma, C. Ling, M. Yu, J. Li**

2:40 Intermission.

3:00 I&EC 26. Performance enhancing amidoxime adsorbent for uranium recovery from seawater. **S. Das, C. Janke, R. Mayes, C. Tsouris, S. Dai**

3:20 I&EC 27. Development of novel porous sorbents for extraction of uranium from seawater. **W. Lin**

3:40 I&EC 28. Carbon materials for seawater uranium extraction. **R.T. Mayes, J. Gorka, Y. Yue, S. Dai, G. Gill, L. Kuo, J. Wood**

4:00 I&EC 29. Novel nanostructured sorbent materials for the collection and recovery of uranium from seawater and other solutions. **R.S. Addleman, W. Chouyok, J.W. Pittman, K.M. Nell, S. Peterson, M.G. Warner, C. Warner**

4:20 I&EC 30. Uranium-from-seawater sorbents from fishing industry waste – from batch to continuous production. **G. Gurau, J.L. Shamshina, S.P. Kelley, R.D. Rogers**

4:40 I&EC 31. Porous polymeric adsorbents for the recovery of uranium from seawater. **Y. Yue**

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

Uranium in Seawater

Sorbents and Analysis

Cosponsored by CEI, MPPG‡ and NUCL

P. F. Britt, R. D. Rogers, Organizers

S. Dai, Presiding

8:00 I&EC 32. Fiber functionalization via novel ligand for uranium recovery from seawater. **S. Chatterjee, S. Brown, J. Johnson, R.T. Mayes, C.A. Grant, B.P. Hay, T. Saito**

8:20 I&EC 33. Synthesis and properties of amidoxime-based fibrous adsorbents for extraction of uranium from seawater by radiation-induced graft polymerization. **G. Wu, J. Hu, Z. Xing, L. Xu, R. Li, S. Li**

8:40 I&EC 34. Effects of crosslinking in polymer brush uranium adsorbents. **J. Johnson, S. Brown, S. Chatterjee, T. Saito**

9:00 I&EC 35. Application of synchrotron radiation technique in extraction uranium from seawater. **L. Zhang, C. Jin, J. Zhou, J. Wang**

9:20 I&EC 36. Adsorption behavior of uranium from seawater on amidoxime-based UHMWPE prepared by radiation induced graft polymerization. **H. Ma, X. Liu, C. Ling, X. Yang, J. Hu, S. Li, Z. Xing, J. Li, G. Wu**

9:40 Intermission.

10:00 I&EC 37. Chemical and structural characterization of high density polyethylene (HDPE) based sorbents developed for the binding of uranium from seawater. **M.G. Warner, S.M. Peterson, B. Arey, I. Arslan, M.H. Engelhard, B. Naes, D. Willingham, C. Barrett, R.S. Addleman**

10:20 I&EC 38. Uranium from seawater marine testing program at the Pacific Northwest National Laboratory: Overview. **G.A. Gill, L. Kuo, J. Wood, J.E. Strivens, M.E. Cobb, G. Bonheyo, R. Jeters, J. Park, T. Khangaonkar, R.S. Addleman, M.G. Warner, S.M. Peterson, K. Buesseler, C. Breier, E. D'Alessandro**

10:40 I&EC 39. Elution of uranium and transition metals from amidoxime-based sorbents for sequestering uranium from seawater. **H. Pan, L. Kuo, G.A. Gill, C.M. Wai**

11:00 I&EC 40. Separation and concentration of Uranium from sea water using aptamer receptors. **R.F. Williams**

11:20 I&EC 41. Matrix elimination for the determination of uranium in seawater using inductively coupled plasma mass spectrometry. **J. Wood, G.A. Gill, K. Choe**

11:40 I&EC 42. Adsorbent pretreatment and batch kinetic experiments for uranium adsorption testing and modeling. **S. Das, W. Liao, R. Mayes, C.J. Janke, S. Dai, C. Tsouris**

ACS Award in Industrial Chemistry: Symposium in Honor of Thomas J. Colacot

Sponsored by BMGT, Cosponsored by ANYL and I&EC

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

Uranium in Seawater

Analysis and Toxicity/Cost

Cosponsored by CEI and MPPG‡

P. F. Britt, R. D. Rogers, Organizers

G. A. Gill, Presiding

1:00 I&EC 43. Characterization and testing of adsorbent materials to extract uranium from natural seawater. **L. Kuo, G.A. Gill, J. Wood, J.E. Strivens, M.E. Cobb, C. Janke**

1:20 I&EC 44. Selectivity and kinetic behavior of heavy metal and radionuclides on supported ion-exchange adsorbent. **W.T. Honeycutt, E.B. Kadossov, A.W. Appleby, N.F. Materer**

1:40 I&EC 45. Toxicity of the adsorbent materials used to extract uranium from seawater. **J. Park, R. Jeters, G.A. Gill, L. Kuo, G. Bonheyo**

2:00 I&EC 46. How biofouling impacts uranium sorbent material performance and what can be done to mitigate the effect. **G.T. Bonheyo, J. Park, R. Jeters, E.M. Winder, L. Kuo, G.A. Gill**

2:20 I&EC 47. Homogeneous blending of chitin with biopolymers for advanced biodegradable sorbents for uranium extraction from seawater. **J. Bandomir, S.P. Kelley, J.L. Shamshina, G. Gurau, R.D. Rogers**

2:40 I&EC 48. Dual functional chitin based sorbents for coextraction of aqueous copper and uranium. **S.P. Kelley, J.L. Shamshina, G. Gurau, R.D. Rogers**

3:00 Intermission.

3:20 I&EC 49. Cost assessment for the recovery of uranium from seawater via a textile adsorbent. **E. Schneider, M. Flicker, X. Chen, H. Lindner**

3:40 I&EC 50. Uranium-from-seawater sorbents from fishing industry waste – cost reduction through solvent recycle. **J.L. Shamshina, G. Gurau, S.P. Kelley, R.D. Rogers**

4:00 I&EC 51. Impacts of seawater uranium extraction on oceanic circulation and transport. **T. Khangaonkar, T. Wang, G.A. Gill**

4:20 I&EC 52. Green process for extraction and recovery of uranium from ground water and seawater. **A.W. Appleby, C. Perkins, H. Albusaidi**

4:40 Panel Discussion.

5:00 Concluding Remarks.

ACS Award in Industrial Chemistry: Symposium in Honor of Thomas J. Colacot

Sponsored by BMGT, Cosponsored by ANYL and I&EC

MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

P. Smith and M. Moore, Organizer

8:00 - 10:00

10, 24, 44. See previous listings.

67, 69, 71, 73-74, 82, 98. See subsequent listings.

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller

Cosponsored by CATL

Financially supported by ExxonMobil Research and Engineering Co

M. Moore, Organizer

J. S. Witzeman, Organizer, Presiding

8:30 I&EC 53. Amido fluorophosphite ligands for the rhodium catalyzed low pressure hydroformylation reaction. **T.A. Puckette**

8:55 I&EC 54. Selective aerobic C-C bond cleavage in lignin models and extracts using oxovanadium complexes. **R. Baker**

9:20 I&EC 55. Epoxybutene: The development of a selective process from butadiene. **J.L. Stavinoha**

9:45 I&EC 56. Acetylene from shale gas. **N. Collins, T. Upshaw**

10:10 I&EC 57. Measuring kinetics of hydrocarbon and oxygenate pyrolysis. **P.R. Westmoreland**

10:35 I&EC 58. Catalytic conversion of C1 reactants to higher value oxygenates. **J.J. Spivey**

11:00 I&EC 59. Tailored transition metal oxides for carbonaceous fuel conversion. **F. Li**

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller

Cosponsored by CATL

Financially supported by ExxonMobil Research and Engineering

M. Moore, Organizer

J. S. Witzeman, Organizer, Presiding

1:30 I&EC 60. Bimetallic cooperativity in homogeneous catalysis: Takes two to tango. **G.G. Stanley**

1:55 I&EC 61. Active state of gold catalysts for carbonylation reactions. **C. Hardacre, M.J. Muldoon, J. Sa', K. Morgan, Q. Cao, A. Goguet, S. Taylor**

2:20 I&EC 62. Molecular active sites in heterogeneous Ir-La/C catalyzed carbonylation of methanol to acetates. **Y. Wang**

2:45 I&EC 63. Pincer-crown ether catalysts for Lewis acid-promoted transformations. **A.J. Miller, J.B. Smith, J. Grajeda, L.C. Gregor**

3:10 I&EC 64. Neutron scattering studies of molecular interactions with pure and decorated metal nanomaterials. **J.Z. Larese**

[†] Cooperative Cosponsorship

- 3:35 **I&EC 65.** Carbonylation of methanol without alkyl halide. A.J. Vetter, J.R. Zoeller, T. Smith, M. Moore, M.K. Wiedmann
- 4:00 **I&EC 66. Award Address** (E. V. Murphree Award in Industrial and Engineering Chemistry sponsored by ExxonMobil Research and Engineering). Role of mechanistic studies in industrial processes. J.R. Zoeller

TUESDAY EVENING

Section A

Colorado Convention Center
Halls C/D

General Posters

P.M. Smith, *Organizer*

5:00 - 6:30

- I&EC 67.** Click chemistry-mediated synthesis of novel functionalized ionic liquids containing TMS moiety. M. Sanchez Zayas, S. Nestor, J.C. Gaitor, A. Mirjafari
- I&EC 68.** Adsorption performance of carbon molecular sieve prepared by carbon deposition with several depositing agents. F. Jin, X. Zhang, M. Gao, J. Zhang, H. Xu, D. Hua
- I&EC 69.** Uranium extraction from seawater using amidoxime modified mesoporous silica. C. Gunathilake, M. Jaroniec, J. Gorka, S. Dai
- I&EC 70.** LbL (layer-by-layer) multilayering on cellulose nanofibrils and its effects on surface charge and suspension dewatering. K. Sim, H. Youn, J. Lee, H. Lee
- I&EC 71.** Withdrawn.
- I&EC 72.** Spectroscopic identifications of inhibition effect by an ionic liquid as a synergist on gas hydrate formation. S. Han, J. Shin, S. Kang
- I&EC 73.** Distinguishing the Rosary and Island form of asphaltene with solid state nuclear magnetic resonance. M. Verma, S. Pradhan, P. Venkataraman, Y. Fang, M. Shammai, S.L. Wellington, W.E. Billups, L. Alemany
- I&EC 74.** Predicting the acid dissociation constants of aqueous amidoximes. N. Mehio, M. Lashley, J. Nudgent, L. Tucker, B. Correia, C. Do-Thanh, S. Vukovic, S. Dai, R.D. Hancock, V. Bryantsev
- I&EC 75.** Nanoparticle tracers for measurement of degree of preferential flow in shale. N. Yang, G. Jiang, E. Zheng, A. Wang, Y. Xu, X. Guo
- I&EC 76.** Polymerized imidazolium ionic liquids containing flexible pendant groups and their properties. J. Lee, H. Kim, J. Lee, H. Kim
- I&EC 77.** Ionic liquids containing ether-functionalized anion and their properties. J. Lee, Y. Kim, S. Park, J. Hwang
- I&EC 78.** Nitrile-functionalized tertiary amines for SO₂ absorption. J. Lee, S. Hong, M. Cheong, H. Kim
- I&EC 79.** Isolation and structural characterization of bicarbonate and carbonate species formed during CO₂ absorption/desorption. J. Lee, J. Im, M. Cheong, H. Kim
- I&EC 80.** Porous carbons derived from biomass for carbon capture. J. Lee, S. Park
- I&EC 81.** Ground calcium carbonate modified by polyelectrolytes multilayering at various salt concentrations for high filler loading in papermaking process. J. Lee, H. Youn, K. Sim, H. Lee, H. Lee
- I&EC 82.** Removal of acid yellow 25 dye onto chitin extracted from waste crab legs. D.D. Wright, L. O'Brien, I. Pathiraja, C. Wei, L. Norcio
- I&EC 83.** Guest gas enclathration in the tetra-n-butyl ammonium chloride (TBAC) semiclatrates: potential application to CO₂ capture. Y. Seo, S. Kim, S. Kang

WEDNESDAY MORNING

Section A

Embassy Suites Denver-Downtown Convention Center
Rexford Room

General Papers

C. J. Murphy, *Organizer, Presiding*

- 8:30 **I&EC 84.** Development of flexible alkaline batteries with carbon nanotube and polymers. Z. Wang, Z. Wu, N. Bramnik, S. Mitra
- 8:50 **I&EC 85.** Two step process for extraction of graphene quantum dots and chemicals/fuels from coal. K. Mondal, A. Sims, K. Tsai, T. Hasan
- 9:10 **I&EC 86.** Amine based mesoporous silica with incorporated metal oxide for carbon dioxide sorption. C. Gunathilake, M. Jaroniec
- 9:30 **I&EC 87.** Study of a novel depressant for reverse cation flotation of iron ore with focused beam reflective measurement. S.A. Kofsky Wofford, X. Yin
- 9:50 Intermission.
- 10:05 **I&EC 88.** Effects of alkyl chain length on lithium salt solubilities in ammonium Tf₂N based ionic liquids. D.P. Fagnant, J.F. Brennecke
- 10:25 **I&EC 89.** Influence of the use of film forming amines in condensate polishing systems on the properties of ion exchange resins. A. Kabir, A. Apblett
- 10:45 **I&EC 90.** Robust block copolymer based RTIL-gel membrane materials for CO₂ separation. D. Wijayasekara, T.S. Bailey
- 11:05 **I&EC 91.** Carbonyl sulfide formation during wide temperature reformate desulfurization on ZnO/SiO₂ and Cu promoted ZnO/SiO₂ adsorbents. A.R. Sujan, B. Tatarchuk, H. Yang

WEDNESDAY AFTERNOON

Section A

Embassy Suites Denver-Downtown Convention Center
Rexford Room

General Papers

C. J. Murphy, *Organizer, Presiding*

- 1:30 **I&EC 92.** Improved kinetic model for ethane pyrolysis at high conversions and high pressures. K. Wang, M.H. Saldana, S. Villano, G. Bogin, A.M. Dean
- 1:50 **I&EC 93.** Electrical discharge enabled plasmachemical activation of methane in microscale reactors. P. Kreider, J. Pommerenck, A.F. Yokochi
- 2:10 **I&EC 94.** Diffusion and aging of wood preservatives in softwood under environmental exposure. K. Ondrusova, V. Martinska, A. Kubatova, E.I. Kozliak
- 2:30 **I&EC 95.** Smoother ride: Paving the voids in thermophysical property data using QSPR. W.H. Carande, A. Kazakov, C. Muzny
- 2:50 Intermission.
- 3:05 **I&EC 96.** Concatenated gas saturation method for vapor pressure measurement: A technique for oxidatively unstable compounds. J.A. Widegren, A.E. Tolbert, T.J. Bruno
- 3:25 **I&EC 97.** Highly selective cation separations in electrodialysis through cation-exchange membranes coated with polyelectrolyte multilayers. N. White, M.L. Bruening, M. Misovich
- 3:45 **I&EC 98.** Extraction of the protein fraction of dry distillers grains with solubles (DDGS), implementing chemical methods. M.F. Villegas Torres, J. Ward, G.J. Lye
- 4:05 **I&EC 99.** Coating for biofouling prevention. Y. Li, H. Yu, K.L. Yeung
- 4:25 **I&EC 100.** Conversion of biodiesel-derived crude glycerol into acrolein. R. Liu, Y. Jin, T. Wang

INOR

Division of Inorganic Chemistry

S. A. Koch and N. S. Radu, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Michael A. Marletta (see BIOL, Sun)

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe (see FLUO, Tue)

Convergence of Theory & Experiment in Heavy Element Chemistry (see NUCL, Wed, Thu)

SOCIAL EVENTS:

Reception: Dow Chemistry of the Energy Water Nexus Reception, 4:30 PM: Tue

SUNDAY MORNING

Section A

Colorado Convention Center
Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry

Coordination Chemistry

C. Nataro, S. R. Smith, *Organizers*
C. Hamaker, *Presiding*

9:00 Introductory Remarks.

9:05 **INOR 1.** Investigating the oxidation of olefins using derivatives of the non-heme iron catalyst [Fe(BPMEN)](OTf). C.A. Lidston, M.R. Davies, R.D. Pike, C. Goh

9:25 **INOR 2.** Metal cation detection using a novel small molecule chemosensor. D.T. de Lili, A.M. Gagnon, M. Brown, K. Shelley, M. DeLuca

9:45 **INOR 3.** Tripodal carbamoylmethylphosphine oxide (CMPO) ligands for f-element chelation: Solution photophysical studies and lanthanide/actinide extraction properties. E.J. Werner, S.M. Biros, S.N. McGraw, D.A. Hardy, H.T. Sertain

10:05 **INOR 4.** Synthesis of a series of first row transition metal complexes containing a tetradentate ligand. H.F. Drake, A. Blake, C.M. Donahue, S.R. Daly, B.J. Bellott

10:25 Intermission.

10:35 **INOR 5.** Lanthanides, chirality, and ionic liquids: Finding a niche with undergraduates. T. Hopkins

10:55 **INOR 6.** Interconversion of eight-coordinate, dodecahedral, rhenium(V) isomers supported by a single chelating ligand. H. Sodni, C.P. Bosko, S. Rashid, G.A. Moehring

11:15 **INOR 7.** Methanobactin-inspired coordination chemistry with new mixed-donor ligands. D. Rabinovich

11:35 **INOR 8.** Utilization of sulfonamides in crystal engineering. C. Hamaker, Z.E. Lawton, M. Oblazny

Section B

Colorado Convention Center
Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, M. C. Buzzeo, S. Delaney, *Organizers*
V. C. Pierre, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 **INOR 9.** Road to genome expansion is paved with good intentions: When DNA repair goes awry. S. Delaney

9:10 **INOR 10.** Snapshots of metallobleomycin-DNA recognition and binding: A tale of two tails. E.C. Long, M.M. Georgiadis

9:40 **INOR 11.** Scrutinizing DNA damage. M. Nunez

10:10 Intermission.

10:20 **INOR 12.** Formation and characterization of platinum adducts on ribosomal RNA. X. Bao, C.S. Chow

10:50 **INOR 13.** Enhancing extracellular proteostasis through the unfolded protein response. J. Genevieux, J.W. Kelly, R. Wiseman

11:20 **INOR 14.** Molecular shape control applied to the dynamic capture and release of bio-relevant substrates. A. Petitjean

11:50 **INOR 15.** Systematic material design using biomolecules. T. Tamaki

Section C

Colorado Convention Center
Room 302

ACS Award in Organometallic Chemistry: Symposium in Honor of William J. Evans

J. R. Walensky, *Organizer*
J. W. Ziller, *Presiding*

8:30 **INOR 16.** Measuring hydride donor ability to guide catalyst design for reduction reactions. J. Yang, C. Tsay, J. Khosrowabadi Kotyk, B. Livesay

8:50 **INOR 17.** Next generation redox-active "ligands" from non-innocent coordination complexes. A.F. Heyduk

9:10 **INOR 18.** Synthetic chemistry as a window into biology: Probing molecular complexity with small molecular species. A. Borovik

9:30 **INOR 19.** Evaluating metal-carbon orbital mixing in metallocene dichlorides. S.A. Kozimor, E.R. Batista, J.N. Cross, D.L. Clark, J.M. Keith, R.L. Martin, S.G. Minasian, D.K. Shuh, C.S. Stieber, J.A. Trujillo, T. Tylicszocek

9:50 Intermission.

10:00 **INOR 20.** Covalency in actinide metallocene complexes. D.L. Clark

10:20 **INOR 21.** Bond strength in molecular f element compounds from the quantum theory of atoms in molecules. Q. Huang, J.R. Kingham, A. Mountain, N. Kaltsoyannis

10:40 **INOR 22.** Group 11 cluster chemistry: What I didn't learn in the Evans Lab. J.R. Walensky, A. Lane, P. Rungthanaphatsophon

11:00 **INOR 23.** Practical models for organometallic chemistry. W. Hehre

Section D

Colorado Convention Center
Room 303

Chemical Approaches to Spintronics Research

R. Beaulac, *Organizer*
K. R. Kittilstved, *Presiding*

8:30 **INOR 24.** Spin coherence transfer using photogenerated spin-correlated radical pairs. M.R. Wasielewski, N.E. Horwitz, B.K. Rugg

9:00 **INOR 25.** Spin transport in organic materials: From single molecules to crystals. S. Sanvito

9:30 **INOR 26.** Probing spin-exciton and spin-charge interactions in open-shell organic semiconductors. T.L. Andrew

10:00 Intermission.

10:30 **INOR 27.** Evaluating magnetic properties of molecules with strong anisotropy based on electronic configuration and geometry. K.R. Dunbar, M. Ballesteros, S. Hill, D. Pinkowicz, M.R. Saber, T.J. Woods, Y. Zhang, H. Zhao

11:00 **INOR 28.** Magnetic ordering and conductivity in heavy atom and multiband radicals. A. Maitman, S.M. Winter, J.W. Wong, D. Tian, C.M. Robertson, P.A. Dube, S.R. Julian, S. Hill, R.T. Oakley

11:30 **INOR 29.** Spin-selective charge recombination in complexes of CdS quantum dots and organic hole acceptors. D.J. Weinberg, S.M. Dyar, Z. Khademi, M. Malicki, S.R. Marder, M.R. Wasielewski, E.A. Weiss

Section E

Colorado Convention Center
Room 201

ACS Award in Inorganic Chemistry: Symposium in Honor of John T. Groves

P. J. Chirik, *Organizer*
R. N. Austin, *Organizer, Presiding*

9:00 INOR 30. Base metal catalysis for hydrocarbon manipulation. P.J. Chirik

9:30 INOR 31. Tandem catalytic hydrogenation of carbon dioxide to methanol. M.S. Sanford

10:00 INOR 32. Functionalization of C-H bonds by iodate and chloride: Mechanistic studies. T.B. Gunnoe, J.T. Groves, G.C. Fortman, N.C. Boaz, S.E. Kalman, R.A. Periana, M.M. Konnick

10:30 Intermission.

10:45 INOR 33. Amazing nonheme high-valent iron-oxo reactivity landscape. L. Que

11:15 INOR 34. Concerted multiple-site proton-coupled electron transfer (PCET): Effects of separating the proton and electron. J.M. Mayer, M.A. Bowling, V. Manner, J.J. Warren, J. Wittman, L.R. Bradshaw, D.R. Gamelin, W.D. Morris, T.F. Markle

Section F

Colorado Convention Center
Room 304

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Emily A. Weiss

Cosponsored by WCC

M. R. Hartings, *Organizer, Presiding*

8:30 INOR 35. Harry Gray as a young investigator: Paradigms lost, found, and going up in gas. R. Eisenberg

8:55 INOR 36. Gray nation: Out of this world. M.L. Cable, J.P. Kirby, A. Ponce, A.M. Stockton, M.F. Mora, P. Willis, T.H. Vu, P.M. Beauchamp, H.B. Gray

9:20 INOR 37. Molecular systems for photocatalytic hydrogen oxidation. M.D. Hopkins, H.B. Vibbert, M. Westwood, N.T. La Porte

9:45 Intermission.

9:55 INOR 38. Artificial hydrogenases for solar hydrogen production. K.L. Bren, B. Kandemir, J.G. Kleingardner, L. Kubie

10:20 INOR 39. Designing metalloproteins with tunable redox potentials and reorganization energies for efficient long-range electron transfer. Y. Lu, N.M. Marshall, P. Hosseinzadeh, O. Farver, S.E. Wherland, I. Pecht

10:45 INOR 40. Time-resolved spectroscopic studies of electron and proton transfer in biologically relevant systems. M.E. Ener, H.B. Gray, T.G. Spiro

11:10 INOR 41. Understanding plasticity in molecular recognition. D.S. Wuttke, T.H. Dickey, M. McKercher

11:35 INOR 42. Bioinorganic chemistry in a gray area. F.A. Tezcan

Section G

Colorado Convention Center
Room 401

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage

Cosponsored by MPPG

A. L. Prieto, *Organizer*
C. Ban, Y. Yang, *Organizers, Presiding*

8:00 INOR 43. Sunlight-driven hydrogen formation by membrane-supported photoelectrochemical water splitting. N.S. Lewis

8:40 INOR 44. Challenges in photoelectrochemical water splitting materials. J.A. Turner

9:20 INOR 45. Enabling solar fuels technology by high throughput discovery of earth abundant oxygen evolution reaction catalysts. J. Haber, D. Guevarra, R. Jones, A. Shinde, N. Becerra, C. Xiang, S. Mitrovic, S. Jung, C. Kisielowski, J. Yano, J. Jin, J. Gregoire

9:40 Intermission.

9:50 INOR 46. Tin nitride spinel semiconductor for photoelectrochemical water oxidation. C. Caskey, J.A. Seabold, V. Stevanovic, D.S. Ginley, N. Neal, R.M. Richards, S. Lany, A. Zakutayev

10:10 INOR 47. Electrolysis of urea for the sustainable production of hydrogen. G. Bötte

10:50 INOR 48. Sulfur Sulfur thermochemical hydrogen production cycle: A new thermochemical cycle employing only earth abundant elements. N. AuYeung, K. Caple, P. Kreider, A.F. Yokochi

11:30 INOR 49. Lithium metalorganic complex used to clean hydrogen sulfide for hydrogen production and/or storage. X. Li, R. Morrish, C.A. Wolden, Y. Yang

Section H

Colorado Convention Center
Room 203

Organometallic Chemistry**Catalysis**

N. S. Radu, *Organizer*
G. Dobreiner, C. Hahn, *Presiding*

9:00 INOR 50. Tetracarbene iron(IV) intermediates for catalytic aziridination. S.A. Cramer, R. Hernandez Sanchez, P.P. Chandrachud, D.F. Brakhage, D.M. Jenkins

9:20 INOR 51. Synthesis and reactions of (η^5 -PCP)Ru(cod)H. B. Thapalyia, G.A. Venegas, N. Arulsamy, D.M. Roddick

9:40 INOR 52. Synthesis and metal coordination chemistry of η^5 (PNP) and η^5 (PONOP) ($R_1 = CF_3$, C_2F_5) chelates. P. Miller, D.M. Roddick

10:00 INOR 53. Experimental and computational investigation of Csp³-N, Csp³-F, and Csp³-Csp² reductive elimination from model palladium (IV) complexes. I.M. Pendleton, P.M. Zimmerman, M.S. Sanford, M. Perez-Temprano

10:20 INOR 54. Investigation of acid and base co-catalysts for the palladium(II) and platinum(II) catalyzed hydroarylation of acetylene. C. Hahn, M. Manjahi

10:40 INOR 55. Synthesis and metal (M = Ir, Ru) coordination chemistry of (Bu)(R)₂(PCP) ($R_1 = CF_3$, C_2F_5) chelates. S. Debnath, D.M. Roddick

11:00 INOR 56. Influence of Lewis acids on migratory insertion: Applications to C-C bond formations. G. Dobreiner

11:20 INOR 57. Cross-coupling catalysis in water – a versatile approach. J. Eppinger, D. Sawant, A.V. Zernickel

Section I

Colorado Convention Center
Room 205

Chemistry of Materials**Materials for Energy and Catalytic Applications**

C. G. Lugmair, *Organizer*
N. C. Anderson, F. Jiao, *Presiding*

8:30 INOR 58. Synthesis of silicon-germanium alloy nanoparticles for thermoelectric applications. A. Hochbaum, T. Cornell

8:50 INOR 59. Energy transfer by demand in well-defined hybrid materials. N.B. Shustova, D.E. Williams, E.A. Dolgoplova

9:10 INOR 60. CdSe sensitized photocathodes on a mesoporous transparent conducting oxide scaffold. M.R. Norris, B.M. Cossairt

9:30 INOR 61. Exploring the potential of nanostructured black silicon toward catalyst-assisted photoelectrochemical reduction of water. N.C. Anderson, Y. Zhao, N.R. Neale, H. Branz, P.W. King

9:50 INOR 62. Zeolite protected nanocatalysts; Using a hard framework for selection and protection. J. Palomba, J.V. Morabito, C. Tsung

10:10 INOR 63. Mesoporous metal sulfides: Synthesis and photocatalysis. F. Jiao

10:30 INOR 64. Control of doping in Cu₂SnS₃, a novel photovoltaic absorber, through defects, alloying, and annealing. L. Baranowski, P. Zawadzki, S. Christensen, S. Lany, L. Gedvilas, E. Töberer, A. Zakutayev

10:50 INOR 65. Symmetry breaking charge transfer in zinc dipyrins for OPVs with open circuit voltage in excess of 1.3 V. A. Bartyński, M.E. Thompson

11:10 INOR 66. Charge storage in cation incorporated α -MnO₂. M. Young, A. Holder, S.M. George, C. Musgrave

11:30 INOR 67. (Cr,Fe,₂)C₂ Solid solution as an efficient electrocatalyst for oxygen reduction and evolution reactions in both acidic and alkaline media. C. Wan, B.M. Leonard

Section J

Colorado Convention Center
Room 402

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*
A. J. Morris, *Presiding*

8:30 INOR 68. Production of chemical feedstocks from pyrolytic lignin using transition metal oxidation catalysts. M.S. Fortin, M.D. Mohadjer Beromi, A. Lai, C.A. Mullen, A.A. Boateng, N.M. West

8:50 INOR 69. On the use of cobalt complexes as mediators in dye sensitized solar cells: Instability of high-potential complexes. J.T. Kirner, C.M. Elliott

9:10 INOR 70. Dipyrrolyl ketone based catalysts for carbon dioxide reduction. H. Meylemans, P. Goodman

9:30 INOR 71. Enhancement of CO₂ absorption utilizing zinc-based homogenous catalysts in primary amine solution. M. Sarma, C. Lippert, R.A. Burrows, L.R. Widger, C. Brandewie, S. Parkin, K. Liu

9:50 Intermission.

10:00 INOR 72. Exploring charge transfer induced spin cross-over redox mediators in quantum dot sensitized solar cells. A.J. Haring, J.D. Godward, M.E. Pomatto, A.J. Morris

10:20 INOR 73. Controlling interfacial energetics for efficient hybrid bulk heterojunction solar cells. A.J. Haring, A.J. Morris

10:40 INOR 74. Oxidation of carbon monoxide in basic solution catalyzed by nickel cyano carbonyls at ambient condition and the prototype of a CO-powered alkaline flow battery type fuel cell. W. Lo, T. Berenson, N. Tracer, D. Shlian, M. Khaloo, J. Jang

11:00 INOR 75. Unassisted energy storage using layered chalcogenide semiconductor. J.R. McKone, R.A. Potash, F.J. DiSalvo, H.D. Abruna

11:20 INOR 76. Heterometallic mixed-valent molecular precursors for the synthesis of transition metal oxides. E. Dikarev, C.M. Lieberman, Z. Wei, A.S. Filatov

SUNDAY AFTERNOON**Section A**

Colorado Convention Center
Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry**Organometallic Chemistry**

C. Nataro, S. R. Smith, *Organizers*
M. Guino-o, *Presiding*

1:30 Introductory Remarks.

1:35 INOR 77. Ruthenium(II) complexes supported by electron-rich aromatic ligands for small molecule activation and catalysis. J.P. Lee, M.J. Hankins, A.D. Riner

1:55 INOR 78. Investigating the mechanism of N-H bond activation by a sterically congested PCP-iridium complex. D.A. Laviska

2:15 INOR 79. Progress toward the synthesis, characterization, and catalysis of iridium complexes containing [N,N,N]-dianionic pincer ligands. H. Sajjad, A.R. O'Connor

2:35 INOR 80. Copper-catalyzed acyloxylation of aromatic halides. F. Barrios-Landeros, B. Ben-Zvi, A.E. Kessler, B.W. Goodman, D.Y. Drory, D.L. Levine

2:55 Intermission.

2:55 INOR 81. Microwave-assisted copper-catalyzed reactions of aryl halides via concurrent tandem catalysis. D.J. Brown, S. Lin, A.H. Roy MacArthur

3:15 INOR 82. Amphiphilic late-metal silyl and silylene complexes for cooperative activation of small molecules. A. Deetz, M.T. Whited

3:35 INOR 83. Modulation of tris(diphenylphosphinomethyl)phenylborane donor ability via introduction of M(CO)₂ units at the boron-bound phenyl substituent. P.J. Fischer, A.B. Weberg, T.D. Bohmann, H. Xu

3:55 INOR 84. Cyclic hydroboration using azaferrrocene-stabilized borenium cations. T.J. Brunker, S. Krause, A.L. Rheingold

4:15 INOR 85. Trends observed during the nickel-catalyzed dehydrogenation of ammonia-borane utilizing asymmetrical triazolylidene ligands. M.O. Talbot, M. Guino-o

Section B

Colorado Convention Center
Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, M. C. Buzzeo, V. C. Pierre, *Organizers*
S. Delaney, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR 86. Roles for metal cofactors of MutY enzymes in preventing DNA mutations. S.S. David

2:05 INOR 87. New ROS-activated agents that specifically target AML cancer cells. E.J. Merino

2:35 INOR 88. Evidence of histidine and aspartic acid phosphorylation in human prostate cancer cells. A.E. Friedman

3:05 Intermission.

3:15 INOR 89. Nitric oxide regulation of bacterial biofilms. E.M. Boon

3:45 INOR 90. DNA-protein self assemblies on millimeter length scales: Artificial light antenna systems. C.V. Kumar

4:15 INOR 91. Assay and mechanistic investigations of iron oxidation catalysts. C.M. Dupureur, Y. Song, H. Mayes, E.B. Bauer

Section C

Colorado Convention Center
Room 302

ACS Award in Organometallic Chemistry: Symposium in Honor of William J. Evans

J. R. Walensky, *Organizer*
J. W. Ziller, *Presiding*

1:30 INOR 92. Synthesis without the solvent: Mechanochemical approaches to organometallic complexes. N.R. Rightmire, D.L. Bruns, T.P. Hanusa

1:50 INOR 93. f-Element single-molecule magnets. K.R. Meihaus, S. Demir, J.D. Rinehart, M. Nippe, J.M. Zadrozny, J.R. Long

2:10 INOR 94. Withdrawn.

2:30 INOR 95. RE-cycle efforts for nationally critical elements: Fundamental coordination chemistry of scandium. T.J. Boyle, J.M. Sears, M.L. Neville, D.T. Yonemoto, R. Cramer, T.N. Lambert, R.F. Hess, L.J. Small

2:50 INOR 96. Role of lanthanide ions in metal-seamed organic nanocapsules. J.L. Atwood, H. Kumari, K. Feaster

3:10 Intermission.

3:20 INOR 97. To cluster or not to cluster. G. Meyer

3:40 INOR 98. iPhone glues: An introduction to the chemistry of reliable and reworkable capillary-flow underfills. T. Champagne

4:00 INOR 99. Synthesis of sodium borohydride without sodium metal. N. Allen, R. Butterick, D.M. Millar, D.C. Molzahn

4:20 INOR 100. Multi-metallic materials containing f-elements. J.H. Farnaby, P.L. Arnold, W.J. Evans, F.N. Cloke

Section D

Colorado Convention Center
Room 303

Chemical Approaches to Spintronics Research

R. Beaulac, *Organizer*
D. J. Weinberg, *Presiding*

1:30 INOR 101. Aggregates of Mn_3 single-molecule magnets: Synthesis, properties, and quantum effects. G. Christou, T.N. Nguyen, M. Shiddiq, A.M. Mowson, K.A. Abboud, S. Hill

2:00 INOR 102. Theoretical approaches to the control of spin states in molecules. C. Hermann

2:30 INOR 103. Development of redox and environmental switches for control of magnetic communication in molecular complexes. M.P. Shores, R. Higgins, C. Klug, i. bhowmick, S. Fiedler, A.K. Rappe

3:00 Intermission.

3:30 INOR 104. Metal silicide nanowires for detection and manipulation of magnetic skyrmions. S. Jin

4:00 INOR 105. Monolayer-protected nanoclusters: Structurally precise building blocks for spintronics applications. K.L. Knappenberger, T.D. Green, C. Yi

4:30 INOR 106. Mechanism of dopant incorporation in $SrTiO_3$ bulk powders and colloidal nanocrystals. K.A. Lehuta, W. Harrigan, K.R. Kittilstved

5:00 INOR 107. Photomagnetic switching in highly conductive Fe(II) spin-crossover complexes with organic radicals. H. Phan, S. Benjamin, E. Steven, J. Brooks, M. Shatruk

Section E

Colorado Convention Center
Room 201

ACS Award in Inorganic Chemistry: Symposium in Honor of John T. Groves

P. J. Chirik, *Organizer*
R. N. Austin, *Organizer, Presiding*

1:30 INOR 108. Inorganic chemistry of biological nitrogen fixation. D. Dean, B.M. Hoffman, D. Lukoyanov, L.C. Seefeldt, S. Shaw, Z. Yang

2:00 INOR 109. Thermodynamics and mechanism of C-H bond activation by the $Cu(III)$ -OH core. W.B. Tolman

2:30 INOR 110. Ligand switching in the control of cytochrome c redox function. E.V. Pletneva

3:00 Intermission.

3:15 INOR 111. Raman spectroscopy and computation reveal how hemoglobin controls oxygen affinity. T.G. Spiro

3:45 INOR 112. Structure/function correlations over non-heme iron enzymes. E.I. Solomon

Section F

Colorado Convention Center
Room 304

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Emily A. Weiss

Cosponsored by WCC
M. R. Hartings, *Organizer, Presiding*

1:30 INOR 113. Singlet fission in carotenoid aggregates and dimers. M.J. Tauber

1:55 INOR 114. Probing pathways of excited-state proton-coupled electron transfer reaction. J.L. Dempsey, T.T. Eisenhart, J.C. Lennox, W.C. Howland

2:20 INOR 115. New sensitizers for solar hydrogen production. R. Sabatini, B. Zheng, W.T. Eckenhoff, A. Orchard, K. Liwosz, D. Watson, M. Detty, R. Eisenberg, D.W. McCamant

2:45 INOR 116. Toward spying on individual working catalyst molecules. R.H. Goldsmith

3:10 Intermission.

3:20 INOR 117. Exploring the mechanism of small molecule metal ion chelators as chemotherapeutic agents against pathogenic bacteria. T. Santos, M. Zhou, M. Lammers, M. Rajendran, K. Hurlley, Y. Eun, D.B. Weibel

3:45 INOR 118. Thermodynamic and kinetic measurements of cation exchange in chalcogenide nanocrystals by isothermal titration calorimetry. N. Sturgis, R.M. Rioux

4:10 INOR 119. Luminescent copper-doped semiconductor nanocrystals. K.E. Knowles, H.D. Nelson, P.J. Whitham, D.R. Gamelin

4:35 INOR 120. Metal nanoparticles trapped in unfolded proteins: Synthesis, characterization, and unique materials properties. M.R. Hartings, D. Fox, A.E. Miller

Section G

Colorado Convention Center
Room 401

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage

Cosponsored by MPPG

C. Ban, Y. Yang, *Organizers*

A. L. Prieto, *Organizer, Presiding*
Y. Zhao, *Presiding*

1:30 INOR 121. Molecular studies of gas clathrate hydrates. C.A. Koh

2:10 INOR 122. Fueling the future: Safe, dense, reversible hydrogen storage in hybrid nanomaterials. J. Urban

2:40 INOR 123. Development of metal hydrides for high temperature thermochemical energy storage. E. Ronnebro

3:20 Intermission.

3:30 INOR 124. Water-mediated cooperative migration of chemisorbed hydrogen on graphene. Y. Zhao, T. Gennett

3:50 INOR 125. Spectroscopic studies of proton-coupled electron transfer in the mechanism of H_2 activation by [FeFe]-hydrogenases. D.W. Mulder, M.W. Ratzloff, M. Bruschi, C. Greco, Y. Guo, E. Koonce, J.W. Peters, P.W. King

4:30 INOR 126. Molecular electrocatalysts for the oxidation of hydrogen: Pendant amines as proton relays. R. Bullock, T. Liu, J.M. Darnon, E.B. Hulley, M. Helm

5:10 INOR 127. Hydrogen fuel cell electric vehicles: new possibilities? Y. Shao

Section H

Colorado Convention Center
Room 203

ACS Award in the Chemistry of Materials: Symposium in Honor of Mark E. Thompson

R. L. Brutchey, *Organizer, Presiding*

1:30 INOR 128. Efficient cyclometalated platinum and palladium complexes for displays and lighting applications. J. Li

1:50 INOR 129. Solvent-dependent fluorescence of substituted quinoxalines. S.P. Sibley

2:10 INOR 130. Excitons and OLEDs: You can't live with them and you can't operate without them. S. Forrest

2:30 INOR 131. Synthetic control of photoinduced structural change and dual emission of phosphorescent molecular butterflies. B. Ma

2:50 INOR 132. Exploiting nonradiative decay of cyclometalated iridium complexes to perform in situ analysis of degradation products in OLEDs. P.I. Djurovich

3:10 Intermission.

3:25 INOR 133. High efficiency phosphorescent OLEDs. J. Brooks

3:45 INOR 134. Stoichiometric and catalytic reactivity based on late-metal/main-group cooperation. M.T. Whited

4:05 INOR 135. Investigating the trap state landscape of cadmium halide-treated CdSe nanocrystals. R.L. Brutchey

4:25 INOR 136. Charge dynamics in next-generation energy conversion materials. C.W. Schlenker

4:45 INOR 137. Photon upconversion and photocurrent generation via self-assembled bilayers on metal oxide surfaces. K. Hanson, S.P. Hill, T. Banerjee

Section I

Colorado Convention Center
Room 205

Division of Inorganic Chemistry Celebration of the Gabor A. Somorjai Award: Symposium in Honor of Maurice Brookhart

K. I. Goldberg, *Organizer*
A. Goldman, *Organizer, Presiding*

1:30 INOR 138. Thermal and photochemical reactions mediated by water-soluble host-guest supramolecular systems. R.G. Bergman

1:50 INOR 139. Cation-modulated hemilability in pincer-crown ether complexes. A.J. Miller, M.R. Kita, J.B. Smith

2:10 INOR 140. Redox reactions of nanoscale oxide materials: Thermodynamics and kinetics of hydrogen-atom and proton-coupled electron transfer processes. J.M. Mayer, C.N. Valdez, M.N. Braten, J. Peper, A. Soria, J.A. Johnson, D.R. Gamelin, A.M. Schimpf, M. Ryoji, C. Tsou, D. Damatov, H. Larson

2:30 INOR 141. Relative reactivity scale of alkanes from C-H bond functionalization reactions. A. Olmos, R. Gava, B. Noverges, D.R. Enrique, K. Jacob, T. Varea, A. Caballero, M. Etienne, G. Asensio, P.J. Perez

2:50 INOR 142. Synthesis and reactivity of high valent organometallic Ni complexes. M.S. Sanford

3:10 INOR 143. Small molecule activation mediated by an iron half-sandwich complex, $[Cp^*FeX]_2$. M.D. Walter, M. Reiners, M. Maekawa, P.G. Jones, J. Hohenberger, J. Sutter, K. Meyer

3:30 Intermission.

3:40 INOR 144. Promoting alkane dehydrogenation by C-H activation at IrIII. A.M. Wright, K. Allen, D. Pahls, T.R. Cundari, A.S. Goldman, D.M. Heinekey, K.I. Goldberg

4:00 INOR 145. Chelate complexes of 1st row transition metals: Redox non-innocence and multiple metal-ligand bonds. P.T. Wolczanski, A. Swidan, B.M. Lindley, S.P. Heins, W.D. Morris, N. Livezey, B.P. Jacobs, R. Agarwal

4:20 INOR 146. Low temperature oxidations of iridium(Cp^*) complexes. C. Turlington, M. Brookhart, J.L. Templeton

4:40 INOR 147. Hydrogenolysis reactions catalyzed by iridium pincer complexes. J.M. Goldberg, G.W. Wong, T. Lekich, K.I. Goldberg, D.M. Heinekey

5:00 INOR 148. Well-defined iron catalysts for the acceptorless reversible dehydrogenation of alcohols and N-heterocycles. S. Chakraborty, W. Brennessel, W.D. Jones

5:20 INOR 149. First row transition metals and Lewis acid co-catalysts for carbon dioxide reduction. W.H. Bernskoetter, N. Hazari

5:40 INOR 150. Applications of tripodal ligands in bioinorganic and organometallic chemistry. G.F. Parkin

Section J

Colorado Convention Center
Room 402

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
M. Fieser, M. Murugesu, *Presiding*

1:30 INOR 151. Isolation of a terminal organocerium acetylide complex and its reactivity with enolizable ketones. J. Kim, D. Weinberger, P. Carroll, E.J. Schelter

1:50 INOR 152. Ligand effects in the synthesis of Ln^{2+} complexes by reduction of tris(cyclopentadienyl) rare earth precursors including C-H bond activation of an indenyl ligand. J.F. Corbey, C.T. Palumbo, D. Woen, J.W. Ziller, W.J. Evans

2:10 INOR 153. Reactivity of the Ln^{2+} complexes $[K(2.2.2\text{-cryptand})][C_2H_5SiMe_2]_2Ln$: Reduction of aromatic hydrocarbons. C. Kofyk, M.R. MacDonald, J.W. Ziller, W.J. Evans

2:30 Intermission.

2:40 INOR 154. Investigation on charge-transfer absorptions of uranyl UO_2^{2+} (VI) and chemical reduction of UO_2^{2+} (VI) to UO_2^+ (V) by UV-visible and EPR spectroscopies. X. Sun, D. Kolling, H. Mazagri, B. Karawan

3:00 INOR 155. Facile synthesis of Npl₁ in solution. A.T. Johnson, J.K. Pfeiffer, M.R. Finck, K.P. Carney, L.R. Martin

3:20 INOR 156. Lanthanide ions in molecular magnets. M. Murugesu

3:40 INOR 157. Lanthanides-TTF complexes: Correlation between single molecule magnet behavior and luminescence. L. Ouahab, F. Pointillart, O. Cador, S. Golhen

4:00 Intermission.

4:10 INOR 158. Ionothermal effects on actinyl coordination chemistry using task-specific ionic liquids. P.A. Smith, P.C. Burns

4:30 INOR 159. Synthesis, structure, and electronic spectroscopy of f-element thiocyanates. J.N. Cross, S.A. Kozimor, C.S. Stieber, J.A. Trujillo, E.R. Batista, R.L. Martin, S.R. Daly

4:50 INOR 160. Unconventional metal-organic frameworks (UMOFs) for separation of lanthanides from actinides and americium from curium. R.M. Silbergagel, J.D. Burns, D.T. Reed, D.T. Hobbs, A. Clearfield

Department, University, and National Models for Faculty Development to Support Adoption of Evidence-Based Teaching

Sponsored by CHED, Cosponsored by INOR, ORGN and PRES

SUNDAY EVENING**Section A**

Colorado Convention Center
Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry**General Posters**

C. Nataro, *Organizer*

6:00 - 8:00

INOR 161. Mg deficient IONiC/VIPEr: An online community for inorganic chemists. M.J. Geselbracht, A.K. Bentley, H.J. Eppley, E.R. Jamieson, A.R. Johnson, C. Nataro, B.A. Reiser, J.L. Stewart, S.R. Smith, N. Williams, L.A. Watson

INOR 162. IONIC VIPEr workshops at the frontiers of inorganic chemistry. S.R. Smith, L.G. Habgood, S.E. Schmidt, K. Young

Section B

Colorado Convention Center
Hall C

Bioinorganic Chemistry**DNA, RNA and Inorganic Drugs**

S. A. Koch, *Organizer*

6:00 - 8:00

INOR 163. Effect of oxidation state on the anti-cancer activity of several gold polypyridyl complexes. D. Gibler, A.C. Ontko

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.

- INOR 164.** Novel gold(III) chelates of 7-substituted dipyrro[3,2-a:2',3'-c] phenazine and their evaluation as antitumor agents. **K. Palanichamy, C. Gatewood, A.C. Ontko**
- INOR 165.** Withdrawn.
- INOR 166.** Synthesis and photolysis of a novel family of photoactivatable HNO donors using the (3-hydroxy-2-naphthalenyl)methyl photolabile protecting group. **Y. Zhou, R.S. Dassanayake, N.E. Brasch, P. Sampson**
- INOR 167.** Correlating cytotoxicity of ruthenium(II) polypyridyl complexes with activation wavelength. **E. Wachter, D.K. Heidary, A. Effinger, E.C. Glazer**
- INOR 168.** E. coli as a screening system to study potential anti-cancer agents with different mechanisms of action. **Y. Sun, Z. Zhang, D. Heidary, C.I. Richards, E. Glazer**
- INOR 169.** New family of rhodium metallointeractors with improved selectivity and potency against DNA mismatch repair deficient cell lines. **K.M. Boyle, A. Komor, J.K. Barton**
- INOR 170.** Development of light activated Ru(II) complexes applicable in photodynamic therapy. **A.M. Kishlock, E.A. Stimmel, A. Jain**
- INOR 171.** Transition metal complexes used for the detection of mismatched DNA base pairs. **T.N. Rohrabough, C. Turro**
- Section B**
Colorado Convention Center
Hall C
- Bioinorganic Chemistry**
Proteins and Enzymes and Model Systems
S. A. Koch, *Organizer*
- 6:00 - 8:00**
- INOR 172.** Spectroscopic studies of the biologically active peptide of low-molecular-weight chromium-binding substance. **H. Arakawa, E. Love, J.B. Vincent**
- INOR 173.** Modeling matrix metalloproteinase inhibition with carbonic anhydrase. **W.A. Richert, D. DeGenova, A. Forchione, R. Patel, A. Plonski, R. Venna, Z. Higgins, M. Morris, S. Al-Abdul-Wahid, D.L. Tierney**
- INOR 174.** Toxic carbon monoxide removal by the soil bacteria *Oligotropha carboxidovorans*: Insights from *In silico* models. **M.C. Dienst, T.A. Large, D. Rokhsana, M. Retegan, F. Neese**
- INOR 175.** Overlap of protein inhibition and metal chelation: A case study. **R. Gautam, E. Akam, E. Tomat**
- INOR 176.** Structural insights of a mononuclear iron center in 2,6-dichlorohydroquinone-1,2-dioxxygenase (PcpA) from *In silico* models. **P.R. Carmichael, D. Rokhsana, T.E. Machonkin**
- INOR 177.** Synthesis and reactivity of manganese(III) complexes with tetradentate ligands that mimic superoxide dismutase enzymes. **S.T. Frey, H.A. Cirka, W.A. Gallopp, P.B. Moses**
- INOR 178.** Biochemical, kinetic, and spectroscopic characterization of a promiscuous metal-dependent DMSP-lyase. **A. Brummert, M. Day**
- INOR 179.** Effect of mutations on the stability of P450_{BM3} as determined by chemical and thermal denaturation. **C. Denning, D.K. Heidary, E. Glazer**
- INOR 180.** Synthesis, characterization, and applicability of reactive biomimetic model complexes toward important biological reactions. **K.J. Meise, E.M. Brandes, R. Theisen**
- INOR 181.** Reduction of copper(II) by thioether sulfur: A synthetic model for the amyloid beta peptide. **M. Wallace, R.P. Houser**
- Section C**
Colorado Convention Center
Hall C
- 2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton**
E. Boon, M. C. Buzzeo, S. Delaney, V. C. Pierre, *Organizers*
- 6:00 - 8:00**
- INOR 182.** Reactivity and electrostatics of ribosomal RNA hairpins with modified nucleotides determined by cationic metal complexes. **G. Dedduwa-Mudalige, S. Elmorh, C.S. Chow**
- INOR 183.** Fluorescently-labeled bioactive protein nanoparticles (prodots) for improved uptake by oral cancer cells. **B. Stromer, I. Deshapriya, A. Pattammattel**
- INOR 184.** New fluorescent probes for peptide nucleic acid (PNA) based diagnostics. **S. Naik, E. Yavin**
- INOR 185.** Efficient DNA photo modulation by PNA-Rose Bengal conjugates. **Y. Shemesh, S. Naik, E. Yavin**
- INOR 186.** Nanoconfinement of gold on the spatial location of titania nanotubes. **S.A. Ferdousi, K.L. Yeung**
- INOR 187.** Lipid signaling through NM23-H1 as a possible suppressor of metastasis. **M.R. Friedman, J.D. Lapek, A.E. Friedman**
- Section C**
Colorado Convention Center
Hall C
- Undergraduate Research at the Frontiers of Inorganic Chemistry**
Bioinorganic Chemistry
C. Nataro, *Organizer*
- 6:00 - 8:00**
- INOR 188.** Probing the effects of environments on pK_a values: Interaction of aniline with reverse micelles as monitored using by ¹H NMR spectroscopy. **J. Sripradite, S.A. Miller, A. Tongraar, M.D. Johnson, D.C. Crans**
- INOR 189.** Electron withdrawing capability of ligating histidine adducts influence the reduction potential of the [2Fe-2S] cluster of the Rieske protein. **L.M. Hunsicker Wang, C. Hertz, N. Karagas**
- INOR 190.** Semiquinone stabilization via de novo designed protein scaffolds. **I. Sokimiy, G. Ulas, W.F. Degrado, A.J. Reig**
- INOR 191.** Structural and functional characterizations of 4-His/3-carboxylate G4DFsc proteins. **K. O'Shea, K. Biernat, A.J. Reig**
- INOR 192.** Creation and characterization of ruberythrin and symerythrin model proteins. **J. Pellegrino, R.Z. Polinski, S.N. Cimerol, A. Jacobs, E.I. Solomon, A.J. Reig**
- INOR 193.** Modeling the activity of the tungsten-containing nitrate reductase of *Pyrobaculum aerophilum*. **K. Scott, R. Page, B. Trujillo, M.A. Cranswick**
- INOR 194.** Toward understanding the reaction mechanism of the tungstoenzyme, acetylene hydratase. **E. Vergunst, B. Trujillo, M.A. Cranswick**
- INOR 195.** Interactions of acrylamide with heme models. **C. Lingafelt, N. Xu**
- INOR 196.** Derivatives of a metallopeptide-based mimic of nickel-containing superoxide dismutase. **T. Detomasi, J. Schmitt, J.M. Shearer**
- INOR 197.** Investigation of sugar-Cu(II) and Zn(II) complexes' interactions in aqueous alkaline media. **M.A. Pedraza, C. Stewart, H. Arman, G.T. Musie**
- Section F**
Colorado Convention Center
Hall C
- Undergraduate Research at the Frontiers of Inorganic Chemistry**
Coordination Chemistry
C. Nataro, *Organizer*
- 6:00 - 8:00**
- INOR 198.** Synthesis and characterization of BIAN iron dihalide complexes. **M.J. Supej, K.A. Wheeler, C.E. Schulz, H.M. Hoyt**
- INOR 199.** Synthesis and reactivity of iron compounds containing acid functionalized 1,4,7-triazacyclononane ligands. **E. Foerster, G. Rowe**
- INOR 200.** Ligand donor effects in copper(I) and copper(II) complexes of polydentate heteroaromatic-amine ligands in the ATRP of styrene. **T. Chidanguro, L. Ma, S.L. Guillot, R.D. Pike, C. Goh**
- INOR 201.** Isolation and characterization of group 13 bis(2-(1-methylimidazolyl)methyl) amine complexes. **N.B. Kingsley, T.J. Doyon**
- INOR 202.** Tuning the photophysical properties in a series of Re(I) charge transfer complexes. **J. Breaux, A. Leeds, J. Yarnell**
- INOR 203.** Bidirectional "ping-pong" energy transfer in an Ir(III) charge transfer complex. **A. Leeds, J. Breaux, J. Yarnell**
- INOR 204.** Development of gold(III) complexes containing ligands designed for chelation-assisted functionalization of strong, sp³-hybridized C-H bonds. **R. Miller, J.E. Thompson, M. Sleck, A. Brown, S. Summi, D. Ohlson, B. Williams, I. Brown, E. Nissen, T. Stutzriem, A.L. Rheingold, D.R. Weinberg**
- INOR 205.** Gold(I) complexes of 2- and 6-mercaptopzozenes: Syntheses, molecular and electronic structures, and reactivity profiles. **B.A. Tappan, A.D. Spaeth, O. Torres-texidor, N. Gerasimchuk, M.V. Barybin**
- INOR 206.** Molybdate hydrolysis of phosphonothioate neurotoxin. **K.M. Dill, L.Y. Kuo, Y. Shari'ati**
- INOR 207.** Withdrawn.
- INOR 208.** Developing a method of copper(II) oxidation catalyst synthesis. **C. Anderson, J. Rumreich, J. Bodwin**
- INOR 209.** Probing the selectivity of luminescent lanthanide complexes toward biologically relevant anions. **K.R. Johnson, K.H. Felix, E.J. Werner**
- INOR 210.** Rational design of catalysts for water-gas shift reaction. **J. Fox, A. Dinescu**
- INOR 211.** Luminescence and extraction properties of novel tripodal CPMO ligands. **D.A. Hardy, M.T. Peruzzi, S.N. McGraw, S.M. Biros, E.J. Werner**
- INOR 212.** Utilizing diphenylacetate lability in the synthesis of mixed ligand copper (II) dimers. **M. Chen, T.W. Clayton**
- Section G**
Colorado Convention Center
Hall C
- ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar**
Cosponsored by WCC
C. P. Berlinguette, D. J. Mindiola, E. J. Schelter, M. Shatruk, *Organizers*
- 6:00 - 8:00**
- INOR 213.** Synthesis, characterization, and photochemical studies of solvated dinuclear Ru(II) compounds with quinoxaline and pyrazine based bridging ligands. **S. Saha, B. Pena, B.A. Albani, C. Turro, K.R. Dunbar**
- INOR 214.** Computational exploration of the noncovalent interactions involved in the inhibition of malate synthase for treatment of tuberculosis. **J.F. Ellenbarger, S.E. Wheeler, J.C. Sacchetti, K.R. Dunbar**
- INOR 215.** "Reinventing the wheel" with heptacyanomolybdate(III). **D.K. Kempe, H. Zhao, T.J. Woods, M.R. Saber, K.R. Dunbar**
- INOR 216.** Cyanide-bridged single chain magnets with hexacyanomanganate. **Y. Zhang, H. Zhao, E.S. Funck, K.R. Dunbar**
- INOR 217.** Ligand effects and geometrical control of the magnetic anisotropy in mononuclear SMMs. **M.R. Saber, K.R. Dunbar**
- INOR 218.** Semiconducting and magnetic properties in metal-TCNQ-based functional materials. **X. Zhang, H. Zhao, Z. Wang, Y. Zhang, K.R. Dunbar**
- INOR 219.** Series of trigonal bipyramidal Co(II) complexes that display SMM behavior. **M.F. Ballesteros-Rivas, T.J. Woods, K.R. Dunbar**
- INOR 220.** Dinuclear lanthanide complexes containing a radical bridging ligand. **T.J. Woods, M.F. Ballesteros-Rivas, K.R. Dunbar**
- INOR 221.** Biological studies of dirhodium(II,II) based compounds and their applications as photochemotherapeutic agents. **A. David, Z. Li, B. Pena, J. Pellois, K.R. Dunbar**
- INOR 222.** Structural study of Prussian blue. **A. Brown, H. Zhao, K.R. Dunbar**
- INOR 223.** Solvent effects on the spin transitions in discrete cyanide-based magnetic material. **C. Sanders, H. Stout, C. Achim, D. Petasis, K.R. Dunbar**
- INOR 224.** Exploring and enhancing the functionality of tetrazine molecular switches. **C. Benson, A.H. Flood**
- INOR 225.** Imaging studies of metal-containing nanoparticle as multimodal platforms for biomedical applications. **P. Promdet, B. Rodriguez-Garcia, A. Henry, C. Blumenfeld, R.A. Moats, R.H. Grubbs, H.B. Gray, J. Galan-Mascaros, K. Sorasaneae**
- INOR 226.** Investigating the magnetic properties of metal complexes containing a tris(amido)amine ligand. **F.J. Birk, K. Schulte, D. Pinkowicz, K.R. Dunbar**
- INOR 227.** Anion-π contacts in supramolecular architectures. **H.T. Chifotides**
- Section H**
Colorado Convention Center
Hall C
- Coordination Chemistry**
Characterization and Applications
D. C. Crans, *Organizer, Presiding*
- 6:00 - 8:00**
- INOR 228.** Heteroleptic polypyridyl ligand cobalt(III) complexes. **S.E. Hightower, B.A. Frenzel, C.T. Kuester**
- INOR 229.** Transition metal complexes as paraSHIFT and paraCEST MRI contrast agents. **P.B. Tsiftovich, J.M. Cox, J.B. Benedict, J.R. Morrow**
- INOR 230.** Carbonato-bridged copper(II) complexes formed via fixation of atmospheric CO₂. **F. Louka, F.A. Mautner, S.S. Massoud**
- INOR 231.** Synthesis and structural characterization of PTA derivative modified transition metals. **J.M. Sears, T.J. Boyle, B.J. Frost, W. Lee, M.L. Neville**
- INOR 232.** Investigation of isomeric single amino acid chelate (SAAc) rhodium series. **N.J. Azzarelli, M.P. Coogan, J.A. Platts, R.P. Doyle, J.A. Zubieta**
- INOR 233.** Electronic structure and reactivity of d⁰ Mo and Ti complexes of a tris-aminophenolate ligand. **T. Marshall-Roth, S.N. Brown**
- INOR 234.** Syntheses and characterizations of luminescent rare earth metals complexes. **P.K. Yuen, C.D. Lau**
- INOR 235.** Designing artificial monoamine transporters based on synthetic superconductors. **U. Sambasivam, Z. Wang**
- INOR 236.** Interactions of coordination complexes with reverse micellar interfaces: The effects on MLCT bands and coordinated ligand pK_a values. **A.A. Cadena, M.D. Johnson, J. Sripradite, S.A. Miller, D.C. Crans**
- INOR 237.** Study of glutathione interactions with anticancer Gold(III) diamines complexes using NMR, UV-VIS and electrochemistry. **A. Isab**
- INOR 238.** Photocatalytic NADH regeneration and hydrogen production using Rh complexes and Pt nanoparticles. **J. Kim, S. Kim**
- INOR 239.** Mechanistic studies of oxidative aliphatic carbon-carbon bond cleavage in Cu(II) chlorodiketone complexes. **S.L. Saraf, J.R. Argue, L.M. Berreau**
- INOR 240.** Coordination chemistry of cyanopyrazoles and cyanoscorpionates. **D.M. Eichhorn**
- INOR 241.** Single and multiphoton turn-off fluorescent sensor for tin and iron. **R.M. Madawala, E. Sinn**

INOR **242.** Synthesis, NMR characterization, and MIC studies of a new series of alpha-(N)-heterocyclic thiosemicarbazone ligands and their Pd²⁺ and Cu²⁺ metal complexes. **J.D. Conner**, S.D. Simpson, A.L. Koch, E.C. Liscic

Section I

Colorado Convention Center
Hall C

Organometallic Chemistry

Applications to Organic Transformations

N. S. Radu, *Organizer*

6:00 - 8:00

- INOR **243.** Borates in biomass conversion processes. **D.M. Schubert**, M.K. McCray
- INOR **244.** Late transition metal complexes for industrially relevant catalysis. **N.A. Swisher**, P. Romero, R.H. Grubbs
- INOR **245.** Cobalt-induced B-H and C-H Activation Leading to Facile B-C Coupling of Carboranedithiolate and Cyclopentadienyl. **H. Yan**

Section J

Colorado Convention Center
Hall C

Organometallic Chemistry

Catalysis

N. S. Radu, *Organizer*

6:00 - 8:00

- INOR **246.** Polynuclear iridium-bismuth carbonyl clusters: Synthesis, chemistry, and applications. **G. Elpitiya**, R.D. Adams, M. Chen, Q. Zhang, R. Raja
- INOR **247.** Alkene vs. alkyne hydroarylation catalyzed by electrophilic palladium(II) and platinum(II) complexes. **M. Manjahi**, C. Hahn
- INOR **248.** Theoretical studies of hydroformylation of butadiene. **C.H. Mendis**, T. Maji, J.A. Tunge, W.H. Thompson
- INOR **249.** Control of *cis*-selectivity and tacticity in ring opening metathesis polymerization using ruthenium metathesis catalysts. **L.E. Rosebrugh**, V.M. Marx, T.S. Ahmed, J. Hartung, R.H. Grubbs
- INOR **250.** Enantioselectivity and substitution effects in rhodium catalyzed intramolecular hydroacylation. **B.P. Schumacher**, L.M. Stanley, J. Scanlon
- INOR **251.** Electrocatalytic reduction of CO₂ to formate using iridium pincer complexes. **P. Kang**, S. Zhang, Z. Chen, C. Chen, T.J. Meyer, M. Brookhart
- INOR **252.** Oxygen atom transfer to iridium(Cp)⁺ complexes. **C. Turlington**, M. Brookhart, J.L. Templeton
- INOR **253.** Synthesis of branched ultra-high-molecular-weight polyethylene using highly active neutral, single-component Ni(II) catalysts. **Z. Chen**, M. Mesgar, P.S. White, O. Daugulis, M. Brookhart
- INOR **254.** Living polymerization of ethylene and copolymerization of ethylene/methyl acrylate using "sandwich" diimine palladium catalysts. **K. Allen**, J. Campos Manzano, O. Daugulis, M. Brookhart
- INOR **255.** Selective cross-dimerization of ethylene with substituted olefins. **P.R. Payne**, M. Brookhart, M.R. Gagne
- INOR **256.** Applications of PC(sp³)P iridium complexes in transfer dehydrogenation of alkanes and ethers. **D. Bezier**, M. Brookhart
- INOR **257.** Regioselective palladium-catalyzed hydrodechlorination of 2,3,5-tribromothiophene. **K.L. Konkol**, S.C. Rasmussen
- INOR **258.** Ligand modification at a remote site to regulate iron-catalyzed olefin hydroboration. **K.T. Tseng**, J. Kampf, N.K. Szymczak
- INOR **259.** Catalytic carbonylation of icosahedral dodecaborates. **K.R. Kamp**, R.J. Staples, J.A. Dopke
- INOR **260.** Copper-catalyzed addition of phenols to icosahedral dodecaborates. **C. Barnhart**, R.J. Staples, A.J. Ramirez, J.A. Dopke

INOR **261.** Ruthenium-catalyzed substitutions of icosahedral dodecaborates. **L.R. Bent**, A.J. Ramirez, J.A. Dopke

INOR **262.** Electrocatalytic oxidation of methylrhenium trioxide to methanol by an electrode-immobilized ruthenium(II) polypyridyl catalyst. **M.K. Coggins**, T.J. Meyer, R.A. Periana

Section K

Colorado Convention Center
Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallic Chemistry

C. Nataro, *Organizer*

6:00 - 8:00

- INOR **263.** Twists and turns: WGS "catalysts" of Fe, Ru, and Os. A. Eschmann, E. Wulff-Fuentes, D. Cunningham, B. Schreiber, L. Burgan, Z. Hecht, G. Seichter, A.L. Rheingold, J.S. D'Acchioli
- INOR **264.** Selective hydrogenation of phenylacetylene over supported gold catalysts. **E. Purdy**, B.D. Chandler
- INOR **265.** Experimental and theoretical studies investigating the effect of solvent on ¹J_{WH} in Cp₂WH₂. **C.I. Viquez Rojas**, T.A. Mobley
- INOR **266.** Low valent metal complexes of tris(diphenylphosphinomethyl)phenylborate. **A.B. Weberg**, T.D. Bohrmann, H. Xu, P.J. Fischer
- INOR **267.** Redox-active NHC pincer ligands for Ni-catalyzed aerobic dehydrogenative C-C cross coupling. **J.E. Hertzog**, C.F. Harris, J.D. Soper
- INOR **268.** Synthesis of palladium(II)-NHC compounds and their employment as cross-coupling catalysts. **D. Colosimo**, **M. Dominguez**, G. Rowe
- INOR **269.** Sulfur-hydrogen bond activation by novel iridium diphosphine complexes. **H.N. Russ**, S.H. Schreiner
- INOR **270.** Synthesis of molybdenum carbon dioxide complexes via oxidation of a carbonyl ligand. **M.A. Pogash**, G.R. Lorzing, J.R. Vasta, X. Duan, R.G. Carden, J.J. Ohane, P.M. Graham
- INOR **271.** Microwave-assisted concurrent tandem catalysis (CTC) methodology for the copper-catalyzed dimerization of aryl halides. **E. Shields**, M. Lee, D.J. Brown, S. Lin, A.R. MacArthur
- INOR **272.** Catalytic transfer hydrogenation of aryl-alkyl ketones using Cp*Ir(III)Cl pyridine-sulfonamide complexes. **A. Ruff**, B.C. Chan, A.R. O'Connor
- INOR **273.** Catalytic transfer hydrogenation of aryl aldehydes using Cp*Ir(III) pyridinesulfonamide complexes. **C. Kirby**, A.R. O'Connor

Section L

Colorado Convention Center
Hall C

Chemistry of Materials

C. G. Lugmair, *Organizer*

6:00 - 8:00

- INOR **274.** pH-dependent ceria-doped titanate nanotubes. **Y. Fam**, S.A. Ferdousi, K.L. Yeung, Y. Du
- INOR **275.** Synthesis and characterization of quaternary misfit-layer-compound-like ferrocyanates. **R. Westover**, D.C. Johnson, J. Ditto
- INOR **276.** Self-assembly of organometallic molecular films based on the azulenic scaffold linearly functionalized with both isocyanide and thiol termini. **M.K. Okeowo**, C.L. Bernie, M.V. Barybin
- INOR **277.** Chiral amplification by metal-ligand conjugation in chiral magnetic nanoparticles. **J. Yeom**, N. Kotov
- INOR **278.** Structure and properties of sodium enneaborate. **D. Neiner**, Y. Sevryugina, D.M. Schubert
- INOR **279.** Wet-spinning of graphene fibers from giant graphene oxide sheets by adopting a series of amine alcohol solution as coagulation solution. **C. Zhao**, W. Zeng, S. Tong, S. Mo, J. Wang, T. Fan, W. Tang, C. Yuan, Y. Liu, Y. Min
- INOR **280.** Water based PAN conductive coatings for antistatic application. **Y. Feng**, X. Liu, C. Ma, J. Shen, Z. Xiao, T. Fan, S. Tong, Y. Liu, Y. Min
- INOR **281.** Facile method to fabricate transparent, flexible conducting graphene thin films via liquid phase deposition. **C. Yuan**, W. Tang, J. Wang, S. Mo, C. Zhao, T. Fan, S. Tong, Y. Liu, Y. Min
- INOR **282.** Supercritical CO₂ method of graphene preparation. **J. Shen**, Y. Feng, C. Ma, X. Liu, Z. Xiao, T. Fan, S. Tong, Y. Liu, Y. Min
- INOR **283.** Production of graphene by dry ice ball milling method. **Z. Xiao**, J. Shen, Y. Feng, C. Ma, X. Liu, T. Fan, S. Tong, Y. Liu, Y. Min
- INOR **284.** Preparation and properties of different phase of hydrothermal synthesis of 3D graphene. **S. Mo**, S. Tong, C. Yuan, W. Tang, J. Wang, C. Zhao, T. Fan, J. Shen, Y. Liu, Y. Min
- INOR **285.** Synthesis and instability of cuprous nitride nanocrystals. **M. Reichert**, J. Vela
- INOR **286.** Categorizing defects in nanowires produced through electrodeposition. **K.J. Kysor**, D. Vu, C. Myers, B.D. Smith
- INOR **287.** Rapid synthesis of carbon nitride materials and composites for use in photocatalysis. **A. Montoya**, E.G. Gillan
- INOR **288.** Thermal and electronic effects on the solvothermal formation of nanocrystalline WSe₂ in aromatic solvents. **M.P. Hanrahan**, **J.S. Edgar**, S.A. Darveau, C.L. Exstrom
- INOR **289.** Formation of WSe₂ thin films via annealing of a solvothermally prepared nanocrystalline precursor. **J.S. Edgar**, M.P. Hanrahan, C.L. Exstrom, S.A. Darveau
- INOR **290.** Metal-sulfur-arene semiconducting frameworks. **H. Hu**, T.P. Vaid
- INOR **291.** Sulfonium derivatives of the [closo-1-CB₁₁H₁₂] anion as polar liquid crystals. **P. Zagorski**, J.G. Pecyna, P. Kaszynski
- INOR **292.** Liquid crystalline derivatives of the [closo-B₁₀H₁₂] anion. **P. Tokarz**, P. Zagorski, P. Kaszynski
- INOR **293.** New network of Mn₁₂ molecules. **A.E. Thujijs**, G. Christou, K.A. Abboud
- INOR **294.** Functionalization of GaP substrates for use in photoelectrochemical cells. **O. Williams**, A.H. Cowley, M.J. Rose
- INOR **295.** Thermodynamic stability of aqueous metal clusters: A dynamic approach. **T.J. Mustard**, L.A. Wills, I. Chang, D.A. Keszler, P.H. Cheong
- INOR **296.** Computational study of polyoxometalate formation mechanisms. **L.A. Wills**, **D.B. Fast**, M. Dolgos, P.H. Cheong
- INOR **297.** Carbon nanofoams as porous scaffolds for iron-air battery electrodes. **M.F. Mayther**, S.D. Murphy, J.C. Lytle
- INOR **298.** Doping Cu₂ZnSnS₄ nanorods with tetrahedral, high spin metals: Co²⁺, Mn²⁺, and Ni²⁺. **M. Thompson**, M. Reichert, J. Vela-Becerra
- INOR **299.** Efficient dye degradation via non-photocatalytic route by perovskite type LaNiO_{3-δ} materials. **W. Zhong**, C. Kuo, S. Chen, S.L. Suib
- INOR **300.** Functionalization of metal oxide surfaces for photoelectrocatalysis of CO₂ reduction. **S.K. Heiskanen**, J.M. Ziegler, D.A. Rider, J.D. Gilbertson
- INOR **301.** Control of the crystalline phase and morphology of CdS deposited on microstructured surfaces by chemical bath deposition. **D. Fernando**, M. Khan, Y. Vasquez
- INOR **302.** Colloidal synthesis of silicon and germanium nanorods and nanowires. **X. Lu**, B. Korgel
- INOR **303.** Graphene oxide assisted hydrothermal carbonization of carbon hydrates. **D. Krishnan**, K. Raidongia, J. Shao, J. Huang

Section L

Colorado Convention Center
Hall C

Inorganic Spectroscopy

S. A. Koch, *Organizer*

6:00 - 8:00

- INOR **304.** New multifunctional Schiff base as fluorescence sensor for AP³⁺ and colorimetric sensor for CN⁻ in aqueous media: an application to bioimaging. **G. You**, Y. Na, S. Lee, K. Ryu, C. Kim
- INOR **305.** Colorimetric organic chemo-sensor for Co²⁺ in a fully aqueous environment. **H. Jo**, **S. Lee**, J. Lee, Y. Kim, C. Kim
- INOR **306.** Water-soluble chemosensor for detecting AP³⁺ in aqueous media and living cells. **J. Lee**, P. Kim, C. Kim
- INOR **307.** Withdrawn.
- INOR **308.** Measurement of NMR relaxation rates in a series of cobalt (II) β-diketonates. **R.R. Baum**, D.L. Tierney
- INOR **309.** Monitoring the ring opening polymerization of hexachlorocyclotriphosphazene through NMR spectroscopy. **J.A. Stiel**, C. Tessier, Z. Tun
- INOR **310.** Scalar and spin-orbit relativistic calculations of ¹J_{WH} in Cp₂WH₂ complexes. **T.A. Mobley**
- INOR **311.** Investigating the stereoelectronic consequences of diphosphine ligands on M-P and M-Cl covalency in late transition metal complexes. **C. Donahue**, B.J. Bellotti, A. Blake, C.M. Forrest, J.M. Keith, S. McCollom, S.R. Daly
- INOR **312.** Photoinduced properties of bimetallic polypyridyl complexes. **T.J. Whittemore**
- INOR **313.** Colorimetric "naked-eye" Cu(II) chemo-sensor and pH indicator in an 100% aqueous solution. **Y. Choi**, M. Lee, G. Park, K. Bok, T. Jo, C. Kim
- INOR **314.** Chiral conducting polymers as efficient spin filters. **P.C. Mondal**, C. Fontanesi, R. Naaman

Section L

Colorado Convention Center
Hall C

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

6:00 - 8:00

- INOR **315.** Synthesis of "rare earths – magnesium" master alloys by high temperature exchange reactions. **A.V. Krylovov**, K.V. Maksimov, I.B. Polovov, V.A. Volkovich, O.I. Rebrin
- INOR **316.** Synthesis, structural characterization, and magnetic properties of dinuclear, tetranuclear, and polynuclear lanthanide(III) complexes of a symmetric ditopic carbohydrazone based ligand (H₂L). **S.S. Tandon**, S.D. Bunge, S.K. Adas, L.K. Thompson, C. Lucas
- INOR **317.** Speciation studies between a novel pincerLigand with lanthanum (III) salts. **D. Kremer**, M. Guino-o, A. De Bettencourt Dias
- INOR **318.** Chiral light emitting ionic liquids. **B. Zercher**, T. Hopkins
- INOR **319.** New calix[4]arene based precursors for stationary phases useful in separation of rare earth metals. **S. Menon**, J.A. Schmidt
- INOR **320.** Magnetic properties of mononuclear uranium-acetylacetonate complexes. **R. Higgins**, B. Newell, A.K. Rappe, M.P. Shores
- INOR **321.** Optimization of rare earth element chromatography. **H. Knutson**, A. Holmqvist, B. Nilsson
- INOR **322.** Stability and cation exchange dynamics of γ-irradiated actinyl peroxide nanocapsules. **T.A. Olds**, B.J. Moeller, P.C. Burns
- INOR **323.** Methylcyclopentadienide as a supporting ligand for a reduced dinitrogen complex of yttrium. **D.H. Woen**, J.W. Ziller, W.J. Evans
- INOR **324.** Synthesis and f-element coordination of phosphine oxide decorated polypyridine ligand. **J. Dehaut**, D.A. Dickie, B.P. Hay, R.T. Paine

INOR 325. Dinitrogen reduction and isoprene polymerization via photochemical activation of bis(cyclopentadienyl) rare earth allyl complexes. *C.W. Johnson, M. Fieser, J.W. Ziller, W.J. Evans*

INOR 326. Tuning of structural dimensionality in lanthanide cyanometallates. *R. Sykora, F.D. White, L. Pham, K. Xaing, A.T. Thames, J. Hendrich, J.D. Taylor*

INOR 327. Dicyanoaurate and tetracyanoplatinate compounds as potential chemical sensors for volatile organic compounds. *F.D. White, R. Sykora, J. Hendrich*

INOR 328. Emissive electropolymerizable lanthanide complexes. *M.V. Tran, D.J. Strohecker, M.T. Raiford, B.J. Holliday*

INOR 329. Lanthanide-organic frameworks as asymmetric heterogeneous catalysts. *D.T. de Lill*

INOR 330. Synthesis and structural characterization of Y^{2+} and Gd^{2+} in heteroleptic tris(cyclopentadienyl) rare earth complexes. *C.T. Palumbo, J.W. Ziller, W.J. Evans*

Section L

Colorado Convention Center
Hall C

Nanoscience

Cosponsored by PRES

R. M. Richards, *Organizer*

6:00 - 8:00

INOR 331. Pt-Au and Pd-Au bimetallic heterostructures using mask assisted seeded growth. *C. Crane, J. Chen*

INOR 332. Effective regulation of post-preparative cation exchange reactions in PbS quantum dots. *B.P. Mainali, P.G. Van Patten*

INOR 333. Incorporation of transition metal cations into PbS QDs via cation exchange. *W. Tiluck, A.D. Evans, J.K. Gurchiek, C.M. Mings, A.L. Morris, P.G. Van Patten*

INOR 334. Supersaturation-precipitation strategies to colloidal hybrid nanoparticles. *C.G. Read, A.J. Bicchii, R.E. Schaak*

INOR 335. Synthesis of acetamide from acetonitrile hydrolysis using EEW catalyzed with metal nanoparticles. *E. Abdelkader, S.W. Buckner, P.A. Jelliss*

INOR 336. Growth kinetics of zinc oxide quantum dots. *B. Colon, H. Egidio-Betancourt, C.P. Mccord, P.P. Vaughan, A.K. Schrock, K.S. Molek*

INOR 337. Effect of synthetic levers on phosphorus incorporation in nickel phosphide nanoparticles: Ni_3P_2 and NiP_2 . *D. Li, S. Brock*

INOR 338. Electrophoretic deposition of gold nanospheres for explosives detection. *K. Roberts, Y.J. Han, T.Y. Olson*

INOR 339. Formation of Ag nanoclusters via the direct dissolution of bulk Ag. *J.R. Changstrom, C.M. Sorensen*

INOR 340. Ion exchange and protection-deprotection chemistry in the total synthesis of colloidal hybrid nanoparticles. *J.M. Hodges, A.J. Bicchii, R.E. Schaak*

INOR 341. Polyaniline/laponite/gold coordination polymer nanoassemblies for solar applications. *P. Quah, M.E. Hagerman*

INOR 342. New routes to clean water: Laponite/copper oxide nanomaterials for bacterial remediation. *A.J. Cavert, M.E. Hagerman*

INOR 343. Synthesis and characterization of titanium oxide nanopowders. *H. Chenoweth, L.F. Barnes, C.J. Van Leeuwen, K.A. Reyes, C.K. Butterfield*

INOR 656. Ligand-induced fate of embryonic seeds in the shape-controlled synthesis of rhodium nanoparticles. *A.J. Bicchii, R.E. Schaak*

Section L

Colorado Convention Center
Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Main Group Chemistry

C. Nataro, *Organizer*

6:00 - 8:00

INOR 344. Synthesis and characterization of spirocyclic monoalkylated organosilicon complexes of 1-hydroxy-2-pyridinone. *J.G. Koch, W.W. Brennessel, B.M. Kraft*

INOR 345. Synthesis and characterization of five-coordinate aluminum complexes that polymerize ϵ -caprolactone. *A.M. Longo, J.M. Fritsch*

INOR 346. Polymerization of ϵ -caprolactone by aluminum alkoxide complexes supported by tridentate ketiminates bearing electron-withdrawing groups. *A.M. McCollum, A.L. Rheingold, J.M. Fritsch*

INOR 347. L-Lactide and sym-caprolactone ring opening polymerization by binary catalysts systems that include bis-ligated magnesium complexes. *R.M. Slattery, A.L. Rheingold, J.M. Fritsch*

INOR 348. Polymerization of lactide by aluminum ion pairs studied with 27Al NMR. *L.A. Schmitz, A.L. Rheingold, D.B. Green, J.M. Fritsch*

INOR 349. Si-H and Ge-H bond activation by a platinum dimer. *L. Matuszewski, S.H. Schreiner*

Section L

Colorado Convention Center
Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Solid State and Materials Chemistry

C. Nataro, *Organizer*

6:00 - 8:00

INOR 350. Investigating the electronic coupling of quantum dots to crystal-bound thiols. *A.M. Fall, S. Castillo, N.K. Brandon, M.J. Turo, A.D. La Croix, J.E. Macdonald*

INOR 351. Synthesis and photovoltaic performances of di-acetylide platinum complexes in dye-sensitized solar cells. *T. Schuyler, S. Gauthier*

INOR 352. New phase discovered in the Cu-Ge-Te system by high-temperature solid state reaction. *B. Hogan, J.A. Aitken*

INOR 353. Spectroelectrochemical determination of the Fe(III)/Fe(II) reduction potential in recombinant, cross-linked hemoglobins. *R. Bangle, C.J. Parker Siburt, R. Kreulen, A.L. Crumbliss*

INOR 354. Green dechlorination via functional models of cyanocobalamin. *D. Marquis, K.M. Van Heuvelen*

INOR 355. Optical and thermal properties of lithium-containing thioacetate with potential nonlinear optical applications. *A. Weiland, J. Brant, J. Zhang, J.A. Aitken*

INOR 356. Surface chemistry of gold nanoparticles in natural environments. *K. Roberts, A.K. Bentley*

INOR 357. Investigation of novel polymorphic Li_2 , -IV-S₂ diamond-like semiconductors utilizing synchrotron X-ray powder diffraction. *K.P. Devlin, K. Daley, M.A. Moreau, J. Brant, J.A. Aitken*

INOR 358. Precursor approach to probing host-guest binding of synthetic superconductors. *A. Hammerstrom, F. Dai, Z. Wang*

MONDAY MORNING

Section A

Colorado Convention Center
Bellico Theatre

ACS National Awards in Inorganic Chemistry: Plenary Session

S. A. Koch, N. S. Radu, *Organizers*

J. M. Boncella, *Organizer, Presiding*

8:30 INOR 359. Award Address (F. Albert Cotton Award in Synthetic Inorganic Chemistry sponsored by the F. Albert Cotton Endowment Fund). Understanding and predicting the behavior of the actinides through organometallic chemistry. *J. L. Kiplinger*

9:00 INOR 360. Award Address (ACS Award in Organometallic Chemistry sponsored by the Dow Chemical Co. Foundation). Importance of organometallic chemistry in the discovery of new oxidation states of the rare earth and actinide elements in molecular complexes. *W. J. Evans*

9:30 INOR 361. Award Address (ACS Award in Inorganic Chemistry sponsored by Aldrich Chemical Co., LLC). Metalloporphyrins in chemical and biological catalysis. *J. T. Groves*

10:00 INOR 362. Award Address (ACS Award for Creative Research and Applications of Iodine Chemistry sponsored by SQM S.A.). Fifty years of Iodine research. *K. O. Christe*

10:30 Intermission.

10:45 INOR 363. Award Address (ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry sponsored by Strem Chemicals). Molecular magnetic and conducting materials inspired by coordination chemistry. *K. R. Dunbar*

11:15 INOR 364. Award Address (Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator sponsored by the Harry Gray Award Endowment). Colloidal quantum dots: Where d10 ions go to glow. *E. A. Weiss*

11:45 INOR 365. Award Address (ACS Award in the Chemistry of Materials sponsored by E. I. du Pont de Nemours & Co.). Use of organometallic complexes to squeeze every last photon out of an organic LED. *M. E. Thompson*

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry

IONIC VIPER on Mg

S. R. Smith, *Organizer*

C. Nataro, *Organizer, Presiding*

A. R. Johnson, *Presiding*

1:30 Introductory Remarks.

1:40 INOR 366. Solvent loss and reuptake in $Na[BH(C_2H_5)_2]$ frameworks. *B.A. Reisner, W.T. Price, A.T. Muetterties*

2:05 INOR 367. Eggs in one basket: Is there a role for riboflavin binding protein in copper transport and storage? *S.R. Smith, M. Benore, J.I. Matchynski*

2:30 INOR 368. Controlling electrochemistry in the synthesis of semiconductor nanoparticles. *A.L. Prieto, E. Nock, P. Reining, G.P. Wheeler*

2:55 INOR 369. Asymmetric hydroamination with titanium and tantalum: experiment and theory. *A.R. Johnson*

3:20 INOR 370. Reactivity of bis(phosphino) ferrocenediyl containing compounds. *C. Nataro*

3:45 Concluding Remarks.

Section B

Colorado Convention Center
Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, S. Delaney, V. C. Pierre, *Organizers*
M. C. Buzzeeo, *Organizer, Presiding*

1:30 INOR 371. Allosteric and unexpected binding sites for small-molecule modulators. *M. Arkin*

2:00 INOR 372. Aptamer technology for biosensing, therapeutics, and targeted release. *M.C. DeRosa*

2:30 INOR 373. Electromechanical tissue reconstruction: A non-invasive surgical modality for reshaping cartilage of the head and neck. *M.G. Hill, J. Kallick, M. Herzog, B. Hunter*

3:00 Intermission.

3:10 INOR 374. 19F MRI: Dream or reality. *V.C. Pierre*

3:40 INOR 375. Real-time metabolic and molecular imaging in vivo by NMR hyperpolarization. *P.K. Bhattacharya*

4:10 INOR 376. Structure and mechanism in the essential stereoinversion in carbapenem biosynthesis. *A.K. Boal*

Section C

Colorado Convention Center
Room 302

ACS Award in Organometallic Chemistry: Symposium in Honor of William J. Evans

J. R. Walensky, *Organizer*

J. C. Gordon, *Presiding*

1:30 INOR 377. Preparation of isotopically labeled active site models for the [FeFe]- and [FeNi]-hydrogenases. *T.B. Rauchfuss, R. Gilbert-Wilson, D. Schiller*

1:50 INOR 378. Studies of metal to ligand charge transfer states involving MM quadruply bonded complexes. *M. Chisholm*

2:10 INOR 379. Bimetallic actinide complexes of constraining macrocycles for small molecule activation. *RL. Arnold, N. Potter, R. White, C. Stevens, M. Dutkiewicz, J. Farnaby, R. Cacluffo, C. Apostolidis, O. Walter, J.B. Love, N. Kaltsayannis, M. Gardiner*

2:30 INOR 380. Rare earth doped alkali metal fluorides — promising new optical materials. *A.V. Mudring*

2:50 Intermission.

3:00 INOR 381. Phosphorus- and arsenic-ligated lanthanide single-molecule magnets. *R.A. Layfield, T. Pugh*

3:20 INOR 382. Catalytic conversion of biomass to fuels. *J.C. Gordon, A.D. Sutton, A.E. King, L.A. Silks, R. Wu, M. Schlaf, F. Waldie*

3:40 INOR 383. Half-sandwich metallacarba-decaboranyl complexes at the interface of main-group and organometallic chemistry. *L.G. Sneddon, E.R. Berkeley, A. Perez-Gavilan, P.J. Carroll*

4:00 INOR 384. Spin-orbit coupling: Not just for f elements. *J. Telsner, S. Fortier, K. Holladack, T.A. Jackson, J. Krzystek, K. Meyer, D.J. Mindiola, J. Nehr Korn, A. Ozarowski, A. Schnegg*

Section D

Colorado Convention Center
Room 303

Chemical Approaches to Spintronics Research

R. Beaulac, *Organizer*

J. K. McCusker, *Presiding*

1:30 INOR 385. Bistability of magnetic molecules on surfaces: An overview. *R. Sessoli, M. Mannini, L. Malavolti, V. Lanzilotto, L. Poggini, I. Cimatti, G. Poneti, S. Ninova, F. Totti, A. Cornia*

2:00 INOR 386. New single-molecule magnets with high blocking temperatures. *K.R. Meihaus, J.M. Zadrozny, S. Demir, X. Feng, P.C. Bunting, J.D. Rinehart, M. Nippe, J.R. Long*

- 2:30 INOR 387.** Molecular control of the magnetic exchange between self-assembled metal-complexes and ferromagnetic surfaces: towards molecular spintronics. V.E. Campbell
- 3:00** Intermission.
- 3:30 INOR 388.** Ligand-field engineering of atomic clock transitions in molecular spin qubits. S. Hill, M. Shiddiq, D. Komijani, Y. Duan, S. Cardona-Serra, A. Gaita-Ariño, E. Coronado
- 4:00 INOR 389.** Magnetic cyanide-based coordination nanoparticles and heterostructures. L. Catala, Y. Prado, M. López Jordá, S. Mazerat, T. Mallah
- 4:30 INOR 390.** Metal-molecule-metal junctions: A versatile platform to investigate molecular electronics/spintronics. R.C. Bruce, J.D. Yablonski, T.W. LaJoie, W. You

Section E

Colorado Convention Center
Room 201

ACS Award in Inorganic Chemistry: Symposium in Honor of John T. Groves

R. N. Austin, *Organizer*

P. J. Chirik, *Organizer, Presiding*

- 1:30 INOR 391.** Transition metal-catalyzed nucleophilic (radio)fluorination. A.G. Doyle
- 2:00 INOR 392.** Formation and reactivity of new primary copper(II)-dioxygen adducts. K.D. Karlin
- 2:30 INOR 393.** Effects of heme ruffling on vibrational dynamics, electronic structure, and electronic coupling. K.L. Bren, N. Lehnert, P.M. Champion, S.J. Elliott, M. Galinato
- 3:00** Intermission.
- 3:15 INOR 394.** Protein-like proton exchange in a synthetic host cavity. K.N. Raymond, R.G. Bergman, D. Toste
- 3:45 INOR 395.** Cytochrome P450 oxidations: A controlled burn of inert organic compounds. M.T. Green

Section F

Colorado Convention Center
Room 304

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers, Presiding*

- 1:30** Introductory Remarks.
- 1:35 INOR 396.** Platinum and other third row transition metals for treating cancer. S.J. Lippard
- 2:05 INOR 397.** Coordination chemistry underlying the promise and pitfalls of Ti(IV) anticancer drugs. A. Valentine
- 2:35 INOR 398.** Covalent photo-adducts of Ru-TAP complexes with DNA guanine bases: Their applications and mechanisms of formation. A. Kirsch-De Mesmaeker, L. Marcelis
- 3:05** Intermission.
- 3:20 INOR 399.** Metalloglycomics approach to antimetastatic platinum. N. Farrell, E. Peterson, M. von Itzstein, C. Parish, A. Bezos, S.J. Berners-Price
- 3:50 INOR 400.** Transient spectroscopic studies of enantiomerically-resolved intercalating ruthenium dipyridophenazine (dppz) complexes bound to defined sequence DNA. J.M. Kelly, C. Cardin
- 4:20 INOR 401.** Selective binding of bifunctional Zn(II) complexes to G-quadruplex DNA. M. Fountain, J.R. Morrow, K.E. Sifers, M. Shapovalova, M. Shively
- 4:50 INOR 402.** Multifunctional supramolecules for interactions with DNA and cancer cells exploiting photochemical activation. R. Padilla, J.A. Rodríguez Corrales, J. Zhu, J. Newman, R. Prussin, K.S. Brewer, E.M. Naughton

Section G

Colorado Convention Center
Room 401

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Cosponsored by WCC

- C. P. Berlinguette, D. J. Mindiola, E. J. Schelter, M. Shatruk, *Organizers, Presiding*
- 1:30 INOR 403.** Molecular spintronics: The role of chemistry. E. Coronado
- 1:50 INOR 404.** Strong magnetic exchange, slow magnetic relaxation, and spin cross-over in iminobenzoquinonoid dinuclear complexes. I. Jeon, J. DeGayer, J.G. Park, A. Gaudette, D. Harris
- 2:10 INOR 405.** Multifunctionality in spin-cross-over complexes: Toward "molecular multiferroics". H. Phan, J.J. Hruocka, J. Lengyel, S. Benjamin, E. Steven, N.S. Dalal, J. Brooks, M. Shatruk
- 2:30 INOR 406.** Recent fun in homo- and heterometallic manganese cluster chemistry. G. Christou, A.E. Thuijs, K. Mitchell, A.M. Mowson, A. Fournet, K.A. Abboud
- 2:50** Intermission.
- 3:05 INOR 407.** Adventures in spin crossover phenomena: (Giant) memory effect in magnetic and in hybrid conducting materials. J. Galan-Mascaros, C. Saenz de Pipaon, P. Maldonado-Illescas, Y. Koo, V. Gomez
- 3:25 INOR 408.** Magnetic metal-cyanide coordination clusters and chains. X. Feng, D. Freedman, T. Harris, H. Choi, B.M. Bartlett, D.M. Jenkins, H. Karunadasa, J. Zadrozny, M. Bennett, J.R. Long
- 3:45 INOR 556.** Halogen photoelimination from Ni(II) complexes: An energy storing transformation. S. Hwang, D.C. Powers, S. Zheng, Y. Chen, D.G. Nocera
- 4:05 INOR 410.** Multifunctionality at extreme conditions: spin cross-over photomagnetic behavior induced by pressure. D. Pinkowicz

Section H

Colorado Convention Center
Room 203

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jacqueline L. Kiplinger

Cosponsored by WCC

D. E. Morris, *Organizer*

G. G. Stanley, *Organizer, Presiding*

- 1:30 INOR 411.** Spectroscopic and computational studies on a bimetallic hydroformylation catalyst system. G.G. Stanley, R. Fernando, M. Moulis
- 1:50 INOR 412.** Activation of C-F bonds: The next stage. T.G. Richmond
- 2:10 INOR 413.** Dehydrocoupling: Then and now. J.Y. Corey
- 2:30 INOR 414.** Interplay between theory and experiment in investigations of organo-actinide complexes: A retrospective. P.J. Hay
- 2:50 INOR 415.** Covalency in the actinides probed with ligand K-edge X-ray absorption spectroscopy. R.L. Martin
- 3:10 INOR 416.** Small molecule activation by complexes of low-valent f elements. M. Mazzanti, J. Pécaut, C. Camp, V. Mougél, J. Andréz
- 3:30** Intermission.
- 3:40 INOR 417.** Selective transformations of organic compounds mediated by transition metal complexes. R.G. Bergman
- 4:10 INOR 418.** Supramolecular chemistry of anions: Inorganic, inorganic and biological studies. K.R. Dunbar
- 4:40 INOR 419.** Technetium halide chemistry. A.P. Sattelberger, F. Poineau, E.V. Johnstone, W.M. Kerlin, C. Malliakas, P.M. Forster, K. Czerwinski
- 5:00 INOR 420.** Computational actinide chemistry: Searching for understanding and holy grails. B.E. Bursten

Section I

Colorado Convention Center
Room 205

Division of Inorganic Chemistry Celebration of the Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Michael A. Marletta

M. A. Marletta, *Organizer, Presiding*

- 1:30 INOR 421.** Reinventing natural product discovery. D. Mitchell
- 2:00 INOR 422.** Metals and Immunity. E.M. Nolan
- 2:30 INOR 423.** Synthetic cluster models of the biological oxygen evolving catalyst from photosystem II. T. Agapie
- 3:00** Intermission.
- 3:15 INOR 424.** Biosynthesis and tailoring of acyl peptidic siderophores. A. Butler, M.P. Kern, H. Naka, H.K. Zane, M.G. Haygood
- 3:45 INOR 425.** Glycocalyx engineering toward probing cancer glycome evolution. C.R. Bertozzi

Section J

Colorado Convention Center
Room 402

Bioinorganic Chemistry

S. A. Koch, *Organizer*

L. A. Finney, *Presiding*

- 1:30 INOR 426.** Second-sphere tuning of enzymatic activity in noncanonical heme oxygenase. M.D. Liptak, A.B. Graves, C.L. Lockhart
- 1:50 INOR 427.** Pf97 as a framework protein for association of organic-inorganic layers of nacre. S. Bahn, B. Jo, Y. Choi, H.J. Cha
- 2:10 INOR 428.** Model compounds of [NiFe]-hydrogenase in the Ni-SI₂ and Ni-L states. G.M. Chambers, T.B. Rauchfuss, E.J. Reijerse, K. Weber, W.W. Lubitz
- 2:30 INOR 429.** Evolution of thioether S-ligated primary Cu/O₂ adducts: The 1st example of Cu⁺-superoxo species with enhanced reactivity. J.C. Lee, S. Kim, R. Cowley, J.W. Ginsbach, M. Siegler, E.I. Solomon, K.D. Karlin
- 2:50 INOR 430.** Fundamental reactivity studies of hydrogen sulfide with metalloporphyrins. D.J. Meininger, H. Arman, Z.J. Tonzetich
- 3:10 INOR 431.** Dioxygen activation under ambient conditions using bio-inspired manganese(II) complexes to generate mid-valent oxidants for catalytic O-H bond oxidations. G.B. Wijeratne, A.D. Burr, B. Corzine, T.A. Jackson
- 3:30 INOR 432.** Short peptides self-assemble to produce catalytic amyloids. C.M. Rufo, Y.S. Moroz, O.V. Moroz, J. Stoehr, T.A. Smith, X. Hu, W.F. Degradó, I.V. Korendovych
- 3:50 INOR 433.** New insights in the chemistry of nickel in urease. L. Mazzei, S. Benini, S. Ciurli
- 4:10 INOR 434.** Understanding the reaction mechanism of the tungstoenzyme, acetylene hydratase. M.A. Cranswick, E. Vergunst, B. Trujillo
- 4:30 INOR 435.** Tethered C,N,S ligands containing an iron-carbamoyl motif as synthetic models of mono-iron hydrogenase. M.J. Rose, G. Durgaprasad
- 4:50 INOR 436.** Family of starch-active polysaccharide monooxygenases. V.V. Vu, W.T. Beeson, D. Suess, E.A. Span, E.R. Farquhar, R. Britt, M.A. Marletta

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

S. A. Koch, N. S. Radu, *Organizers*

8:00 - 10:00

- 4, 79, 161-162, 165, 167, 171, 180, 182, 184, 197, 204, 211, 213, 217-218, 224, 226, 228-229, 238-239, 241, 243-244, 248, 256, 260, 270-273, 287, 291, 295, 307, 310-311, 318, 320, 323, 329, 331-332, 336, 348, 356.** See previous listings.
- INOR 437.** Investigation of copper exchange between the avian egg proteins riboflavin binding protein, phosvitin and vitellogenin. J.I. Matchynski, A.W. Chamoun, M. Benore, S.R. Smith
- 509, 585, 590-591, 595, 598, 600-601, 604, 607, 610-611, 614, 623-624, 631-632, 634-635, 644-647, 649-650, 653, 659, 663, 666, 670, 672, 674-676, 688, 694, 697-698, 709, 713, 715, 719, 723, 725.** See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry

Bioinorganic Chemistry

C. Nataro, S. R. Smith, *Organizers*

A. J. Reig, *Presiding*

9:00 Introductory Remarks.

- 9:05 INOR 438.** Biochemical and molecular modelling studies of the interaction of organometallic ruthenium complexes containing thiosemicarbazones or curcuminoids as ligands with DNA and proteins. F.A. Beckford, K.L. Hall, K.R. Webb
- 9:25 INOR 439.** Formation and characterization of Langmuir-Blodgett films of lipid rafts. D.L. Calkins, I. Kuznetsov, E. Magallanes, C. Menoni, D. Crick, D.C. Crans
- 9:45 INOR 440.** Functional model of the first and second coordination spheres of type 2 copper nitrite reductase. G. Rowe, S.L. Behnke, S. Weaver, E. Foerster, M. Bezpalko, B.M. Foxman
- 10:05** Intermission.
- 10:15 INOR 441.** Voltammetric studies of the Rieske protein. K.R. Hoke, R.J. Quarles
- 10:35 INOR 442.** X-ray crystallographic analysis of reduction potential mutants of the Rieske protein from *Thermus thermophilus*. L.M. Hunsicker Wang
- 10:55 INOR 443.** Understanding functional tuning in binuclear non-heme iron enzymes through systematic variation of the G4DFsc active site. A.J. Reig, S. Cimerol, J. Pellegrino, R. Polinski, K.A. Drost, C.L. Kanya, K. Biernat, K. O'Shea
- 11:15 INOR 444.** Homoleptic transition metal complexes of the 7-azaindolide ligand featuring κ^1 -N1 coordination. M. Kewit, Z.J. Tonzetich

Section B

Colorado Convention Center
Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

M. C. Buzzeo, S. Delaney, V. C. Pierre, *Organizers*

E. Boon, *Organizer, Presiding*

8:30 Introductory Remarks.

- 8:35 INOR 445.** Coupling oxygen consumption with substrate oxidation in bacterial multi-component monooxygenases. S.J. Lippard
- 9:05 INOR 446.** Are metal-associated misfolded proteins involved in Alzheimer's disease? M. Lim
- 9:35 INOR 447.** Cephalopod-derived materials for photonic and protonic devices. A.A. Gorodetsky
- 10:05** Intermission.

10:15 INOR 448. Exploring the physiological role of selenium redox chemistry. **M.C. Buzzo**

10:45 INOR 449. Nucleic acids in quadruplexes. **F. Shao**

11:15 INOR 450. Photochemical dynamics of stacked peryleneimide assembly constructed on DNA. **T. Takada**

Section C

Colorado Convention Center
Room 302

ACS Award in Organometallic Chemistry: Symposium in Honor of William J. Evans

J. R. Walensky, *Organizer*

J. C. Gordon, *Presiding*

8:30 INOR 451. Highly selective chemical processes for tailored electronic materials: Interfaces, depositions, and treatments. **R.D. Clark**

8:50 INOR 452. Progress toward fluid materials for chemical hydrogen storage. **B.L. Davis, A. Carre-Burritt, B.D. Rekkon**

9:10 INOR 453. Effects of fast charging on lithium-ion cells. **I. Bloom**

9:30 INOR 454. Peptidomimetic sequence-defined polymers based on a new synthetic architecture. **J.W. Grate, K. Mo, M. Daily, C. Chen**

9:50 Intermission.

10:00 INOR 455. Development of a 3D composite for NASA's Orion spacecraft compression pad. **J.D. Feldman**

10:20 INOR 456. Optimizing the performance of polyolefins via stabilization chemistry and effects. **R.E. King**

10:40 INOR 457. Natural gas to ethylene in one step: Siluria technologies OCM (oxidative coupling of methane). **G. Nyce**

11:00 INOR 458. Cobalt complexes containing pendant amines in the second coordination sphere as electrocatalysts for energy storage. **M. Fang, E.S. Wiedner, R. Bullock**

Section D

Colorado Convention Center
Room 303

Chemical Approaches to Spintronics Research

R. Beaulac, *Organizer, Presiding*

8:30 INOR 459. Zero-field spin polarization effects on Dexter transfer. **J. Kouzelos, M. Soler, J.K. McCusker**

9:00 INOR 460. Theoretical characterization of conduction-band electrons and magnetic exchange interactions in photodoped and aluminum-doped diluted magnetic semiconductors. **X. Li, J. Goings**

9:30 INOR 461. Near-infrared paramagnetic manganese-doped PbS nanocrystals. **L. Turyanska**

10:00 Intermission.

10:00 INOR 462. Chirality induced spin selectivity (CISS) effect-chiral molecules for spintronics. **R. Naaman**

10:30 INOR 463. Decoherence in crystals of quantum molecular magnet. **S. Takahashi**

11:00 INOR 464. Effects of the addition of spin on donor-acceptor excited state electronic structure. **B. Stein, C. Tichnell, D. Stasiw, D. Shultz, M.L. Kirk**

11:30 INOR 465. π -System superexchange in cross-conjugated donor-bridge-acceptor triads: Electronic structure contributions to quantum interference. **D. Shultz, D. Stasiw, B. Stein, D. Habel-Rodriguez, M.L. Kirk**

Section E

Colorado Convention Center
Room 201

Chemistry of the Energy Water Nexus: Focus on Fracking

C. McInnis, *Organizer, Presiding*

9:00 INOR 466. Thinking constructively about hydraulic fracturing fluid design in the new resource landscape. **B.A. MacKay**

9:30 INOR 467. Review of industrial biocides used for microbial control in hydraulic fracturing. **T.M. Williams**

10:00 Intermission.

10:10 INOR 468. Electrochemically produced biocides: A greener disinfectant for waters used in hydraulic fracturing. **A.K. Boal**

10:40 INOR 469. Reclaiming produced water: Using chemistry to convert a waste stream into a resource. **K. Sikkema**

Section F

Colorado Convention Center
Room 304

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers*

P. C. Glazer, *Presiding*

8:30 INOR 470. Noncovalent recognition of "unusual" but active DNA and RNA structures. **M.J. Hannon**

9:00 INOR 471. Tuning in *cellulo* targeting and function of metal complex bioprobes. **J.A. Thomas**

9:30 INOR 472. Platinum biomolecule target analysis using click chemistry. **J.D. White, A.D. Moghaddam, R. Cunningham, K. Plakos, M.F. Osborn, M.M. Haley, V. DeRose**

10:00 Intermission.

10:30 INOR 473. Catalytic metallodrugs: Structure-function and activity studies of a broad therapeutic platform. **J.A. Cowan**

11:00 INOR 474. Tuning the pharmacological properties of platinum-acridine anticancer agents using novel prodrug and subcellular targeting strategies. **U. Bierbach**

11:30 INOR 475. Unusual synergism of serum transferrin titanium(IV) coordination brings insight into its potential transport and bio-activity in the human body. **A.D. Tinoco**

Section G

Colorado Convention Center
Room 401

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Cosponsored by WCC

C. P. Berlinguette, E. J. Scheller, M. Shatruk, *Organizers*

D. J. Mindiola, *Organizer, Presiding*

8:30 INOR 476. Drug membrane interactions and uptake as key aspects of drug action. **D.C. Crans**

8:50 INOR 477. Understanding anion- π interactions: from substituted benzenes to N-heterocycles. **S.E. Wheeler**

9:10 INOR 478. Role of inorganic chemistry in the activities of antimicrobial peptides. **A.M. Angeles Boza**

9:30 INOR 479. Highly unsaturated cationic metal complexes supported by pincer ligands. **O. Ozerov, J.C. DeMott, R. Huacuja**

9:50 Intermission.

10:05 INOR 480. Nonexistent compounds. **C.C. Cummins, R. Field, M. Nava, B. Park, W. Transue, A. Velian**

10:25 INOR 481. New Carbon-Hydrogen Activation Reactions by Titanium Alkylidynes and Phosphino-Alkylidynes. **D.J. Mindiola**

10:45 INOR 482. Ligand and reagent effects in C-H borylation. **M.R. Smith**

11:05 INOR 483. Carbene-stabilized allotropes: Synthesis, structure, and reactivity. **G.H. Robinson**

11:25 INOR 484. Mobile zinc signaling in the brain – learning, memory, hearing, olfaction, and vision. **S.J. Lippard**

Section H

Colorado Convention Center
Room 203

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger

Cosponsored by WCC

G. G. Stanley, *Organizer*

D. E. Morris, *Organizer, Presiding*

8:30 INOR 485. Covalency in lanthanides.

S.A. Kozimor, J.M. Keith, A.B. Altman, E.R. Batista, D.L. Clark, R.L. Martin, S.G. Minasian, T. Tylicszczak, D.K. Shuh, M.P. Wilkerson

8:50 INOR 486. Uranium-element multiple bond formation facilitated by redox-active pyridine(diimine) ligands: Synthesis, characterization, and reactivity of a unique class. **S.C. Bart**

9:10 INOR 487. Reactions of oxygen with late transition Metal Complexes. **K.I. Goldberg**

9:30 INOR 488. DFT studies of Cp2An(P)2 complexes as catalysts for pyridine and thophene ring opening. **E.R. Batista, A.W. Pierpont, R.L. Martin, N.E. Travia, J.L. Kiplinger**

9:50 INOR 489. Pursuits of rare oxidation states in actinide chemistry. **M.R. Antonio, L. Soderholm**

10:10 INOR 490. Perturbation of the electronic properties of non-innocent vanadium(V) complexes and the chemical properties of vanadium and copper coordination complexes in inhomogeneous environments. **D.C. Crans, I. Sánchez Lombardo, J. Koehn, E. Magallanes**

10:30 Intermission.

10:40 INOR 491. Formation, characterization, and uses of metallocycles via coordination directed self-assembly. **P.J. Stang**

11:10 INOR 492. Interplay of metal ions and oxidative damage in DNA G-quadruplexes. **C.J. Burrows**

11:40 INOR 493. Reduction chemistry with group 3 metals supported by a ferrocene diamide ligand. **P. Diaconescu**

12:00 INOR 494. Uranium imido complexes: A window into actinide-ligand bonding and reactivity. **J.M. Boncella, N.C. Tomson, E.R. Batista, B. Scott**

Section I

Colorado Convention Center
Room 205

Molecular Catalysts for Solar Fuels

Cosponsored by MPPG

A. M. Appel, M. Helm, J. Y. Yang, *Organizers, Presiding*

8:30 INOR 495. Bimetallic hydrides inspired by the hydrogenase active sites. **T.B. Rauchfuss, G.M. Chambers, U.C. Olbelina, W. Wenguang**

9:00 INOR 496. Enzyme-like behavior achieved with amino acids in the outer coordination sphere of H₂ oxidation catalysts. **W.J. Shaw, A. Dutta, D. DuBois, J. Roberts**

9:30 INOR 497. Theoretical design of hydrogen-evolving molecular electrocatalysts. **S. Hammes-Schiffer**

10:00 INOR 498. Molecular proton reduction catalysts in metal-organic frameworks. **S. Ott**

10:30 Intermission.

10:45 INOR 499. Production of C1 sources via reduction of CO₂ on redox active iron ligand platforms. **J.D. Gilbertson**

11:15 INOR 500. Harnessing heterobimetallic complexes for CO₂ activation and reduction. **J. Yang, S. Pooteet, J. Ritter**

11:45 INOR 501. Deep photoreduction of carbon dioxide to methanol and formate by ruthenium polypyridyl chromophores with pendant pyridyl sites. **F.M. MacDonnell, M. West, D.J. Boston, N. de Tacconi**

Section J

Colorado Convention Center
Room 402

Soluble Inorganic Semiconductors: Synthesis, Properties, and Applications

R. L. Brutchey, B. M. Cossairt, *Organizers, Presiding*

8:30 INOR 502. Magic-size II-VI nanoclusters as semiconductor precursors. **Y. Wang, Y. Zhou, F. Wang, W.E. Buhro**

9:00 INOR 503. High throughput investigations of colloidal metal chalcogenide nucleation and growth. **J.S. Owen, M.P. Hendricks, M.P. Campos, S. Hong, G.T. Cleveland, E. Chan**

9:30 INOR 504. Photochemical reactions of semiconductor nanocrystals coupled with redox catalysts. **G. Dukovic**

10:00 Intermission.

10:15 INOR 505. All-inorganic design of colloidal nanocrystals: New inorganic ligands and new atomistic insights into their surface binding. **M. Kovalenko**

10:45 INOR 506. Novel fabrication strategies for heterostructured PbS and PbSe QDs via controllable cation exchange reactions. **M.C. Beard, J. Zhang, J. Luther, E. Miller, J. Gao**

11:15 INOR 507. Near-infrared photoluminescence enhancement in Ge/CdS and Ge/ZnS core/shell nanocrystals: Utilizing IV/II-VI semiconductor epitaxy. **J. Vela-Becerra**

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe

Sponsored by FLUO, Cosponsored by INOR

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry Solid State and Materials Chemistry

C. Nataro, S. R. Smith, *Organizers*

M. T. Whited, *Presiding*

1:30 Introductory Remarks.

1:35 INOR 508. Infrared Spectroscopic tracking of Q-state particle formation in ionomers. **FA. Meyer, J.H. Doan, E. Kingston, K.P. Anderson, A.K. Vong, E.S. Smolkin**

1:55 INOR 509. Ultrasmall Cu nanoparticles: A greener synthesis and catalytic studies. **G.A. Ferko, A.D. Brumbaugh, S.K. St Angelo**

2:15 INOR 510. Synthesis, characterization, and utility of trifluoroacetic acid and fluoroalkoxy lanthanide precursors for production of fluorinated lanthanide nanomaterials. **D. Yonemoto, T.J. Boyle, M.L. Neville, R.F. Hess, S.P. Bingham**

2:35 INOR 511. Phenoxy-mercapto derivatives of group 4 alkoxides as core-shell precursors to group 4 ceramic-coating metal nanomaterials. **M.L. Neville, T.J. Boyle, P. Lu, M.V. Parkes**

2:55 Intermission.

3:05 INOR 512. Oxidizing aldehydes with water: Catalysts for the aldehyde-water shift. **J.C. Tran, T. Brewster, D.M. Heinekey, K.I. Goldberg**

3:25 INOR 513. Multifunctional nanoclusters for biomedical applications. **S. Park, S.K. Cho, W. Park**

3:45 INOR 514. Student explains international undergraduate research and cultural experiences. **A. Walker, G. Royal, T.J. Hubin, R. Duran**

4:05 INOR 515. Computational and synthetic study of organic-inorganic conjugate dyes for solar energy harvesting. **R.E. Bachman, A.E. Connor, S.A. Parks, M.R. Leidy, N.J. Deyonker**

4:25 Concluding Remarks.

Section B

Colorado Convention Center
Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, M. C. Buzzeo, S. Delaney, V. C. Pierre, *Organizers*
A. K. Boal, *Presiding*

1:30 INOR 516. Targeting mitochondrial DNA. S.O. Kelley

2:00 INOR 517. Novel development of electrolytes in lithium ion battery. Y. Tanaka

2:30 INOR 518. Peptide nucleic acids (PNAs) as diagnostic and therapeutic molecules. E. Yavin

3:00 Intermission.

3:10 INOR 519. Controlling molecular display and cell behavior with nanocrystals. C.J. Murphy

3:40 INOR 520. Sensitive and selective real-time electrochemical monitoring of DNA repair. J. Slinker, M. McWilliams, F. Anka, K.J. Balkus

4:10 INOR 521. Evolution of an idea born in my postdoc with Jackie Barton: From rhodium-peptide conjugates to Alzheimer's disease. R.P. Houser

Section C

Colorado Convention Center
Room 302

Solid-State Inorganic Chemistry

C. G. Lugmair, *Organizer*
V. Poltavets, *Organizer, Presiding*
M. Dolgos, *Presiding*

1:30 Introductory Remarks.

1:35 INOR 522. Low temperature synthesis of (noncentrosymmetric) oxide-fluoride materials. K.R. Poeppelmeier, K.B. Chang, A. Vinokur, M. Marvel

2:15 INOR 523. Low temperature synthesis of bimetallic carbide nanomaterials and their electrocatalytic activity. S.M. Schmucker

2:35 INOR 524. Single source precursor approach to metastable molybdate phases. A.W. Abblett, A.M. Moneeb, A. Alabdulrahman, A. Bagabas, C. Perkins

2:55 INOR 525. Mechanistic studies in kinetically controlled solid state synthesis: The case of $[(\text{SnSe})_{1-x}(\text{VSe})_x]$. M. Esters, M. Falmberg, D.C. Johnson

3:15 INOR 526. Following the journey from aqueous polyoxometalate to metal oxide. Y. Hou, D. Fast, L.B. Fullmer, M.D. Nyman, M. Dolgos

3:35 Intermission.

3:50 INOR 527. Synthesis of metal sulfides in sulfur/iodine flux using furnace or microwave reactions. R. Groom, S.E. Lattumer

4:10 INOR 528. Extraction behavior of mesoporous silica SBA-15 for soluble uranyl peroxo clusters. Y. Liu, A. Czarnecki, J.E. Szymanski, M. Dembowski, G. Sigmon, P.C. Burns

4:30 INOR 529. Negative thermal expansion and other anomalous properties in rock salt ordered mixed metal fluorides $\text{M}^{\text{II}}\text{ZrF}_6$ with a ReO_3 -type structure. J.C. Hancock, C.R. Morelock, L.C. Gallington, K.W. Chapman, G.J. Halder, B.S. Kaplan, A. Bongiorno, C. Han, S. Zhou, **A.P. Wilkinson**

4:50 INOR 530. Dark reactions project: a machine learning approach to materials discovery. A.J. Norquist

5:10 INOR 531. Ferromagnetic behavior in non-metal anionic element reagent complexes. M.P. Rowe, R. Desautels, E. Skoropata, J. van Lierop

Section D

Colorado Convention Center
Room 303

Inorganic Catalysts

S. A. Koch, *Organizer*
Y. Zhang, *Presiding*

1:30 INOR 532. Novel CeO_2 yolk-shell structures loaded with tiny Au nanoparticles for highly catalytic reduction of *p*-nitrophenol. C. Fan, A. Xu

1:50 INOR 533. Diphenyl ether based secondary phosphine oxide as preligand for nickel-catalyzed carbon-sulfur cross-coupling reactions. N.P. Nambukara Wellala, H. Guan

2:10 INOR 534. Dehydration and dehydrogenation of ethanol over Au-exchanged ZSM-5 zeolite: A DFT study. T. Maihom, B. Boekfa, J. Limtrakul

2:30 INOR 535. Withdrawn.

2:50 INOR 536. Mesoporous Co_2O_3 catalyst for CO oxidation at -60C: Controlled porosity, reaction mechanism, and deactivation reason. W. Song, A. Poyraz, Y. Meng, Z. Ren, S. Chen

3:10 Intermission.

3:20 INOR 537. Dinitrogen silylation facilitated by a dicobalt catalyst. R.B. Siedschlag, K.D. Vogiatzis, V. Bernales, N. Ptasas, L. Gagliardi, C.C. Lu

3:40 INOR 538. Cyclic alkyl amino carbene (CAAC) ruthenium complexes as remarkably active catalysts for ethenolysis. V.M. Marx, A.H. Sullivan, M. Melaimi, S.C. Virgil, G. Bertrand, R.H. Grubbs

4:00 INOR 539. Iron porphyrin carbenes as catalytic intermediates: Structures, Mössbauer and NMR spectroscopic properties, and bonding. R. Khade, Y. Zhang

4:20 INOR 540. Electrochemical studies of cobalt (II) N_2Py_2 complexes and a nickel (II) bis(diphosphine) complex toward catalytic proton reduction. J.F. Khosrowabadi Kotyk, J. Yang

Section E

Colorado Convention Center
Room 201

Chemistry of the Energy Water Nexus: Focus on Fracking

Cosponsored by MPPG†

C. McInnis, *Organizer, Presiding*

1:30 INOR 541. Development of advanced polymers for hydraulic fracturing applications. C.R. Hilliard, C. Meza, R. Schlemmer, J. Donovan

2:00 INOR 542. Shale gas and oil flowback and produced water modeling and treatment. M.B. Tomson, Z. Zhang, Z. Dai, V. Bolanos, A.T. Kan, F. Yan, R. Tomson

2:30 INOR 543. Dynamic microbial communities in hydraulic fracturing water: Implications for chemistry and water management. K.B. Gregory

3:00 INOR 544. Characterizing oil and gas exploration and production waste streams: Collaborative inter-laboratory comparison. T.Y. Cath

3:30 Panel Discussion.

Section F

Colorado Convention Center
Room 304

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers*
U. Bierbach, *Presiding*

1:30 INOR 545. In vitro selection and characterization of metallo-DNAzymes and their delivery into cells for sensing and imaging applications. Y. Lu, K. Hwang, P. Wu, S. Torabi

2:00 INOR 546. Is the geometry of Vanadium in active site of phosphatases important for inhibitor design and antidiabetic properties of vanadium compounds. D.C. Crans, B.J. Peters, M.L. Tarlton, G.R. Willisky, C.C. McLauchlan

2:30 INOR 547. Metal ion incorporation in peptide nucleic acid triplexes. C. Achim, D. Jayarathna, Y. Bae, H. Stout

3:00 Intermission.

3:15 INOR 548. Development of redox-active ruthenium polypyridyl complexes as an anticancer agents for the treatment of platinum resistant tumors. F.M. MacDonnell, N. Alatrash, E. Narh, C. Griffith

3:45 INOR 549. Cobalt Schiff base complexes as targeted inhibitors of transcription factors. M.C. Heffern, T.J. Meade

4:15 INOR 550. Inhibition of cysteine proteases with ruthenium-caged compounds. J.J. Kodanko

4:45 INOR 551. Strategies for the photochemical uncaging of bioactive small molecules. P.C. Ford, J.V. Garcia, A. Pierri, M. Crisalli, A.W. DeMartino, P. Huang

Section G

Colorado Convention Center
Room 401

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Cosponsored by WCC

C. P. Berlinguette, D. J. Mindiola, M. Shatruk, *Organizers*
E. J. Schelter, *Organizer, Presiding*

1:30 INOR 552. Lewis acidic properties of organotin compounds: From bidentate distorboranes to perfluorinated stibonium cations. F.P. Gabbai

1:50 INOR 553. Platinum diimine dithiolate chromophores and dyads for the light-driven generation of hydrogen. R. Eisenberg

2:10 INOR 554. Manipulation of the electronic structures of cerium complexes toward the development of a new class of photosensitizers. E.J. Schelter, H. Yin, P. Carroll

2:30 INOR 555. Control of excited states of transition metal complexes: Optimizing multiple excited state pathways. C. Turro, K.R. Dunbar

2:50 Intermission.

3:05 INOR 409. How to get what you want: A control freak's guide to inorganic nanoparticle synthesis. R.E. Schaak

3:25 INOR 557. How nickel/iron films catalyze the oxygen evolution reaction. C.P. Berlinguette, R.D. Smith

3:45 INOR 558. Inorganic chemistry, solution processed solar cells, and the era of perovskites. M.G. Kanatzidis

4:05 INOR 559. Cyanide-bridged iron complexes as analogues of tri-iron arrangements in hydrogenase active site precursors. A.M. Lunsford, C. Beto, M.Y. Darensbourg

Section H

Colorado Convention Center
Room 203

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger

Cosponsored by WCC

D. E. Morris, *Organizer*
G. G. Stanley, *Organizer, Presiding*

1:30 INOR 560. Microfluidic separations for actinide processing and analysis. R.M. Chamberlin, S.L. Yarbro, N. Xu

1:50 INOR 561. Production of Mo-99 for nuclear medicine. A. Anderson, L. Bittaker, M. Connors, R. Copping, M. Cover, W. Crooks, G. Dale, D. Dalmás, M. Gallegos, E. Garcia, J. Gioia, R. Gonzales, D. Graves, W.K. Hollis, M. Janicke, C. Kelsey, I. May, M. Mocko, M. Pieck, M. Rawool-Sullivan, S.D. Reilly, D. Rios, T. Romero, F. Stephens, F. Taw, D. Thorn, K. Woloshun

2:10 INOR 562. CO_2 conversion using organometallic and organic molecular catalysts. T. Cantat

2:30 INOR 563. Organometallic thorium azide complexes. M.J. Monreal, J.L. Kiplinger, B. Scott

2:50 INOR 564. Pursuit of high-oxidation state phosphinidene complexes of the group 6 metals for metathesis reactivity. R.K. Thomson

3:10 INOR 565. Aluminum chemistry featuring nitrogen-based ligands for stabilization of cations and radicals. J.D. Masuda, W.L. McClennan, N.A. Giffin

3:30 Intermission.

3:40 INOR 566. Actinide speciation in aqueous chloride and pseudochloride solutions. L. Soderholm, S. Skanhakumar

4:00 INOR 567. Synthesis and combustion of nitrogen-rich f-element complexes. J.M. Veauthier, J.L. Kiplinger, B.C. Tappan, N.E. Travia, K. Browne, B.L. Scott, N.J. Henson, A.H. Mueller, D.E. Chavez, A.T. Nelson

4:20 INOR 568. Actinide-arene interactions and their use in carbon-element bond forming reactions. P.L. Arnold, J. McKinven, J. Hlina, R. Lord, R. Batrice, N. Kaltsayannis, M. Eisen, M. Gardiner, J.B. Love

4:50 INOR 569. Covalency and the relative roles of 5f and 6d orbitals in actinide metal-ligand bonds. D.L. Clark

5:20 INOR 570. Enabling the exploration of metal-ligand bonding in light actinides: One of Jackie Kiplinger's many synthetic legacies. D.E. Morris

Section I

Colorado Convention Center
Room 205

Molecular Catalysts for Solar Fuels

Cosponsored by MPPG

A. M. Appel, M. Helm, J. Y. Yang, *Organizers, Presiding*

1:30 INOR 571. Selective heterogeneous electrocatalytic reduction of CO_2 to CO or HCOO using iron porphyrin complexes. A. Dey

2:00 INOR 572. Navigating structure-activity relationships in molecular electrocatalysts for CO_2 reduction. R.J. Nielsen, S.I. Johnson, Y. Lam, W.A. Goddard

2:30 INOR 573. Ir-H species as key intermediates in CO_2 hydrogenation, formic acid dehydrogenation and photochemical CO_2 reduction. E. Fujita, J.T. Muckerman, Y. Himeda

3:00 INOR 574. Reduction of CO_2 to methanol by an organo hydride via hydride transfer/proton transfer steps. J.T. Hynes, C. Musgrave, C. Lim, A. Holder

3:30 Intermission.

3:45 INOR 575. Homogeneous reduction of CO_2 by $[\text{Ni}(\text{cyclam})]^{2+}$; poisoning by CO, detoxification by CO sponge, and useful conversion of CO by tandem catalysis. C.P. Kubiak, J. Froehlich, J. Tillman

4:15 INOR 576. What theory can reveal about carbon dioxide reduction and the role of molecular catalysts. E.A. Carter

4:45 INOR 577. Molecular catalysis of SO_2 reduction in dye sensitized photoelectrosynthesis cells (DSPEC). T.J. Meyer, J. Concepcion, Z. Chen, M. Norris, M. Zhang, M. Coggins, R. Binstead, N. Song, D.L. Ashford, M. Sheridan, P. Kang, S. Zhang, N.Y. Iha, M. Brookhart, J.L. Templeton

Section J

Colorado Convention Center
Room 402

Soluble Inorganic Semiconductors: Synthesis, Properties, and Applications

R. L. Brutchey, B. M. Cossairt, *Organizers*
G. Dukovic, J. S. Owen, *Presiding*

1:30 INOR 578. Single junction CZTSSe and tandem CZTSSe/hybrid perovskite solar cells from molecular-inks: Mapping the effects of composition on material quality and device performance. H.W. Hillhouse

2:00 INOR 579. Solution-processed electrochromic and photovoltaic thin films from nanocrystal building blocks. D.J. Milliron, A. Llordes, A. Singh

- 2:30 INOR 580.** Synthesis of transition metal chalcogenide and pnictide nanoparticles for applications in photovoltaics. **A.L. Prieto**, D. Agocs, M.B. Braun, S. Fredrick, L. Korala, R.C. Miller
- 3:00 Intermission.**
- 3:15 INOR 581.** Photophysics in metal enriched and stoichiometric quantum dots. **M. Sfeir**, E. Busby, N.C. Anderson, J.S. Owen
- 3:45 INOR 582.** New matrix engineering strategies for efficient charge transport in quantum dot solids. **M. Law**
- 4:15 INOR 583.** Designer semiconductor nanocrystal electronic and optoelectronic materials and devices. **C.R. Kagan**, S. Oh, J. Choi, Y. Lai, D. Kim, E.D. Goodwin, A.T. Fafman, B. Diroll, C.B. Murray

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christie

Sponsored by FLUO, Cosponsored by INOR

TUESDAY EVENING

Section A

Colorado Convention Center
Hall C

Bioinorganic Chemistry

DNA, RNA and Inorganic Drugs

S. A. Koch, *Organizer*

6:00 - 8:00

- INOR 584.** Luminescent ruthenium probe for DNA mismatches. **A.N. Boynton**, A.S. McConnell, J.K. Barton
- INOR 585.** 1H- and 19F-NMR spectroscopic studies of 4-fluorophenylbiguanide with the interface of reverse micelles. **J. Sripradite**, N. Samart, A. Tongraar, D.C. Crans
- INOR 586.** N-hydroxysulfonamides RSO₂NHOH as nitroxyl (HNO) donors: Improved preparation and kinetics of nitroxyl generation. **S.K. Adas**, N.E. Brasch, P. Sampson
- INOR 587.** Exploring the cellular activity of polyazine bridged Ru(II)-Rh(II) supramolecules in rat malignant glioma F98 cells. **J. Zhu**, K.S. Brewer
- INOR 588.** Cytotoxic and DNA binding properties of Mn(II) and Re(II) carbonyl perhenato complexes. **J. Taylor**, S.K. Pramanik, J.A. Krause, S.K. Mandal
- INOR 589.** Photosensitization of singlet oxygen by ruthenium(II) polypyridyl complexes for DNA photocleavage. **S. Yang**, K. Wang, B.R. Williams, S.J. Niefer Burgmayer
- INOR 590.** Evaluation of heme peripheral groups interactions in low-dielectric constant media. **A. Stockhausen**, J. Cerda

Section B

Colorado Convention Center
Hall C

Bioinorganic Chemistry

Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

6:00 - 8:00

- INOR 591.** Spectroscopic methods to characterize non-heme iron enzymes (monooxygenase and dioxygenase). **B. Subedi**, B.S. Pierce
- INOR 592.** Formation, characterization, and O-O bond activation of a bio-inspired peroxomanganese(III) complex. **H.E. Colmer**, T.A. Jackson

- INOR 593.** Binuclear complexes: Analogs for superoxide dismutase enzyme substrate binding studies. **J.W. Kreft**, E. Sinn
- INOR 594.** Crystallization of protein models of non-coupled dinuclear copper proteins. **A. Sauer**, M. Ladd, S. Pedersen, S.M. Berry
- INOR 595.** Modeling oxidoreductase enzymes in the protein azurin. **T. Roach**, G. Stoddard, S.M. Berry
- INOR 596.** Role of halogen substituents and substrate pK_a in defining the substrate specificity of 2,6-dichlorohydroquinone 1,2-dioxygenase (PcpA). **J.E. Burrows**, M.Q. Paulson, T.E. Machonkin
- INOR 597.** Nitrite reduction activity of azurin variants. **B. Khaiwada**, J. Strange, S.M. Berry
- INOR 598.** Synthetic models for nickel superoxide dismutase. **S.K. Senaratne**, D.M. Eichhorn
- INOR 599.** Job's method and high resolution NMR studies of trinuclear bis(bis(O-ethyl-L-cysteinato)₂Ni)₂NP⁺. **R.J. Dougherty**, K.V. Krishnan, M.L. Golden

Section C

Colorado Convention Center
Hall C

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers*

6:00 - 8:00

- INOR 600.** Tuning mechanisms of action of Ru(II) polypyridyl complexes as anticancer targets by changing charge states. **Y. Sun**, M. Dickerson, B. Howerton, D. Heidary, E. Glazer
- INOR 601.** Selective recognition of G-quadruplex and thymine bulge DNA using bifunctional Zn(II) complexes. **K.E. Sifers**, S.A. Sander, J. Devlin, J.R. Morrow
- INOR 602.** Evaluation of the binding of Zn(II) complexes to G-quadruplexes using a PCR-stop assay. **M. Shively**, M. Shapovalova, M. Fountain, J.R. Morrow, K.E. Sifers
- INOR 603.** Determining titanium (IV) transport for its potential use by humans. **T.M. Planas-Fontanez**, S. Gonklin Lopez, A. Lopez-Cubero, A.D. Tinoco
- INOR 604.** Non-covalent interactions of a Ru-Rh supramolecular complex with DNA and their effect on covalent modification of the biomolecule. **J.A. Rodriguez Corrales**, K.S. Brewer
- INOR 605.** Light-activated drug release using heterobimetallic ruthenium and cobalt complexes. **R. Whitman**, C. Turro

Section D

Colorado Convention Center
Hall C

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*

6:00 - 8:00

- INOR 606.** Synthesis, characterization, and reactivity of pyridazine-oxime metal complexes. **S.O. Elsdiedig**, F.R. Fronczek, A.W. Maverick
- INOR 607.** "Super Bulky" guanidines for the support of low-coordinate metal complexes. **L. Griego**, A.K. Maity, S. Fortier, A.J. Metta-Magana
- INOR 608.** Synthesis and characterization of a new guanidinate-guanidinate ligand featuring an imidazol-2-iminate backbone. **B. Barraza**, J. Lu, R. Aguilar, A. Maity, S. Fortier, A.J. Metta-Magana
- INOR 609.** Reactivity of group 11 formamidate complexes. **A. Lane**, J.R. Walensky, W.E. Antholine
- INOR 610.** Vanadium(V) catecholates: Correlating redox potential with 51V NMR chemical shifts. **J. Koehn**, P. Chatterjee, A. Waterhouse, T. Lucia, T.E. Polenova, M.D. Johnson, D.C. Crans
- INOR 611.** Octahedral to trigonal prismatic distortion in Ruthenium and Osmium bis-homoleptic complexes of a noninnocent ligand. **J. Cipressi**, S.N. Brown

- INOR 612.** Recent developments in cyano-substituted polypyrazoloborates chemistry. **L. Kadel**, D.M. Eichhorn
- INOR 613.** Synthesis, structural and spectroscopic studies of six-coordinate iron and cobalt phosphasalen complexes. **J.M. Fritsch**, **C.M. Bakewell**, A.J. White, C.K. Williams
- INOR 614.** Electron transfer between metal and ligand in chromium complexes with tetrazine-containing pincer ligand. **A.V. Polezhaev**, C. Chen, N.A. Maciulis, K.G. Caulton
- INOR 615.** Pyrazolate and polypyrazoleborate complexes of platinum and palladium. **A. Oberley**, D.M. Eichhorn
- INOR 616.** Chemistry of copper and nickel pyridyltriazole complexes. **T.M. Wheat**, U.R. Pokharel, F.R. Fronczek, A.W. Maverick
- INOR 617.** Synthesis and characterization of bis-bipyridyl ruthenium(II) complexes with high nitrogen content tetrazole aromatic ligands. **R.R. Ruminski**, M.A. Hiskey, R. Malkan, B. Powell
- INOR 618.** Novel synthesis of a dinuclear ruthenium(II) polypyridyl complex based on a polymeric carbonyl complex. **L.M. Puckett**, B. Durham
- INOR 619.** 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 620.** Synthesis and characterization of [M(tacn)(dppz)(solvent)]ⁿ⁺ complexes of Ru, Rh, and Ir: New DNA metallointercalators possessing modifiable groups. **H.L. Hancock**, M. Pham, G. Culcu, **S.C. Haefner**
- INOR 621.** Combined experimental and theoretical investigation of electronic structures and anion sensing aspects of Os^(bpy)(HL²⁻) AND [Os^(bpy)]₂(μ-HL²⁻)⁺. **A. Das**

Section E

Colorado Convention Center
Hall C

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*

6:00 - 8:00

- INOR 622.** Dehydrohalogenation as an effective route to unsaturated bimetallic and monometallic systems featuring a proton-responsive pincer ligand. **B. Cook**, C. Chen, M. Pink, R.L. Lord, K.G. Caulton
- INOR 623.** Low-valent organometallics incorporating the 2,2'-biazulenyl motif. **M.D. Hart**, D.M. McGinnis, B.M. Neal, M.V. Barybin
- INOR 624.** Six-coordinate 16-electron complexes of tungsten (II): Synthesis, electrochemistry, and density functional theory. **A.F. Greene**, S. Dahlhauser, J.T. Mague, J.P. Donahue
- INOR 625.** Structural trends for triple-decker organometallic sandwiches formed by highly charged π-bowls with mixed alkali metal cores: Li/K vs. Li/Rb. **S.N. Spisak**, A.S. Filatov, A. Zabula, A.Y. Rogachev, **M.A. Petrukhina**
- INOR 626.** Novel, multizonal, crystalline composite based upon self-assembled, helical coordination polymers and exhibiting seven primary zones in the solid state. **S.R. Seidel**, R. Wilkens
- INOR 627.** Synthesis of new diethylene-type ligands. **E. Haas**, J.P. Donahue, J.T. Mague
- INOR 628.** Cd(II) complexation with 1,1-dithiolate and nitrogen donors: Synthesis, luminescence, crystal structure and antifungal activity. **A. Das**
- INOR 629.** Reversible addition of alcohols across C=N bonds of a N₂ Schiff base ligand coordinated to copper (II). **W. Zhang**, H. Nie, M.S. Mashuta, C.A. Grapperhaus, R.M. Buchanan
- INOR 630.** Design and synthesis of lightweight MOFs for gas storage. **M. Shimazu**, X. Bu, X. Zhao

- INOR 631.** First row transition metal complexes of tetrazine based ligands as a new class of energetic materials. **T.W. Myers**, S.K. Hanson, J. Veauthier, D.E. Chavez
- INOR 632.** Role of ligand modifications in structural outcomes of dinucleating, criss-crossed cobalt peroxo (μ-OH, μ-O₂) complexes. **Y. Cho**, M. Ward, M.J. Rose
- INOR 633.** Investigations of the reaction of PMe₃Ph with a Pt-Ru heterometallic complex. **Z.J. Manning**, N.C. Dopke
- INOR 634.** Chemo-induced spin-state switching using tunable iminopyridine ligands. **T. Ozumerzifon**, J. Kolanowski, M.P. Shores
- INOR 635.** Iron(II) complexes of the dimethylated tris(pyrazolyl)ethane ligands. **M.S. Goodman**, M.A. Goodman, A.Y. Nazarenko
- INOR 636.** Atropisomerism of iron 5,10,15,20-tetrakis(2-chloro-6-fluorophenyl)porphyrinates. **D.J. Meiningner**, N. Muquizz, Z.J. Tonzetich
- INOR 637.** Electrochemical analysis of iron nitriotriscetate complexes. **P.A. Defnet**, L.N. Ball, U.J. Williams

Section F

Colorado Convention Center
Hall C

Main Group Chemistry

T. W. Hudnall, *Organizer*

6:00 - 8:00

- INOR 638.** Exploring the impact of ligand variation on arsenic-sulfur bonding using X-ray Absorption Spectroscopy (XAS). **A.V. Blake**, C.M. Donahue, S.R. Daly
- INOR 639.** Cytoselectivity of organotin and transition metal-substituted organotin compounds on cancer cells. **J.S. Enriquez**, J.A. Muniz, A. Varela, K.H. Pannell, R. Aguilera
- INOR 640.** Synthesis of novel bismuth complexes for small molecule activation. **M. Castillo**, O. Barreda, R. Aguilar, S. Fortier, A.J. Metta-Magana
- INOR 641.** Synthesis and reactivity of a novel doubly base stabilized five-coordinate "silene" derivative, [k²-C(SiMe₂benzimid²⁺)₂]SiMe₂: Addition of a Zn-Me bond of Me₂Zn to afford [k²-C(SiMe₂)₂(SiMe₂benzimid²⁺)₂]ZnMe. **S. Ruccolo**, G.F. Parkin

Section G

Colorado Convention Center
Hall C

Organometallic Chemistry

Applications to Materials and Polymer Science

N. S. Radu, *Organizer*

6:00 - 8:00

- INOR 642.** Multistep synthesis of the biocompatible lactone 3,6-dihydro-2H-pyran-2-one. **B.S. Cundiff**
- INOR 643.** Coupling of cyclohexadiene oxide and CO₂ via metal catalysts. **C.J. Arp**, W. Chung, F. Tsai, S.J. Kyran, D.J. Darensbourg
- INOR 644.** Synthesis and characterization of aluminum β-diketiminato complexes and their application in ring opening polymerization of lactides and synthesis of cyclic carbonates. **S. Bian**, G. Du
- INOR 645.** Synthesis, characterization, and polymerization of thieryl phosphine palladium(II) complexes. **J.L. Shott**, B.J. Reeves, B.M. Boardman
- INOR 646.** Extending π-conjugation for metal-organic photon harvesting. **M.H. Chisholm**, J. Leizeman
- INOR 647.** Theoretical study of the sodium mediated coupling of organochlorosilanes: Stable α-chloro-ω-sodium cycloosilane intermediates in the Wurtz synthesis of polysilanes? **S.J. Holder**

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

[†] Cooperative Cosponsorship

Section H

Colorado Convention Center
Hall C

Nanoscience

R. M. Richards, *Organizer*

6:00 - 8:00

- INOR **648.** Synthesis of aluminum nanoparticles capped with *o*-carborane. A. Benziger, P.A. Jelliss, S.W. Buckner
- INOR **649.** Stability of gold nanoparticle-based films deposited on plasma-etched borosilicate glass via a layer-by-layer physisorption technique. R.L. Svatora, S.A. Darveau, C.L. Exstrom
- INOR **650.** Stabilization of anisotropic gold nanoparticle shapes by Protein A. B.A. Lueck, S.A. Darveau, C.L. Exstrom
- INOR **651.** Heat-mediated drug release from inorganic nanoparticles. N.D. Klein, K.R. Hurlay, H.L. Ring, J.T. Buchman, C.L. Haynes
- INOR **652.** Soft inorganic oxide nanofibrous membranes and their applications. X. Mao, B. Ding
- INOR **653.** Design and synthesis of precursors for surface plasmon mediated chemical solution deposition of metal nanoparticles. N. Richey, Y. Wu, J. Qiu, W.D. Wei, L. McElwee-White
- INOR **654.** Role of oxygen vacancy in nanocrystalline perovskite oxides for electrochemical reactions. J. Kim, X. Yin, K. Tsao, S. Fang, H. Yang
- INOR **655.** Direct assembly of zeolite beta into mesoporous nanoparticles. T. Chen, Y. Liu, C. Mou
- INOR **657.** Binding and static quenching behavior of iridium (I) dyes on monodispersed zinc oxide nanocrystals. T.J. Morin, D.A. Blank, W.L. Gladfelter, K.R. Mann
- INOR **658.** Digestive ripening of gold nanorods in aqueous solution: Effect of CTAB and Au concentration. P. Guimera Coll, C.M. Sorensen
- INOR **659.** Design and controllable synthesis of Au@MOF Core@Shell Nanostructures. C. Tian, S.G. Boyes, A. Worcester
- INOR **660.** Studies of CdSe and CdSe/CdS core-shell quantum belts. Y. Zhou, F. Wang, Y. Wang, L. Mu, W.E. Buhro

Section I

Colorado Convention Center
Hall C

Inorganic Catalysts

S. A. Koch, *Organizer*

6:00 - 8:00

- INOR **661.** Synthesis of palladium diphosphine complexes for XAS analysis. C.M. Forrest, C.M. Donahue, A. Blake, S.R. Daly, B.J. Bellott
- INOR **662.** Transition metal carbides as noble metal fuel cell support materials. J.M. Thode
- INOR **663.** Synthesis and analysis of heterobimetallic cobalt-zirconium complex for artificial photosynthesis. S. Chapp, N. Cella, A. Hill
- INOR **664.** Nonheme iron complex-catalyzed efficient alcohol oxidation by *t*-BuOOH with *N*-hydroxyphthalimide as a cocatalyst. S. Lee, P. Kim, C. Kim
- INOR **665.** Versatile syntheses of optically pure ECE' pincer complexes. X. Yang, W. Tay, Y. Li, P.A. Sumod, P. Leung
- INOR **666.** Toward inner-sphere photoactivation of carbonyl and imine groups using Earth-abundant Schiff-base photocatalysts. D.J. Boston, F.J. Sarabia, M.P. Nguyen, C. Midkiff, E.M. Ferreira, A.K. Rappe, M.P. Shores
- INOR **667.** Synthesis, electrochemistry, and catalytic properties of hexacoordinate bis-bipyridylsilicon(IV) complexes. C. Maguilo, S. Garofalo, T. Le, T. Huynh, T.A. Schmedake
- INOR **668.** Investigation of substituted bidentate polypyridyl vanadium chromophores for photocatalysis. M.P. Nguyen, A.K. Rappe, M.P. Shores

Section J

Colorado Convention Center
Hall C

Organometallic Chemistry**New Ligand Platforms**

N. S. Radu, *Organizer*

6:00 - 8:00

- INOR **669.** Synthesis of dual gunction *ansa*-metallocene ligands via hydrocarbon radical anion coupling of 1,3-diphenyl-6-(alkyl/aryl)fulvenes. M.M. Lai, G.J. Balaich, S.T. Iacono
- INOR **670.** Novel binuclear pincer ligands for applications in catalysis and energy. C. Palit, O. Ozerov
- INOR **671.** Probing molecular and electronic structures of conjugated molecular linkers based on linear polyazulenic motifs. N. Erickson, A.D. Spaeth, M.V. Barybin
- INOR **672.** Efficient synthesis and heterobimetallic complexation of the first aromatic π -linker featuring mercapto and isocyanato junctions within the same molecule. J. Applegate, N. Gerasimchuk, M.V. Barybin
- INOR **673.** Synthesis of amphiphilic nickel-silyl complexes for cooperative small molecule activation. C.A. Olivares, M.T. Whited
- INOR **674.** E-H bond activation and hydrofunctionalization via bifunctional bis(pyridyl-imino)zincindolate complexes. J.B. Geri, N.K. Szymczak
- INOR **675.** Synthesis of ligand platforms for metalloenzyme mimics. O.M. Crandell, J.A. Dopke
- INOR **676.** Withdrawn.

Section K

Colorado Convention Center
Hall C

Organometallic Chemistry**Synthesis and Characterization**

N. S. Radu, *Organizer*

6:00 - 8:00

- INOR **677.** Organometallic complexes of 1,6-methano[10]annulene: DFT investigation of structure and dynamic behavior. D.A. KIssounko, Y.F. Oprunenko, I.P. Gloriovov
- INOR **678.** Room temperature carbon-sulfur bond activation by a reactive (dippe) Pd fragment. L. Munjanja, W. Brennessel, W.D. Jones
- INOR **679.** Synthesis and characterization of ruthenium(II) complexes with hydrosilyl pincer-type ligands. B.D. Nguyen, M.T. Whited
- INOR **680.** Scope, limitations, and mechanistic aspects of a regioselective acylation of cycloplatinated complexes. J.S. Carroll, H.G. Woolard, R. Mroz, C.A. Nason, S. Huo
- INOR **681.** Organosilver scaffolds for small-molecule activation and catalysis. B. Tate, C.M. Wyss, J.P. Sadighi, J.T. Nguyen, J. Bacsa, L. Gelbaum
- INOR **682.** Synthesis, structure, and cross-coupling of 2,3,5-tris(4-ferrocenylethynylphenyl)boroxine. D.A. KIssounko, V.P. Dyadchenko, V.N. Okulov, M.A. Dyadchenko, A.V. Churakov, L. Wang, D.A. Lemenovskii
- INOR **683.** Complexation studies of bipyridine aza-crown macrocycles. B. Carpenter, M. Harris
- INOR **684.** Synthesis of bis(diorganodithiocarbamato)iron(II) by the thermal decomposition of *cis*-dicarbonylbis(diorganodithiocarbamato)iron(II). J.E. Coffield, N.V. Duffy
- INOR **685.** Computed structures of cyclic platinum-metal-directed self-assembled complexes. E.A. Buchanan, J. Michl
- INOR **686.** Dual-metal NHC phenanthroline complexes. A.J. Landis, J.O. Hoberg
- INOR **687.** Fused siloles for electronic applications. D.A. Lee, T.A. Schmedake
- INOR **688.** Actinide high-nitrogen chemistry. K.P. Browne, D.E. Morris, B.L. Scott, D.E. Chavez, A.T. Nelson, B.C. Tappan, J.L. Kiplinger, J. Veauthier

INOR **689.** New synthetic pathways to (C₆Me₆)₂ThS₂. J.M. Dorhout, A. Lichtscheidl, N.E. Travia, P.K. Dorhout, B. Scott, K. Czerwinski, J.L. Kiplinger

- INOR **690.** Actinide metal fluorides: Synthesis, characterization, and chemistry. A.G. Lichtscheidl, M.J. Monreal, K. Browne, D.E. Morris, B. Scott, A. Nelson, J.L. Kiplinger
- INOR **691.** Molecular chemistry of thiophene with actinide complexes. N.E. Travia, A.W. Pierpont, B.J. Barker, K. Browne, M.J. Monreal, E.R. Batista, J.M. Berg, R.L. Martin, R. Michalczyk, D.E. Morris, B. Scott, M.P. Wilkerson, J.L. Kiplinger

Section K

Colorado Convention Center
Hall C

Soluble Inorganic Semiconductors: Synthesis, Properties, and Applications

R. L. Brutchey, B. M. Cossairt, *Organizers*

6:00 - 8:00

- INOR **692.** Low-temperature solution processing of stibnite thin films. C.L. McCarthy, R.L. Brutchey
- INOR **693.** Synthesis and characterization of metal chalcogenide nanomaterials for potential application in nanoelectronic devices. A.J. Bicchieri, A.R. Hight Walker
- INOR **694.** Colloidal cinnamic acid capped PbSe quantum dots: Solution phase ligand exchange, thin film formation, and electrical conductivity for photovoltaic applications. D.M. Kroupa, A. Sellinger, M.C. Beard
- INOR **695.** Probing structure-property relationships at the nanoscale: Combined X-ray and spectroscopic methods for the study of colloidal cadmium selenide. A. Beecher, P. Chen, Z. Norman, J.S. Owen
- INOR **696.** Effect of precursor reactivity on nickel phosphide nanocrystal synthesis. H. Andaraarachchi, J. Vela-Becerra
- INOR **697.** Rational control over electron-transfer using inorganic cluster-anions directly coordinated to anatase-TiO₂ cores in water. M. Raula, I. Weinstock

Section L

Colorado Convention Center
Hall C

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage

Cosponsored by MPPG

C. Ban, A. L. Prieto, Y. Yang, *Organizers*

6:00 - 8:00

- INOR **698.** Electrocatalytic and photocatalytic hydrogen evolution using iron phosphide nanoparticles. J.F. Callejas, J.M. McEnaney, C.G. Read, R.E. Schaak
- INOR **699.** Amorphous MoP and WP nanoparticles as electrocatalysts for the hydrogen evolution reaction. J. McEnaney, R.E. Schaak
- INOR **700.** Fast kinetics of Ni-doped nanomagnesium for hydrogen storage and the difficulty of effectively comparing material performance in literature. D.J. Shissler, M.B. Braun, S.J. Fredrick, A.L. Prieto
- INOR **701.** Solution synthesized magnesium nanoparticles: The role of synthesis, particle size, structure, and dopant incorporation on hydrogenation kinetics. M.B. Braun, D. Shissler, A.L. Prieto
- INOR **702.** Efficient method of cleaning hydrogen sulfide at ambient temperature and pressure for hydrogen storage. X. Li, R. Morrish, C.A. Wolden, Y. Yang

Section L

Colorado Convention Center
Hall C

Electrochemistry

B. L. Lucht, *Organizer*

6:00 - 8:00

- INOR **703.** Electrochemistry of neodymium in chloride-fluoride melts. D.A. Shuklin, I.B. Polovov, M.V. Chernyshov, V.A. Volkovich, O.I. Rebrin

- INOR **704.** Functionalization of Si(111) photocathodes: Interplay between steric spacing of molecular linkers and ALD-deposited metal oxide films. R. Pekarek, M.J. Rose
- INOR **705.** Stable 4 volt electrolytes for high energy electrochemical capacitors. C. Sun, R.E. Ruther, F.M. Delnick, J. Nanda
- INOR **706.** Patterned electrodeposition of cobalt selenide nanostructure arrays as effective ORR catalysts. J. Masud, A. Swesi, M. Nath

Section L

Colorado Convention Center
Hall C

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

6:00 - 8:00

- INOR **707.** Humidity effects on the methylamine lead iodide perovskite solar cells with TiO₂ mesoporous structure. F. Zheng, Y. Ding, Z. Zhu
- INOR **708.** Photoelectrochemical characterization of natural semiconducting minerals. B.K. Durant, B.A. Parkinson
- INOR **709.** Synthesis and characterization of rhenium and manganese electrocatalysts containing diaminophenyl ligands for CO₂ reduction. B.A. Corbin, B. Dhakal, D.A. Kurtz, G.S. Nichol, G.A. Felton
- INOR **710.** Bioaccumulation of arsenic in the bryophyte *Hygrohypnum ochraceum* in Fountain Creek watershed, Colorado. J.S. Carsella, D.C. Crans, S.J. Bonetti, D.R. Nimmo, S.J. Herrmann, D. Lehmpuhl
- INOR **711.** Protein folding thermodynamics of cytochrome *c*₂₂ from mesophilic and psychrophilic microbes. N.K. Asous, E.A. Benzik, J. Chou, N. Dalchand, G.E. Gallagher, G.J. Salerno, J.S. Magee
- INOR **712.** Improved lithium ion transference numbers in electrolytes for lithium-ion batteries with organosilyl and fluoroalkyl solvents. J. Gnrke, M.I. Bakhira, L.J. Lyons
- INOR **713.** Ionic conductivity studies of lithium electrolytes with organosilyl and carbonate solvent blends. V. McGraw, N. George, L.J. Lyons
- INOR **714.** Ruthenium incorporated platinum copper nanotubes for electro-oxidation of methanol. L.E. Mathurin, J. Chen
- INOR **715.** Oxidative cleavage of pyrolytic lignin using transition metal catalysts. A. Lai, M.S. Fortin, M.D. Mohadjer Beromi, C. Mullen, A.A. Boateng, N.M. West
- INOR **716.** Preparation and applications of carbon interdigitated array electrodes (IDA). F. Liu, G. Kolesov, B.A. Parkinson

Section L

Colorado Convention Center
Hall C

Molecular Catalysts for Solar Fuels

Cosponsored by MPPG

A. M. Appel, M. Helm, J. Y. Yang, *Organizers*

6:00 - 8:00

- INOR **717.** Withdrawn.
- INOR **718.** Developing dirhodium(II,II) complexes that function as single-component photocatalysts for proton reduction to hydrogen. T.A. White, S. Witt, L. Zhanyong, K.R. Dunbar, C. Turro
- INOR **719.** Pendant base groups in the secondary coordination sphere of pyridinediimine compounds for syngas conversion. Y. Kwon, J. Adams, J.D. Gilbertson
- INOR **720.** Photocatalytic and photoelectrochemical generation of hydrogen from water Using CdSe quantum dots and CdSe quantum dot-sensitized photocathodes. P. Ruberu, A. Das, Y. Dong, R. Eisenberg
- INOR **721.** FTIR studies of interactions between carbon dioxide and surface molecular photocatalysts. M.E. Louis, T. Fenton, G. Li

Section E

Colorado Convention Center
Room 201

Inorganic Catalysts

S. A. Koch, *Organizer*
A. K. Vannucci, *Presiding*

- 1:30 INOR 867.** "Innocent" role of Sc³⁺ on a non-heme Fe catalyst in an O₂ environment. A. Poater, S. Chaitanya Vummaleti, L. Cavallo
- 1:50 INOR 868.** Electrocatalytic reductive carbon-carbon cross coupling using well defined Ni catalysts. A.K. Vannucci
- 2:10 INOR 869.** Characterization of BIOX compounds as photocatalysts for the degradation of pharmaceuticals in water. J.C. Ahern, R. Fairchild, J. Thomas, J. Carr, H.H. Patterson
- 2:30 INOR 870.** Molybdenum complexes for effecting organophosphate hydrolysis. L.Y. Kuo, Y. Shari'ati
- 2:50 INOR 871.** Chiral pincer complexes: A study on the influence of catalyst design in an asymmetric P-H bond addition reaction. W. Tay, X. Yang, Y. Li, P.A. Sumod, P. Leung
- 3:10 Intermission.**
- 3:20 INOR 872.** Incorporation of Lewis acidic or Lewis basic group in the secondary coordination sphere of metal complexes for the modulation of C-H bond formation and cleavage. Z. Thamavongsy
- 3:40 INOR 873.** Electronic tuning of H₂ production catalyzed by Co complexes with pentadentate ligands. X. Zhao, M. Vennampalli, G. liang, L. Katta, C.E. Webster
- 4:00 INOR 874.** Rigid tetraphenylelement linker scaffolds for immobilizing catalysts on oxide supports. E.M. Steffensmeier, J.H. Baker, B. Beele, J. Bluemel
- 4:20 INOR 875.** Active catalysts for oxygen containing substrates: Actinide coordination complexes. I. Karmel, N. Fridman, T. Bannenberg, M. Tamm, M. Eisen

Section F

Colorado Convention Center
Room 304

Organometallic Chemistry

New Ligand Platforms

N. S. Radu, *Organizer*
M. V. Barybin, D. V. Peryshkov, *Presiding*

- 1:30 INOR 876.** New developments in the chemistry of low-valent organometallics featuring linear azulenyl π -linkers. M.V. Barybin
- 1:50 INOR 877.** Flexible coordination of PC=C-P ligands to late transition metals. B. Barrett, V.M. Iluc
- 2:10 INOR 878.** Proton-switchable nitrile hydrogenation by a rationally designed bifunctional ruthenium complex. J.B. Geri, N.K. Szymczak
- 2:30 INOR 879.** New pyrrole-based PNP pincer complexes with late transition metals. J.A. Kessler, V.M. Iluc
- 2:50 INOR 880.** Carborane clusters in metal-ligand cooperative substrate activation. D.V. Peryshkov, B.J. Eleazer
- 3:10 INOR 881.** Synthesis, reactivity, and catalytic behavior of heterobimetallic cooperative complexes based on a β -oxo- δ -diiminate ligand. H. Chiu, I.A. Tonks

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

- 3:30 INOR 882.** Flexible, open chain tetracarbene ligands: Diversity in structural motifs depending on ligand structure and metal center. D.T. Weiss, S. Haslinger, C. Jandl, A. Pothig, M. Cokoja, J.M. Basset, F.E. Kuehn
- 3:50 INOR 883.** Withdrawn.
- 4:10 INOR 884.** Synthesis, structure, and reactivity of bis(oxazoline)-substituted cyclopentadienyl and fluorenyl rhodium and iridium complexes. B. Schmidt, A.D. Sadow
- 4:30 INOR 885.** Development of new ligands for [M(CO)₂]⁺ (M= Re, ^{99m}Tc) complexes with enhanced chemical properties and stability. T.R. Hayes, P.A. Lyon, C.L. Barnes, S.L. Trabue, P.D. Benny
- 4:50 INOR 886.** Hydrogen bonding behavior of amide-functionalized α -diimine palladium complexes. F. Zhai, R.F. Jordan

Section G

Colorado Convention Center
Room 401

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*
M. Emmert, *Presiding*

- 1:30 INOR 887.** Photocatalytic CO₂ reduction from organic/inorganic hybrid system. S.O. Kang, H. Son, D. Won
- 1:50 INOR 888.** Water splitting with Prussian blue-type catalysts. J. Galan-Mascaros, B. Rodriguez-Garcia
- 2:10 INOR 889.** Fixation of carbon dioxide to oxalate and carbonate by copper complexes. U.R. Pokharel, F.R. Fronczek, A.W. Mawerick
- 2:30 INOR 890.** Mechanism of the doped hercynite cycle for solar thermal water splitting. C. Muhich, K. Weston, D. Arifin, A.H. McDaniel, E.N. Coker, B. Ehrhart, V. Witte, A.W. Weimer, C. Musgrave
- 2:50 Intermission.**
- 3:00 INOR 891.** Peroxo-based oxygen-rich compounds for potential use as new high energy-dense oxidizers. N.H. Gamage, B. Stiasny, J. Stierstorfer, P.D. Martin, T.M. Klapötke, C.H. Winter
- 3:20 INOR 892.** Plasmonic behavior of copper iron sulfide nanoparticles. K. Plass, N.J. Freymeyer, C. Kim, C.J. Wisdo, Z. Georgieva
- 3:40 INOR 893.** Combining separation science and synchrotron X-ray fluorescence for fuels. L.A. Finney, S. Vogt, R.E. Winans
- 4:00 INOR 894.** A p-GaN/P₃ photoelectrode for water reduction stabilized with TiO₂ and a molecular cobalt catalyst. J. Gu, Y. Yan, J. Young, N.R. Neale, J.A. Turner
- 4:20 INOR 895.** Sustainable methods for rare earth recycling: Chemical perspectives on critical materials. M. Emmert
- 4:40 INOR 1058.** Consequences of chloromethane (R40) mixed in with tetrafluoroethane (R134a); production of trimethylaluminum, reactivity of TMA and various refrigerant oils and methods to deactivate trimethylaluminum. R.L. Luck, Z. Chen, J.M. Marciniok, A.W. Schultz

Section H

Colorado Convention Center
Room 203

Electrochemistry

B. L. Lucht, *Organizer*
N. Bedford, *Presiding*

- 1:30 INOR 896.** Perfluoroalkyl-fluorophosphate anions for high voltage electrolytes in lithium cells: A DFT study. S. Brutti, R. Spezia, M. Carboni
- 1:50 INOR 897.** Bromine-free quinone flow battery chemistries. M.P. Marshak, M.J. Aziz, R.G. Gordon
- 2:10 INOR 898.** Non-platinum group metal bimetallic electrocatalyst for alternative fuel oxidation and ammonia production. N. Bedford, L.F. Greenlee, A.M. Herring

- 2:30 INOR 899.** Hemi-cage 5,5' substituted cobalt bipyridine complexes for use as dye sensitized solar cell mediators. J.D. Thomas, C.M. Elliott, A.L. Prieto
- 2:50 INOR 900.** Photoelectrochemical properties of p-type GaP(111)A after deliberate surface chemisorption. E. Brown, S. Maldonado
- 3:10 INOR 901.** Hybrid molecular/materials passivation of p-silicon(111) photocathodes: Band-edge modulation with organic surface linkers and thin film Al₂O₃ or TiO₂. M.J. Rose, H. Kim, J. Seo, L. Le

Section I

Colorado Convention Center
Room 205

Organometallic Chemistry Applications to Materials and Polymer Science

N. S. Radu, *Organizer*
B. Boardman, R. Wright, *Presiding*

- 1:30 INOR 902.** Influence of π - π Stacking, π -cation interactions and axial steric blockage on the ethylene polymerization behavior of asymmetric phosphine-sulfonate palladium methyl complexes. G. Feng, J.J. Defoe, R.F. Jordan
- 1:50 INOR 903.** Cobalamin-fluorophore based photoinitiators for hydrogel curing with tissue penetrating light. Z. Rodgers, R.M. Hughes, L. Doherty, J.R. Shell, B. Moleisky, A. Brugh, A.M. Moran, M.D. Forbes, D.S. Lawrence
- 2:10 INOR 904.** Synthesis and characterization of chiral C₂-symmetric bimetallic zinc complexes of amido-oxazolines: Active initiators for asymmetric copolymerization of CO₂ and cyclohexene oxide. S. Abbina, V.K. Chidara, S. Bian, G. Du
- 2:30 INOR 905.** Hydrophilic polycarbonates derived from coupling of cyclohexadiene and CO₂ utilizing metal salen catalysts. W. Chung, D.J. Darensbourg
- 2:50 INOR 906.** Withdrawn.
- 3:10 INOR 907.** In situ tacticity control in lactide polymerization reactions. J. Byers, C.M. Manna, L. Yablon
- 3:30 INOR 908.** Synthesis, characterization, and the applications of novel zinc alkyl complexes for polylactide synthesis. O. Falola, J.S. Matthews
- 3:50 INOR 909.** Synthesis, characterization, and investigation of cobalt chalcogenide clusters with thienyl phosphine ligands as new acceptor materials for P3HT. B.M. Boardman, B.J. Reeves, D.M. Shircliff, J.L. Shott
- 4:10 INOR 910.** Formation of stoichiometric GaAs from thin films of [tBu(H)AsGaEt₂]₂: Mechanistic studies and isolation of the novel cluster {[tBu(H)AsGaEt₂]₂}[tBuAsGaEt₂]₂. R. Wright, A. Sokolov, G. Athens, A. Krasovskiy, R. Frosse, L. Spencer, B. Gerhart, P.N. Nickias, J.C. Stevens
- 4:30 INOR 911.** Synthesis of unprecedented solution-stable metal organic oligomers via iClick and Au-Au bond formation. X. Yang, A. Powers, I. Ghiviriga, K.A. Abboud, A.S. Veige
- 4:50 INOR 912.** Solvent control of surface plasmon mediated chemical deposition of Au nanoparticles from phosphorus based organo-gold precursors. C. Muhich, J. Qiu, A. Holder, W. Wei, L. McElwee-White, C. Musgrave

Section J

Colorado Convention Center
Room 402

Inorganic Spectroscopy

S. A. Koch, *Organizer*
S. R. Daly, *Presiding*

- 1:30 INOR 913.** Photoluminescence decay dynamics of white light emitting ultrasmall cadmium selenide nanocrystals: Mechanistic insights to foster the development of an energy-efficient solid state sunlight-mimicking device. N. Orfield, J. Keene, T. Frecker, L.M. Davis, S.J. Rosenthal

- 1:50 INOR 914.** Impact of structure on metal-ligand covalency in late transition metal complexes: Do variations in diphosphine bite angle matter? S.R. Daly, C. Donahue, A. Blake, B.J. Bellotti, C.M. Forrest, J.M. Keith, S. McCollom
- 2:10 INOR 915.** Fluorescent d10 metal complexes for the presumptive identification of substances of abuse and the implementation of a cell phone fluorimeter for field identification. D.J. Nash, R.G. Blair
- 2:30 INOR 916.** High temperature X-ray absorption spectroscopic investigation of Sr₂Fe₃Mo₂O₁₅ solid oxide fuel cell electrodes. B.C. Eigenbrodt, T. Sultana, A. D'Orazio, T. Marshall, J. Gerardi, C.U. Segre
- 2:50 INOR 917.** Measurement of the activation energies of exciton migration in ruthenium(II) and rhodium(III) polypyridyl and phenanthroline complexes via luminescence at cryogenic temperatures. J.W. Kenney, J. Macwillie, p. weaver, R. Ramos, N. Nunez, G.A. Crosby
- 3:10 INOR 918.** Variable-temperature multinuclear NMR spectra of the [Mn_nO₁(O,CR)_n(H₂O)]⁺ family of single-molecule magnets in solution. A. Fournet, K.A. Abboud, G. Christou
- 3:30 Intermission.**
- 3:40 INOR 919.** Iron(II) and cobalt (II) paraCEST MRI contrast agents responsive to pH and redox environment. P.B. Tsvitovich, J.R. Morrow
- 4:00 INOR 920.** Optical properties of Ag nanocrystals self-assembled in thin 3D crystalline superlattices. J. Wei, N. Schaeffer, M. Pileni
- 4:20 INOR 921.** Investigation of valence tautomerism in cobalt-dioxolene complexes using K X-ray emission spectroscopy. W. Liang, D. Nordlund, T. Weng, D. Sokaras, C.G. Pierpont, K. Gaffney
- 4:40 INOR 922.** Bromine atom formation by visible light driven bromide oxidation with a Ru polypyridyl compound. G. Li, G.J. Meyer
- 5:00 INOR 923.** d- and f-Orbital mixing in open-shell systems. S.E. Stieber, E.R. Batista, D.L. Clark, M.W. Lölble, R.L. Martin, S.G. Minasian, J.A. Trujillo, S.A. Kozimor
- 5:20 INOR 924.** Surface and bulk characteristics of Zn/Ni substituted cobalt oxide spinel p-type semiconductors. C.C. Mercado, C.L. Donley, C. Flynn, A. Zakutayev, K. Zhu, J. Cahoon, A.J. Nozik

THURSDAY MORNING

Section A

Colorado Convention Center
Room 105

Bioinorganic Chemistry

- S. A. Koch, *Organizer*
K. E. Splan, *Presiding*
- 8:00 INOR 925.** Interaction of amino-acids with ferredoxin-like centers in a designed metalloprotein. J. Schmitt, J.M. Shearer
- 8:20 INOR 926.** DNA-mediated signalling by the *E. coli* helicase, DinG. M.A. Grodick, T.J. Zwang, J.K. Barton
- 8:40 INOR 927.** Ferromagnetically coupled (S = 1) peroxodioxycopper(II) complex. N. Kindermann, S. Dechart, S. Demeshko, E.J. Reijerse, E. Bill, F. Meyer
- 9:00 INOR 928.** Spectroscopic characterization of Cu(I) binding at the BIR2 domain of the X-linked Inhibitor of apoptosis protein. K.E. Splan, Y. Liang
- 9:20 INOR 929.** Label-free electrochemical detection of human methyltransferase from tumors. A.L. Furst, N. Muren, M.G. Hill, J.K. Barton
- 9:40 Intermission.**
- 9:50 INOR 930.** Ru(II) complex-antibody conjugation for targeted photochemotherapy. J.D. Knoll, C. Turro
- 10:10 INOR 931.** Arming anticancer platinum(IV) complexes as prodrugs for targeted chemotherapy. W. Ang, D. Wong, J. Lim

- 10:30 INOR 932.** Ruthenium anticancer agents with redox-active intercalating ligands (RAILs): Correlation of reduction potential with DNA cleavage activity. E.S. Narh, J. Nguyen, F.M. MacDonnell
- 10:50 INOR 933.** Characterization and reactivity of metallosalphen complexes with G-quadruplexes. M.J. Ross, J.A. Cowan
- 11:10 INOR 934.** New dirhodium (II,II) complex with potential dual-binding to DNA upon photoactivation. R. Akhime, C. Turro
- 11:30 INOR 935.** Construction and application of a Rh-Pt DNA metalloinsertor conjugate. A.G. Weidmann, J.K. Barton
- 11:50 INOR 936.** *Mycobacterium tuberculosis* and cobalt: A new approach to the fight against *M. tb* resistance. T.J. Greenfield

Section B

Colorado Convention Center
Room 301

Chemistry of Materials

Nanomaterials

C. G. Lugmair, *Organizer*
L. V. Frolova, J. R. Soliz, *Presiding*

- 8:30 INOR 937.** Grain structure and transport in nanocrystalline cadmium selenide. Z. Norman, J.S. Owen
- 8:50 INOR 938.** Nanocrystals of lithium group 14 compounds: Synthesis, stability, and carbon encapsulation. J.E. Cloud, Y. Wang, X. Li, T. Yoder, L. Taylor, Y. Yang, Y. Yang
- 9:10 INOR 939.** How the crystalline structure of Co nanocrystals plays a role in the Kirkendall processes. Z. Yang, N. Yang, M. Pileni
- 9:30 INOR 940.** Graphene as the test material for chemical modifications of bulk graphite. L.V. Frolova

9:50 INOR 941. Cation-vacancy and electron-hole relaxation in single-walled aluminosilicate nanotubes: A linear-scaling density functional theory study. E. Poli, G. Teobaldi

10:10 Intermission.

- 10:25 INOR 942.** Synthesis and characterization of magnetic nanoparticles for toxic gas adsorption. J.R. Soliz, A.J. Hauser, K.M. Bussmann, M.S. Osolfsky, C.J. Karwacki
- 10:45 INOR 943.** First stoichiometric metal chalcogenide nanocrystal. P. Chen, N.C. Anderson, Z. Norman, J.S. Owen
- 11:05 INOR 944.** Chromium-based chalcospinel nanocrystals: Syntheses and magnetism. K. Ramasamy, A. Gupta
- 11:25 INOR 945.** Synthesis, functionalization, and surface modification of layered zirconium phosphate nanoplatelets. Y. Kan, A. Clearfield
- 11:45 INOR 946.** Effects of the spatial location of Ag in titania nanotube on its photocatalytic activity and toxicity. S.A. Ferdousi, Y. Li, K.L. Yeung, Y. Xu

Section C

Colorado Convention Center
Room 302

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*
D. Harris, M. Harris, *Presiding*

- 8:00 INOR 947.** Closed-shell metal complexes of caffeine sulfide and selenide. M. Styron, D. Rabinovich
- 8:20 INOR 948.** 1D1 coordination polymers of metallacrowns. C.M. Zaleski
- 8:40 INOR 949.** Multireceptor host-guest complexation studies of novel ruthenium(II) ethylene-oxide oligomers, polyamine macrocycles, and tripodal cage complexes. M. Harris, B. Carpenter, T. Carroll, W. Lewis, A. Thomas, M. McBride, A. Smale
- 9:00 INOR 950.** Synthesis and crystal structures of oxo-molybdenum(VI), oxo-vanadium(V) and alkaline earth cations-based clusters. A. Moneeb, A. Apblett, A. Alabdulrahman, A. Bagabas

9:20 INOR 951. Polyoxometalate complexes of anatase-TiO₂ cores. M. Raula, G. Gan Or, M. Saganovich, Y. Wang, R. Gobetto, I.A. Weinstock

9:40 INOR 952. Novel transition metal(II)-2,5-diamino-2(difluoromethyl)pentanoic acid hydrochloride-1-hydrate complexes: Syntheses, characterization, structural elucidation, and their biological potency. J.A. Obaleye, W.A. Osunniran, A.C. Tella, J.O. Adebayo, M.O. Bamigboye

10:00 Intermission.

- 10:10 INOR 953.** Coordination chemistry of a fluorescein-decorated phosphine ligand. A. DeLaRosa, F.P. Gabbai
- 10:30 INOR 954.** Updating Richman-Atkins for the 21st century: Simpler, faster, and greener azamacrocyclic synthesis. M. Wasilewski, M. Wetzel
- 10:50 INOR 955.** Synthesis and characterization of tris-(2-aminoethyl)amine copper complexes incorporating para-substituted electron withdrawing functional groups. A.R. McGlone
- 11:10 INOR 956.** Withdrawn.
- 11:30 INOR 957.** Tetrahedral Sn-silsesquioxane: Synthesis, characterization, and adsorption properties. E.V. Beletskiy, Z. Shen, M.V. Riotski, X. Hou, J.R. Gallagher, J.T. Miller, Y. Wu, M.C. Kung, H.H. Kung
- 11:50 INOR 958.** Generalization of the donor-acceptor charge transfer complexation of Pt(bipyridine)(dithiolate) donors and nitrofluorenone acceptors to exhibit "black-absorber" behavior in the solid state and solution. C. Browning

Section D

Colorado Convention Center
Room 303

Nanoscience

Applications

Cosponsored by PRES

R. M. Richards, *Organizer*
B. G. Trewyn, *Presiding*

- 8:30 INOR 959.** New and efficient surface modification of NaYF₄: Yb³⁺, Er³⁺ upconversion phosphor nanoparticles (UCNPs) for biomedical imaging and organic photovoltaic applications. S.K. Cho, S. Ahn, L. Su, T.W. Flaig, W. Park
- 8:50 INOR 960.** Cholera toxin subunit B-modified mesoporous silica nanoparticles as vehicles for the improved intracellular delivery of proteins. W. Walker, J.L. Vivero
- 9:10 INOR 961.** Incorporating enzyme and metal nanoparticle catalysts on mesoporous silica supports for tandem reactions. M.M. Otting, X. Sun, B.G. Trewyn
- 9:30 INOR 962.** Power of rust and sand at the nanoscale: Iron oxide and mesoporous silica nanoparticles for theranostic applications. K. Hurley, H. Ping, M. Etheridge, J. Zhang, N. Klein, V. Szlag, C. Chung, Q. Shao, T.M. Reineke, M. Garwood, J. Bischof, C.L. Haynes
- 9:50** Intermission.
- 10:00 INOR 963.** Withdrawn.
- 10:20 INOR 964.** Nanostructured organosilica hybrids as highly efficient and regenerable sorbents for rare earth extraction. J. Florek, A. Mushtaq, E. Juerre, F.G. Fontaine, D. Larivere, F. Kleitz
- 10:40 INOR 965.** Effects of bis[3-(triethoxysilyl)propyl]tetrasulfide on gold nano particle formation in gold intercalated in the wall of mesoporous silica. Y. Ji, R.M. Richards
- 11:00 INOR 966.** Tackling environment and energy challenges with mesoporous nanomaterial technology. B.G. Trewyn
- 11:20 INOR 967.** Selectively inner-surface methylated single-walled aluminosilicate nanotubes, toward integration of chemical separation and (photo)-catalysis in confined volumes? J.D. Elliott, G. Teobaldi

Section E

Colorado Convention Center
Room 201

Organometallic Chemistry

Catalysis

N. S. Radu, *Organizer*
S. C. Chmely, N. P. Mankad, *Presiding*

- 9:00 INOR 968.** Withdrawn.
- 9:20 INOR 969.** Deoxygenation of CO₂ and N₂O enabled by bimetallic cooperativity: Control of reactivity and selectivity using tunable bimetallic effects. N.P. Mankad, S. Bagherzadeh, S. Parmelee, U. Jayarathne
- 9:40 INOR 970.** Light-activated iron bifunctional catalysts for transfer hydrogenations of polar double bonds. S.C. Chmely, P. Das
- 10:00 INOR 971.** Studies on the reductive elimination of C-X (X = C, N, S) bonds from a Co(III) center and its applications in catalysis. C. Palit, S. Timpa, O. Ozerov
- 10:20 INOR 972.** Regulation of iron-catalyzed olefin hydroboration by ligand modifications at a remote site. K.T. Tseng, J. Kampf, N.K. Szymczak
- 10:40 INOR 973.** Understanding H₂ oxidation by [Fe-Fe] hydrogenase: From enzymatic function to functional mimics. N. Kumar, S. Raugai, B. Ginovska-Pangovska, M. Dupuis, M. Helm, M. Bullock
- 11:00 INOR 974.** Cooperative catalysts for the synthesis of polyesters. R.J. Hue, I.A. Tonks
- 11:20 INOR 975.** Rhodium-catalyzed reduction of secondary and tertiary amides to amines using phenylsilane. Z. Weinstein, A.D. Sadov

Section F

Colorado Convention Center
Room 304

Main Group Chemistry

T. W. Hudnall, *Organizer*
C. Martin, K. H. Pannell, *Presiding*

- 8:00 INOR 976.** Functionalization of nine-atom deltahedral germanium clusters. F. Li, S.C. Sevov
- 8:20 INOR 977.** Exploration of aluminum(II) chemistry: Reactions involving AlX (X = Cl or Br). S.M. De Carlo, B.W. Eichhorn
- 8:40 INOR 978.** Steric bulk as both inhibitor and promoter of reactivity: the case of group 15 M[N(SiMe₃)₂]₃ complexes. N.C. Boyde, T.P. Hanusa
- 9:00 INOR 979.** Inverse FLP and related acid-base chemistry of Verkade's superbase. S. Mummadi, C. Krempler
- 9:20 INOR 980.** Cationic carbon Lewis acids in frustrated Lewis pairs. L. Curless, M. Ingleson
- 9:40 INOR 981.** Hexacoordinate polypyridyl-silicon(IV) chemistry for electronic and catalytic applications. T.A. Schmedake, B.T. Donovan-Merkert, C. Maguillo, D.M. Pelouquin
- 10:00** Intermission.
- 10:10 INOR 982.** Stepwise anion-induced polarity reversal of an antimony-transition metal bond. J. Jones, F.P. Gabbai
- 10:30 INOR 983.** Synthesis, spectroscopic, and structural characterization of structurally unique trialkylboranes: Evidence of unusual geometries stabilized by dispersion effects. M.A. Faust, P.P. Power
- 10:50 INOR 984.** Investigating ring expansion reactions with pentaphenylborole. K. Huang, C. Martin
- 11:10 INOR 985.** Synthesis, spectroscopic properties, and structural characterization of new BODIPY fluorophores. L.I. Saucedo, E. William, Y. Li, L. Tan, P. Tu, R. Roacho, A.J. Metta-Magana, E. Pena-Cabrera, K.H. Pannell
- 11:30 INOR 986.** Stabilization of reactive main group species by coordination to carbonyl-decorated carbenes. T.W. Hudnall, C.L. Dearthoff, R.E. Sikma, K.M. Melancon, M.B. Gildner
- 11:50 INOR 987.** Polyborates as coordination compounds. D.M. Schubert, D. Neiner, M.K. McCray

Section G

Colorado Convention Center
Room 401

Nanoscience

Metal Oxides

Cosponsored by PRES

- R. M. Richards, *Organizer*
F. Kleitz, *Presiding*
- 9:00 INOR 988.** Fe-doped ZnO colloidal nanocrystals: Synthesis, characterization, and photodoping. D. Zhou, K.R. Kittilstved
- 9:20 INOR 989.** High-surface-area nanostructured mixed metal oxides for catalytic applications. H. Yen, F. Kleitz
- 9:40 INOR 990.** Preparation and characterization of magnesium oxide and nickel oxide nanostructures with polar surfaces. S.M. Shulda, F. Lin, D. Nordlund, T. Weng, R.M. Richards
- 10:00 INOR 991.** Cu- and Ni-doped α-MnO₂ electrocatalysts for reversible oxygen electrochemistry. T.N. Lambert, J.A. Vigil, S.E. White, B.S. Swartzentruber
- 10:20** Intermission.
- 10:30 INOR 992.** Growth and characterization of LaNiO₃ nanostructures using chemical vapor deposition. J.S. Page, A.L. Prieto
- 10:50 INOR 993.** Low-temperature synthesis of compositionally complex scheelite-structured nanocrystals. S. Culver, R.L. Brutchey
- 11:10 INOR 994.** Design of magnetically recoverable catalysts via controlled aggregation of iron oxide and catalytic nanoparticles. R. Easterday, Y. Losovj, M. Pink, B. Stein, D. Morgan, V.Y. Doluda, L.Z. Nikosvili, E.M. Sulman, W. Mahmood, A.A. Al-Ghamdi, L. Bronstein

Section H

Colorado Convention Center
Room 203

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*
D. Rabinovich, C. M. Zaleski, *Presiding*

- 8:00 INOR 995.** Synthesis, structure, and volatility of alkali and alkaline earth element hexafluoroacetylacetonate complexes. D.B. Rego, P.M. Forster, K. Czerwinski
- 8:20 INOR 996.** Effect of precursor ligand on particle size/morphology of zinc oxide nanomaterials. E. Rukundo, A. Apblett
- 8:40 INOR 997.** Unexpected facile access to dimetallic cryptates containing an elaborate hydrogen bonding network. J.B. Gordon, G. Guillet, K.A. Abboud, L.J. Murray
- 9:00 INOR 998.** Preparation and properties of a molecular analog of a perovskite-like structure. A.E. Thuijs, Y. Oh, S. Cheong, K.A. Abboud, G. Christou
- 9:20 INOR 999.** Supramolecular aggregates of single-molecule magnets. A.M. Mowson
- 9:40 INOR 1000.** Ligand field modification of cobalt-H₂bip complexes to control field induced magnetic relaxations. I. Bhowmick, A.K. Rappe, M.P. Shores
- 10:00** Intermission.
- 10:10 INOR 1001.** Dinuclear complexes as model systems to explore magnetic coupling through tetrazine-based radical ligands. T.J. Woods, M.F. Ballesteros-Rivas, K.R. Dunbar
- 10:30 INOR 1002.** Investigation of spin-cross-over behavior in cobalt tetrazene complexes with chelating ligands. A.C. Bowman, H.J. Zecca, H. Kim
- 10:50 INOR 1003.** Electronic effects on dinuclear iron(II) spin crossover complexes bridged by diiminobenzoquinonoid. J.G. Park, I. Jeon, D. Harris
- 11:10 INOR 1004.** Employing hydrogen-bonding interactions to modulate magnetic relaxation in a Co(II) tripodal iminopyridine-based complex. C.M. Klug, I. Bhowmick, A.K. Rappe, M.P. Shores

11:30 INOR 1005. Strong magnetic coupling in dinuclear transition metal complexes bridged by redox-active ligands. I. Jeon, D. Harris

11:50 INOR 1006. Magnetic and spectroscopic properties of linear two-coordinate transition metal complexes. C. Lin, G.J. Long, P.P. Power

Section I

Colorado Convention Center
Room 205

Inorganic Catalysts

S. A. Koch, *Organizer*
T. J. Hubin, *Presiding*

8:30 INOR 1007. Structure-function relationships for electrocatalytic water oxidation by molecular $[Mn_2O_2]$ clusters. Y. Yan, D.A. Ruddy

8:50 INOR 1008. Functional ordered mesoporous metal carbides. M. Xu, M.R. Nimlos, B.G. Trewyn, R.M. Richards

9:10 INOR 1009. Withdrawn.

9:30 INOR 1010. Single-crystal to single-crystal structural and chemical transformation of a Fe-based mononuclear electrocatalyst for hydrogen production. X. Wang, T. Liu, M. Bullock

9:50 Intermission.

10:00 INOR 1011. Two 4-step mechanisms for nanoparticle nucleation, growth, bimolecular agglomeration, and then autocatalytic agglomeration or secondary autocatalytic growth. P. Kent, R.G. Finke

10:20 INOR 1012. Progress in developing an aerobic hydrocarbon oxidation catalyst. C.C. Scarborough, G.J. Karahalas, C.T. Buru, A. Thangavel

10:40 INOR 1013. Measurement of aqueous hydricities of transition-metal hydrogen evolution catalysts. C. Tsay, B. Livesay, J. Yang

11:00 INOR 1014. Activation of CO, utilizing Lewis acid/base cooperativity from a NiFe bimetallic Robson-type complex. S. Poteet, J. Yang

11:20 INOR 1015. Synthesis, structural studies, and oxidation catalysis of the late first row transition metal complexes of a 2-pyridylmethyl pendant armed ethylene cross-bridged cyclam. T.J. Hubin, D.G. Jones, A.D. Shirofll, G. Yin, T.J. Prior

Section J

Colorado Convention Center
Room 402

Organometallic Chemistry

Synthesis and Characterization

N. S. Radu, *Organizer*

S. Fortier, V. M. Iluc, *Presiding*

8:30 INOR 1016. Metal-ligand interactions: E-H activation and metal-element multiple bonding. V.M. Iluc

8:50 INOR 1017. Synthesis, characterization, and coordination chemistry of a new guanidinate ligand class possessing ketimine backbones. A. Maity, S. Fortier, L. Griego, A.J. Metta-Magana

9:10 INOR 1018. Identification and characterization of an η^2 nitrogen-nitrogen complex between diazoalkanes and lithium dimethylcuprate. J. Morse, M.D. Murphy, S.H. Bertz, C. Ogle

9:30 INOR 1019. U(bpy)₂: A mistaken case of U(O)³⁺. S. Fortier, J. Le Roy, K. Ghiassi, M.M. Olmstead, D. Villagrán, M. Murugesu, A.J. Metta-Magana

9:50 INOR 1020. Structural and chemical study of iron supported by “super bulky” guanidinates. S. Fortier, A. Maity, L. Griego, A.J. Metta-Magana

10:10 INOR 1021. Mechanochemical vs. solution syntheses of group 15 bulky allyl metal complexes. N.R. Rightmire, D.L. Bruns, T.P. Hanusa

10:30 INOR 1022. C–H bond activation by iridium(III) pincer dicarboxylate complexes. A.M. Wright, K.I. Goldberg

10:50 INOR 1023. Synthesis, characterization, and reactivity study of a masked “Ti(II)” complex. R. Aguilar, S. Fortier, A. Metta-Magana

11:10 INOR 1024. Size effect and odd-even alternation in the melting of single and stacked silver alkanethiolate layers: Experiment and phenomenological model. Z. Ye, L. de la Rama, L. Hu, M. Efremov, L. Allen

11:30 INOR 1025. Molecular switches: Exploring the counter-ion problem. J.A. Christie, R. Forrest, S. Corcelli, N.A. Wasio, R. Quardokus, S.A. Kandel, Y. Lu, C.S. Lent, A.G. Oliver, K.W. Henderson

THURSDAY AFTERNOON

Section A

Colorado Convention Center
Room 105

Nanoscience

Semiconductors

Cosponsored by PRES

R. M. Richards, *Organizer*

N. R. Neale, M. Zamkov, *Presiding*

1:30 INOR 1026. Progress towards complete photocatalytic water splitting utilizing hybrid nanoparticles. A.D. LaCroix, J. Macdonald

1:50 INOR 1027. Phase dependent visible to near-infrared photoluminescence of CuInS₂ nanocrystals. A. Leach, J. Macdonald

2:10 INOR 1028. Silicon monoxide: A convenient precursor for near infrared emitting silicon nanocrystals and switching-on quantum size effects. W. Sun, C. Qian, G.A. Ozin

2:30 INOR 1029. Growth of CuInS₂ nanoplatelets by cation exchange and mechanism study. L. Mu, W.E. Buhro

2:50 Intermission.

3:00 INOR 1030. Sub-diffraction imaging of exciton diffusion in semiconductor nanocrystal solids. M. Zamkov, N.N. Kholmicheva, P. Moroz

3:20 INOR 1031. Surface passivation of group 14 nanocrystals. N.R. Neale

3:40 INOR 1032. Cu₂ZnSnS₄/Cu₂Se core/shell nanocrystal thin films: Manipulation of charge carrier transport through surface modification. L. Korala, A.L. Prieto

Section B

Colorado Convention Center
Room 301

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

P. C. Burns, N. E. Travia, *Presiding*

1:30 INOR 1033. Withdrawn.

1:50 INOR 1034. Coordination chemistry of the rare-earths in a tripodal nitroxide ligand framework: New chemistry for magnet recycling. J.A. Bogart, C.A. Lippincott, P.J. Carroll, E.J. Schelter*

2:10 INOR 1035. Interactions of uranium and plutonium with phosphonate-functionalized mesoporous silica. E.C. Urbe, J. Shusterman, A. Bruchet, H. Mason, H. Nitsche

2:30 INOR 1036. Exploring the chemistry of the f-elements with nitrogen-rich ligands. N.E. Travia, K. Browne, J.L. Kiplinger, D.E. Morris, A. Mueller, A. Nelson, A.J. Parkison, B. Scott, B.C. Tappan, J. Veauthier

2:50 Intermission.

3:00 INOR 1037. Synthesis, characterization, and reactivity of U²⁺ in the $[(C_6H_5)_3(SiMe_3)]_2U^{2+}$ anion. C.J. Windorff, J.W. Ziller, W.J. Evans

3:20 INOR 1038. Examining covalency in uranium-ligand multiple bonds through synthesis, spectroscopy, and theory. N.C. Tomson, L. Spencer, R.L. Shook, E.R. Batista, J.M. Boncella

3:40 INOR 1039. Mechanistic insights into the early stages of crystallization of REE-carbonate. J. Rodriguez Blanco, K. Dideriksen, D. Tobler, K. Sand, B. Vallina, L. Benning, S.S. Stipp

4:00 Intermission.

4:10 INOR 1040. Increasing the reactivity of actinide coordination compounds: Imdiazoloni-2-iminato actinide complexes. I. Karmel, N. Fridman, T. Bannenberg, M. Tamm, M. Eisen

Section C

Colorado Convention Center
Room 302

Chemistry of Materials

Metal-Organic Frameworks

C. G. Lugmair, *Organizer*

J. Jiang, J. V. Lockard, *Presiding*

1:30 INOR 1041. Metal-organic frameworks for natural gas storage. J.A. Mason, M.K. Taylor, M.R. Hudson, Z. Hulvey, A. Guagliardi, C.M. Brown, N. Masciocchi, J.R. Long

1:50 INOR 1042. Ultra-stable piezofluorochromic metal-organic frameworks. Q. Zhang, H. Zhou

2:10 INOR 1043. In situ spectroscopy studies of CO₂ adsorption in a dually functionalized microporous metal-organic framework. Y. Chen, H. Wang, J. Li, J.V. Lockard

2:30 INOR 1044. Highly stable meso porous MOFs. D. Feng, K. Wang, T. Liu, J. Park, H. Zhou

2:50 INOR 1045. Mechanistic insights into the gelation of cyanide-bridged coordination polymers. I.C. Fortmeyer, P.A. Højmeier, Y. Yan, I. Pelczar, A.B. Bocsarsly

3:10 INOR 1046. Alternative UiO-66 synthesis for HCl-sensitive nanoparticle encapsulation. K.S. Walton, K. Tulig

3:30 INOR 1047. Prussian red: A carbon monoxide fused cyano bridging mixed valence FeII/III coordination polymer with unprecedented packing pattern and anisotropic negative thermal expansion. W. Lo, O. Ishal, D. Sultan, J. Jiang

3:50 INOR 1048. Photochromic metal-organic frameworks toward control of singlet oxygen generation. J. Park, D. Feng, S. Yuan, H. Zhou

4:10 INOR 1049. Solvothermally grown porphyrin metal-organic framework (MOF) thin films: Post metalation and electrocatalysis. C. Kung, T. Chang, L. Chou, J.T. Hupp, O.K. Farha, K. Ho

4:30 INOR 1050. Novel phosphine coordination materials based on bis(phosphine) and methyl triarylphosphonium groups for applications in gas storage, separations, and sensing. N. Waggoner, A. Bohnsack, L. Cinninger, T. Kornfuehrer, B.J. Holliday, S.M. Humphrey

4:50 INOR 1051. Pressure-induced switching in functional molecular materials. G.J. Halder, K.W. Chapman, A.A. Yakovenko, P.J. Chupas, A.M. dos Santos

Section D

Colorado Convention Center
Room 303

Coordination Chemistry

Characterization and Applications

D. C. Crans, *Organizer, Presiding*

A. C. Bowman, *Presiding*

1:30 INOR 1052. Proton-responsive pincers: Enabling bifunctional Lewis acidic/Bronsted basic late metal complexes. B. Cook, C. Chen, M. Pink, R.L. Lord, K.G. Caulton

1:50 INOR 1053. Synthesis and photocatalytic properties of a boron-centered ionic metal organic framework. X. Zhang, X. Zhang, Y. Chen, J. Zhang

2:10 INOR 1054. Mechanism for ligand exchange processes in metal organic frameworks. J. Byers, C. Tsung, J.V. Morabito, L. Chou, Z. Li, R. Kiyada

2:30 INOR 1055. Highly dynamic coordination chemistry and redox chemistry of aromatic polyphosphorus complexes. M. Fleischmann, M. Scheer

2:50 INOR 1056. [Ru(bpy)₃]²⁺ linked with methyl viologen and phenothiazine substituted aminoethylglycines. B. Biber, M. Williams

3:10 INOR 1057. Utilizing TREN-based copper complexes to calculate activation rate constant values in ideal atom transfer radical addition (ATRA) reactions. K.A. Bussey, K.D. Oshin

MEDI

Division of Medicinal Chemistry

W. B. Young, *Program Chair*

SUNDAY MORNING

Section A

Colorado Convention Center
Mile High Blrm 2A/2B

Applications of Positron Emission Tomography in Drug Discovery

D. Donnelly, C. D. Jesudason, *Organizers, Presiding*

9:00 MEDI 1. Synthesis of radiopharmaceuticals and applications in functional positron emission tomography (PET) imaging. P.J. Scott

9:30 MEDI 2. 18F-T807: A PET imaging compound for detecting tau in Alzheimer's and non-Alzheimer's neurodegenerative diseases. G. Attardo, A.T. Hoyer, H. Xiong, X. Li, C.L. Horchler, K. Fan, N. Lim, F. Gomez, Y. Lin, Q. Liang, K. Conway, H. Kolb, D. Skovronsky, M. Mintun

10:00 MEDI 3. Development of PET radioligands for imaging brain mGlu1 receptors. P.W. Victor

10:30 MEDI 4. Preclinical peripheral enzyme occupancy and PK/PD modelling: A retrospective analysis of sildenafil. C.D. Jesudason, V.N. Barth, T.E. Eessalu, E. Yuen

11:00 MEDI 5. Design, synthesis, and development of fluorine-18 and carbon-11 labeled lysophosphatidic acid receptor 1 (LPA1) PET radioligands for lung receptor occupancy imaging. D. Donnelly, S. Bonacorci, S. Du, A. Pena, J. Kim, W. Hayes, N. Nabulsi, J. Gallezot, Y. Huang, R. Carson

11:30 MEDI 6. ImmunoPET imaging in the development of therapeutic antibodies. J. Mark

Section B

Colorado Convention Center
Mile High Blrm 1A/1B

Targeting the Microbiome

S. M. Firestine, *Organizer, Presiding*

9:00 MEDI 7. Gut reactions: Understanding and manipulating chemistry from the human microbiota. E.P. Balskus

9:35 MEDI 8. Chemical library in food presents the natural ligands for the gastrointestinal microbiome. M.L. Heiman

10:10 MEDI 9. Discovery of small molecule therapeutics based on microbiome-host interaction analysis in inflammatory bowel disease. T.Z. DeSantis

10:45 MEDI 10. Incorporation of therapeutic bacteria into the gut microbiome for treatment of obesity. S.S. Davies

11:20 MEDI 11. Pharmaceutical control of the microbiome. M. Redinbo

Section C

Colorado Convention Center
Mile High Blrm 2C

General Oral Session

W. B. Young, *Organizer*

J. B. Schwarz, *Presiding*

8:30 MEDI 12. γ-AApeptides as a new class of peptidomimetics. H. Wu, Y. Niu, J. Cai

8:50 MEDI 13. Improved inhibitors of inducible nitric oxide synthase (iNOS) through fragment assisted lead generation and optimization. F. Edfeldt

- 9:10 MEDI 14.** SAR enablement of multifunctional BACE templates: Thioamidines. **B.T. O'Neill**, E. Beck, M.A. Brodney, M.W. Bundesmann, C. Butler, L. Buzon, L. Chenard, J. Davoren, J. Dutra, C.J. Helal, K.E. Henegar, J.M. Humphrey, E.A. LaChapelle, B. Li, R. Lira, L.A. Martinez-Alsina, J.C. Murray, K. Ogilvie, L. Price, T.P. Tran, S. Sakya, Y. Zhang, A. Yu
- 9:30 MEDI 15.** Development of novel NLRP3 inflammasome inhibitors and their potential application. **S. Zhang**, J. Chojnacki, C. Marchetti, S. Toldo, A. Abbate
- 9:50 MEDI 16.** Methionine aminopeptidases (MetAPs) as promising targets toward discovery of novel anti-infective agents. P. Wangtrakuldee, **C. Chen**, B. Staker, J.M. Wilk, J.R. Horn, T.J. Hagen
- 10:10 MEDI 17.** Development of pyridopyrimidine-based inhibitors of HIV-1 reverse transcriptase. **C. Labbay**, J. Mancuso, Y. Lin, N. Bennett, M. Menni, M. Gotte, Y.S. Tsantrizos
- 10:30 MEDI 18.** Open source malaria: A new approach to drug discovery. **A.E. Williamson**, M.H. Todd, P. Willis, O. Consortium
- 10:50 MEDI 19.** Development of non-incorporating small molecule inhibitors of antibody fucosylation. **M.J. Frohn**, J.G. Allen, C.H. Fotsch, M. Mujacic, T. San Miguel, O.R. Thiel, J. McCarter, A.J. Pickrell, M. Lo, J.B. Jordan
- 11:10 MEDI 20.** Discovery and opioid receptor SAR of AT-076, the first small-molecule opioid pan antagonist with nanomolar affinity at mu, delta, kappa and nociceptin opioid receptors. **V.B. Journigan**, N.T. Zaveri, W.E. Polgar
- 11:30 MEDI 21.** Discovery of oral FSHR (follicle stimulating hormone receptor) allosteric modulators. **H.N. Yu**
- 11:50 MEDI 22.** Small molecule activators of Pro-apoptotic BAX for cancer therapy. **E. Gavathiotis**

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

SUNDAY AFTERNOON

- Section A**
 Colorado Convention Center
 Mile High Blrm 1A/1B
General Oral Session
 W. B. Young, *Organizer, Presiding*
- 1:30 MEDI 23.** Discovery of TAK-063, a novel phosphodiesterase 10A (PDE10A) inhibitor. **M. Fushimi**, J. Kunitomo, M. Yoshikawa, A. Kawada, J.F. Quinn, H. Oki, H. Kokubo, M. Kondo, K. Nakashima, T. Taniguchi
- 1:55 MEDI 24.** Discovery of a novel and potent dual orexin 1/orexin 2 receptor antagonist, E2006, for the treatment of sleep disorders. **T. Terauchi**
- 2:20 MEDI 25.** Discovery of the clinical candidate BMS-816336, an adamantyl acetamide based 11 β -hydroxysteroid dehydrogenase type-1 (11 β -HSD1) inhibitor. **X. Ye**, S. Chen, S. Wu, D.S. Yoon, H. Wang, Z. Hong, S.P. Oconnor, J. Li, J. Li, S. Walker, L.J. Kennedy, A. Apedo, A. Nayeem, S. Sheriff, P. Morin, D. Carnac, T. Harrity, R. Zebo, J. Taylor, N. Morgan, R. Ponticello, R. Golla, R. Seethala, M. Wang, T. Harper, B. Sloczka, B. He, M. Kirby, J. DiMarco, R. Scaringe, R.L. Hanson, Z. Guo, J. Li, J. Sun, M.K. Wong, B. Chen, L. Haque, D.K. Leahy, C. Chan, Y. Li, T. Zvyaga, L. Hansen, C. Patel, D.A. Gordon, J.A. Robl
- 2:45 MEDI 26.** Discovery, optimization, and human microdosing study of a novel series of H3 antagonists. **M. Chytil**, S. Engel, K. Fang, K. Spear
- 3:10 MEDI 27.** Cholesteryl ester transfer protein inhibitor BMS-795311. **J.X. Qiao**, T.C. Wang, A. Chen, D.S. Taylor, R.Z. Yang, P.G. Steph, J.P. Li, D. Li, M. Chang, X. Chen, C. Xu, J. Li, D. Smith, D. Wu, L. Leith, L.S. Hanikrishnan, M. Kamau, R. Rampulla, M.M. Miller, D. Bilder, R. Lawrence, M.A. Poss, P. Levesque, C.S. Huang, L.P. Adam, R.R. Wexler, H.J. Finlay, M.S. Salvati

- 3:35 MEDI 28.** Discovery of potent and kinase-selective p21-activated kinase 1 (PAK1) inhibitors. **J. Rudolph**, I. Aliagas, E. Blackwood, T. O'Brien, J. Crawford, J. Drobnick, L. Gazzard, C. Heise, W. Lee, L. Murray, C. Ndubaku, W. Wang, X. Zhao, K.P. Hoeflich
- 4:00 MEDI 29.** Liver targeted HIF-PHD inhibitors for the treatment of anemia. **C. Sinz**, Y. Chen, V.J. Colandrea, Q. Dang, B. DuBois, P. Liu, P.T. Meinke, R. Liu, J. Tan, F. Ujjainwalla, L. Wang, J.J. Hale, J. Cai, D. Stickens, B. Bishwokama, M. Zielstorff, D. Zaller, C. Chiu, M. Cheng, C. Alpert, J. Metzger, L. Yang, S. Vincent, K. Bleasby, M. Hatley, R. Houle
- 4:25 MEDI 30.** Discovery of BMS-852927, a potent LXR partial agonist possessing LXRbeta functional selectivity. **E.K. Kick**, B. Busch, R. Martin, Y. Xie, M. Nanao, T. Stout, A. Plonowski, I. Schulman, G. Yan, W. Stevens, M. Nyman, L. Nguyen, R. Narayanan, K. Behnia, G. Cantor, J. Lupisella, P. Slep, D. Grimm, J. Ostrowski, T. Kirchgessner, R.R. Wexler, R. Rohan
- 4:50 MEDI 31.** Building ERK inhibitors. Mitigating their clearance. **J.T. Bagdanoff**, D. Poon, W. Han, S. Zhu, R. Jain, M. Lindvall

- Section B**
 Colorado Convention Center
 Mile High Blrm 2A/2B
Biased Agonism: An Emerging Paradigm in GPCR Drug Discovery
 J. Herr, Z. Rankovic, *Organizers, Presiding*
- 1:30 MEDI 32.** Harnessing ligand-directed signaling to improve pain therapeutics. **L.M. Bohn**, C.L. Schmid, K. Lovell, N.C. Ross, T.D. Bannister
- 2:10 MEDI 33.** Engineering enhanced, receptor-specific, and signaling-biased arrestins. **V. Gurevich**
- 2:50 MEDI 34.** Discovery of TRV130, a G protein biased agonist of the μ -opioid receptor, for the treatment of acute severe pain. **A.L. Crombie**, X. Chen, P.M. Pittis, G. Liu, C. Yuan, D. Gotchev, D.S. Yamashita, J.D. Violin
- 3:30 MEDI 35.** Discovery of functionally selective ligands of fopamine D_2 receptors. **K. Butler**, J. McCornay, X. Chen, M. Caron, W. Wetsel, B.L. Roth, J. Jin
- 4:00 MEDI 36.** Novel GPR40 agonists for the treatment of type-2 diabetes: The effect of b-arrestin signaling. **C. Hamdouchi**
- 4:30 MEDI 37.** Biased signaling with allosteric modulators of GPCRs. **C.W. Lindsley**
- 5:00** Concluding Remarks.

- Section C**
 Colorado Convention Center
 Mile High Blrm 2C
Young Investigator in Medicinal Chemistry
 Cosponsored by YCC
 T. E. Prisinzano, *Organizer, Presiding*
- 2:00 MEDI 38.** First structural disclosure, discovery, preclinical characterization, and FTIH pharmacokinetics for GSK2878175, a second generation boron-based inhibitor of the HCV RNA-dependent RNA polymerase. **J. Shotwell**
- 2:30 MEDI 39.** Hedgehog pathway modulators as therapeutic agents. **M.K. Hadden**
- 3:00 MEDI 40.** Discovery of halogenated phenazine and halogenated quinoline small molecules with antibacterial and antibiofilm activities against *staphylococcal* biofilms. **R. Huigens**
- 3:30 MEDI 41.** Novel small molecule immunomodulators that target toll-like receptors. **H.H. Yin**
- 4:00 MEDI 42.** Discovery and adverse safety findings of two new mGluR5 NAM chemotypes. **A.F. Stepan**
- 4:30 MEDI 43.** Efficient small molecule inhibitors of the HDM2-p53 protein-protein interaction. **M.R. Machacek**

Drug Discovery
Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

SUNDAY EVENING

- Section A**
 Colorado Convention Center
 Hall C
General Poster Session
 W. B. Young, *Organizer*
- 7:00 - 9:00**
- MEDI 44.** Design, synthesis, and biological evaluation of novel tubulysin analogs as payloads for antibody-drug conjugates for the targeted treatment of cancer. **Y. Huang**, H. Xie, J. Jia, H. Guo, S. Gai, X. Li, L. Qu, X. Zuo, X. Zhou, S. Sun, Q. Yang, W. Li, C. Lin, H. Ye, R.Y. Zhao
- MEDI 45.** Withdrawn.
- MEDI 46.** New flash purification capabilities decrease run times up to 67%. **J.R. Bickler**
- MEDI 47.** New high-performance C18 flash cartridge significantly improves resolution and fraction purity. **J.R. Bickler**
- MEDI 48.** Rapid cleanup of peptides with mass-directed flash chromatography and spherical C18 silica. **W.J. Hartsack**, J.R. Bickler, V. Vandell, F.A. Kero
- MEDI 49.** Purification of peptides by flash chromatography. **J.E. Silver**, R. Lewis
- MEDI 50.** Design, synthesis, and biological evaluation of *Rickettsia prowazekii* methionine aminopeptidase (MetAP) inhibitors. **T.R. Helgren**, C. Chen, P. Wangtrakuldee, C. Long, M. Hathuc, R. Small, B. Curran, J.R. Horn, T.J. Hagen
- MEDI 51.** Mutual solubilities of the antibiotic/ β -lactamase inhibitor drug combinations vancomycin, piperacillin, and tazobactam in aqueous solution. **H.S. Gray**, H.N. Gray, S.C. Butler, R.N. Mason
- MEDI 52.** Molecular mechanism and ligand design of a PLP/GABA-dependent bacterial transcription regulator GabR. **E. Cybulla**, R. Wu, C. Reid, D. Gawron, D.P. Becker, D. Liu
- MEDI 53.** Synthesis, conformational analysis, and pharmacokinetics of fluorinated antitubercular nucleosides. **S. Dawadi**, K. Viswanathan, H. Boshoff, C.E. Barry, C.C. Aldrich
- MEDI 54.** Protein structure-based virtual screening led to identification of novel natural product-derived hits as cannabinoid receptor 1 modulators. **P. Pandey**, K.K. Roy, R.J. Doerksen
- MEDI 55.** Building on the success of the first generation of N-alkylthiol beta-lactams yields a multimodal, multiaction prodrg therapy for MRSa. **J.L. Borja**
- MEDI 56.** Investigating the conformational states and ligand binding of voltage gated sodium channels by multiple spectroscopic techniques. **M. Colledge**, B. Wallace
- MEDI 57.** Incorporation of triazoles as disulfide mimics in chimeric AGRP-melanocortin peptide template. **S.R. Tala**, A. Singh, C. Haskell-Luevano
- MEDI 58.** Drug discovery and large-scale synthesis for 7-azaindoline derivatives as potent, orally available, selective M1 and M4 muscarinic acetylcholine receptors agonists. **Y. Urano**, Y. Inoue, Y. Konishi, A. Suwa, K. Takai, K. Hashimoto, H. Matsuda, T. Nakako, M. Sakai, G. Hashimoto, T. Enomoto, A. Kitamura, Y. Uematsu, A. Kiyoshi, T. Sumiyoshi
- MEDI 59.** Design, synthesis, and structure-activity relationships of flupirtine derivatives for the treatment of neuronal ceroid lipofuscinosis. **N. Kinarivala**, J. Makoukji, F. Saadeh, R. Boustany, P.C. Trippier
- MEDI 60.** Exploiting the Sigma-2 receptor as a therapeutic target for cancer and various CNS diseases. **J. Chan**, J. Sahn, S.F. Martin, L. Scott, J. Pierce-Shimomura

- MEDI 61.** Optimization of synthetically novel agonists of the putative cannabinoid receptor, GPR55, using an activated state model. **M.A. Lingerfelt**, L. Alifakhori, D.P. Hurst, P. Zhao, M.P. Croatt, M.E. Abood, P.H. Reggio
- MEDI 62.** Rational fesign of dual-site scetylcholinesterase inhibitors: Multifunctional lead for Alzheimer's disease therapy. **W. Yang**, S. Yang, G. Yang
- MEDI 63.** Discovery of novel, potent γ -secretase inhibitors. **Z. Zhao**
- MEDI 64.** Novel amyloid binding compounds: A search for PET imaging probes for neurofibrillary tangles. **B. Hurtle**, L. Cai, B. Qu, V.W. Pike
- MEDI 65.** Crystallographic evaluation of chelidamic acid congeners. **A.L. Green**, K.M. Lincoln, R.E. Saunders, K.N. Green
- MEDI 66.** Rational design and bioevaluation of novel acetylcholinesterase inhibitors for treating Alzheimer's disease. **Q. Sun**, G. Yang, . Yang
- MEDI 67.** Structural insights into the mechanism of activation of the human cannabinoid type 2 (CB₂) receptor: Molecular dynamics study of an agonist-bound state. **K.K. Roy**, P. Pandey, R.J. Doerksen
- MEDI 68.** Discovery, SAR, and biological evaluation of a novel series of piperazine-based inhibitors of glycine transporter-1 (GlyT-1). **C.L. Cioffi**, S. Liu, M.A. Wolf, P.R. Guzzo, K. Sadalapure, V. Parthasarathy, J. Maeng, E. Carulli, D.T. Loong, X. Fang, P. Gupta, S. Panduga, K.N. Kaesh, L. Matta, S. Choo, R.N. Buckle, R. Davis, S.A. Sakwa, M. Hu, D.H. Dethe, B. J. Sargent, N.A. Moore, M.M. Luche, Y.L. Khmelintsky, J. Ismail, H. Decornez, D.B. Kitchen, P.L. Love, M.A. Watson, J. Adolphson, G. Padilla, K. Waikins, S. Tom, A. Ngo, M. Chung, M. Bai, N. Johal, S. Swaminathan, A.J. Mhyre
- MEDI 69.** Arylguanidine NAMs for α 7 nAChRs: Where do they bind and why? **O.I. Alwassil**, S. Khatri, M.K. Schulte, M. Dukat
- MEDI 70.** Structure activity relationship of tetrahydroisoquinoline N-methyl-D-aspartate receptor positive allosteric modulators can be modified to target GluN2B-containing receptors. **K.L. Strong**, D.S. Menaldino, K.K. Ogden, S.F. Traynelis, D.C. Liotta
- MEDI 71.** CPM: A potential moiety to reduce opioid dependence. **Z. Wu**, V.J. Hruby
- MEDI 72.** Curcumin/melatonin hybrids as neuroprotective agents for Alzheimer's disease. **J. Saathoff**, K. Liu, J. Chojnacki, S. Zhang
- MEDI 73.** Application of machine learning and regression techniques in developing novel homologous recombination inhibitors. **J. Zhu**
- MEDI 74.** Simple and integrated approach to compound progress and work-request tracking. **J.W. Sager**, T.E. Mansley, P. Mountney, C.P. Snyder
- MEDI 75.** In silico modeling workflows in support of exploratory computational toxicology. **M.R. Goldsmith**, D. Chang, A. Deschenes, C. Williams, A. Ajamian
- MEDI 76.** Importance of visualization in lead discovery: Supporting the medicinal chemist in designing compounds more efficiently. **C. Detering**
- MEDI 77.** Cheminformatics analysis of natural products databases: Toward the identification of tubulin polymerization inhibitors. **R. Aguayo-Ortiz**, R. Castillo-Bocanegra, A.M. Hernandez Campos, J.L. Medina-Franco
- MEDI 78.** Discovery and synthesis of triphenylethanamine derivatives as highly potent cholesteryl ester transfer protein Inhibitors. **T. Wang**, J.X. Qiao, A. Chen, D.S. Taylor, R.Z. Yang, P.G. Steph, J.P. Li, D. Li, M. Chang, X. Chen, C. Xu, J. Li, P. Levesque, C.S. Huang, L.P. Adam, M.S. Salvati, H.J. Finlay, R.R. Wexler
- MEDI 79.** Identification of a novel class of covalent modifiers of hemoglobin as potential antisickling agents. **A.M. Omar**, M.A. Mahran, M. Ghatge, N. Chowdhury, F.H. Bamine, M.E. El-Araby, O. Abdulmalik, M. Sato

MEDI 80. Process of blood coagulation investigated through the interactions of aspirin with bovine red blood cell lipid extract membrane monolayers. **K.A. Miller,** A. Sostarecz

MEDI 81. Novel coumarin based monocarboxylate transport 1 & 4 inhibitors as anticancer agents. **L. Solano, C. Ronayne, G.L. Nelson, S. Gurrappu, S.K. Jonnalagadda, V. Mereddy**

MEDI 82. Potent dual monocarboxylate transporter 1 & 4 inhibitors for triple negative breast cancer treatment. **L. Solano, G.L. Nelson, C. Ronayne, V. Mereddy, S.K. Jonnalagadda, S. Gurrappu**

MEDI 83. Development of collagen films coated with synthetic photoreactive peptides that support cardiovascular repair and regeneration. **J. Malcor, D. Bax, D. Bihan, S. Hamala, R. Farnedale**

MEDI 84. Withdrawn.

MEDI 85. Total synthesis of clavadinone A analogs to produce a viable reverse inhibitor for factor XIa. **C.E. Malmberg, S. Chamberland**

MEDI 86. Discovery of novel, potent, and highly selective factor xla inhibitors from HTS hit with X-ray crystallography-based rational design. **T. Nishiyama, T. Kondo, K. Hisaichi, K. Ochi, A. Kinoshita, R. Miwa, A. Imagawa, S. Flanagan, C.J. Yarnold, S. Courtney, M. Gohda, K. Suzuki, T. Ono, S. Koyama, T. Hagio, M. Sakai, H. Habashita, K. Kawabata**

MEDI 87. Structure-based design, synthesis, and evaluation of novel peptide inhibitors of thrombin-induced activation of platelets aggregation. **C.C. Clement, J. Gonzalez, A. Babinska, M. Philipp**

MEDI 88. Picomolar K_{i} ligands can be obtained by increasing the binding rate instead of decreasing the dissociation rate: Surprising structure-kinetic relationship among very similar thrombin inhibitors. **M.T. Khayat, A.S. Murkin, M.M. Murphy, T.e. Ryan, B. Sathyamoorthy**

MEDI 89. Synthesis of resorfin derivatives as inhibitor indicators of cytochrome P450 enzymes. **L. Lovings, J. Liu, M. Foroozesh**

MEDI 90. Radical-induced oxidation of tobacco-specific nitrosamines under physiological conditions. **B.R. Daws, S.P. Mezky, J.J. Kiddle**

MEDI 91. Pyrano- and furanochromones as specific inhibitors of human cytochrome P450 1A2. **J. Liu, P. Pham, L. Lovings, N. Goyal, M. Foroozesh**

MEDI 92. Investigation of regulation of cytochrome P450 2J2 in adult human primary cardiomyocytes. **R. Rowlands, E. Evangelista, B. Raccor, R. Totah**

MEDI 93. Metabolic stability assessment of tumor-targeted drug delivery systems with fluorine-labeled taxoid probes by ¹⁹F NMR. **B. Lichtenhal, J.D. Seitz, J.G. Vineberg, L. Wei, C. Lin, J. Kahn, I. Ojima**

MEDI 94. Drug release by remotely controlled magnetic anisotropy. **M. Shin, B. Kang, S. Han, E. Jang, J. Suh, Y. Huh, S. Haam**

MEDI 95. Modular platform for the synthesis of a targeting and pH-responsive lipopeptide ligand in nanovectors. **M. Salinas, G.R. Negrete**

MEDI 96. Fibrosis toolbox: Small molecules to investigate fibrosis pathways and mechanisms. **R. Hatley**

MEDI 97. Novel Nrf2 activators from microbial transformation products suppress oxidant stress-induced cellular damage in ARPE-19 cells. **Y. Nakagami, K. Masuda, E. Hatano, T. Inoue, S. Komoriya**

MEDI 98. Discovery of potent and selective S1P2 antagonists. **K. Kusumi, A. Naganawa, H. Kurata, K. Shinozaki**

MEDI 99. Monster Mx agonist: Revealing the beauty in the beast. **J. Redmond, S. Peace, G. Inglis, G. Vitulli, J. Barrett**

MEDI 100. Quaternary-ammonium salt derivatives as bifunctional muscarinic antagonist and beta2 agonist (MABA) for the treatment of COPD and asthma. **J. Igarashi, E. Mitsuyama, T. Ida, H. Sugiyama, K. Segawa, J. Nomura**

MEDI 101. Novel strategy for the treatment of asthma by targeting GABA_A receptors in the lung. **R. Jahan, M.R. Stephen, G. Gallos, C.W. Emala, J.M. Cook**

MEDI 102. Design and synthesis of anti-inflammatory steroids with improved therapeutic index: Discovery of an inhaled dissociated steroid (selective glucocorticoid receptor modulator). **P.J. Biju**

MEDI 103. Achieving desired levels of selectivity for a series of "acyclic-based" JAK inhibitors. **J. Kempson, S.H. Spergel, S. Wrobleski, J. Das, L.M. Doweiko, J. Guo, J. Hynes, J. Duan, B. Jiang, Z. Lu, R.V. Moquin, S. Lin, H. Wu, B.V. Yang, S.M. Stachura, J.S. Tokarski, A. Gupta, J.C. Barrish, P.H. Carter, G.L. Schieven, W.J. Pitts**

MEDI 104. Determinants of activity at human toll-like receptors 7 and 8: Quantitative structure-activity relationship (QSAR) of diverse heterocyclic scaffolds. **E. Yoo, D.B. Salunke, D. Sil, X. Guo, A.C. Salyer, A.R. Hermanson, M. Kumar, S.S. Malladi, R. Balakrishnan, W.H. Thompson, H. Tanji, U. Ohto, T. Shimizu, S.A. David**

MEDI 105. Enhancement of potency of the TLR7 ligand by conjugation to polysaccharide. **H. Shinchi, T. Hayashi, M. Chan, A. Ahmadiyeli, S. Zhang, B. Crain, Y. Suda, H.B. Cottam, D. Carson**

MEDI 106. Design and synthesis of a dual-targeting liposomal spherical nucleic acid. **J. Ferrer, N. Chernyakh, J. Wertheim, C.A. Mirkin**

MEDI 107. Human toll-like receptor 8-selective agonistic activities in 1-alkyl-1H-benzimidazol-2-amine. **M. Beesu, S.S. Malladi, L.M. Fox, C.D. Jones, A. Dixit, S.A. David**

MEDI 108. Design, synthesis, and testing of macrocyclic β -strand as protease inhibitors. **A.D. Pehera, M. Pietsch, N.M. Paul, D.F. Callen, M. Gütschow, A.D. Abell**

MEDI 109. Single cell imaging and analysis for macrophage uptake of nanoparticles using fluorescent organosilica nanoparticles. **M. Nakano, M. Nakamura, K. Hayashi, T. Kanadani, K. Miyamoto**

MEDI 110. Mitochondria targeted cardiolipin based high density lipoprotein mimicking nanoparticles for atherosclerosis. **R. Wen, S. Dhar**

MEDI 111. Investigation on cellular uptake of functionalized gold nanoparticles and their biological effects. **N. Ma, C. Ma, X. Mou, N. He**

MEDI 112. Molecular beacon-functionalized gold nanoparticle as miRNA detecting probe for cellular classification in gastric cancer. **K. Jisun**

MEDI 113. Wire-framed gold nanoparticles for a multistep photothermal driven drug release system. **T. Lee, D. Bang, J. Suh, Y. Huh, S. Haam**

MEDI 114. Virus-mimicking antimicrobial polymer brushes: The nanostructure and activity. **Y. Jiang, W. Zheng, H. Liang**

MEDI 115. Targeting mitochondrial genome by cisplatin prodrug and its nanoparticle formulation to overcome chemoresistance. **R. Pathak, S. Marrache, S. Dhar**

MEDI 116. Syntheses, characterization, and biomedical applications of novel organosilica nanoparticles. **M. Nakamura**

MEDI 117. Activatable two-component photosensitizer: selective targeting and killing of cancer cells. **J. He, Y. Wang, M.P. Bruchez**

MEDI 118. Withdrawn.

MEDI 119. Silybin derivatives as antiprostata cancer agents: Synthesis and antiproliferative activity. **B. Vue, S. Zhang, X. Zhang, K. Parisis, Q. Chen**

MEDI 120. Fluorescein hydrazones as novel nonintercalative topoisomerase catalytic inhibitors with low DNA toxicity. **A.M. Rahman, S. Park, Y. Kwon, A.A. Kadi**

MEDI 121. Design and synthesis of a novel tri-branched asymmetric bowtie PAMAM dendrimer-based drug conjugate as a cancer theranostic agent. **L. Wei, T. Wang, Y.G. Teng, I. Ojima**

MEDI 122. Synthesis and antitumor activity of *N,N'*-bisnaphthylated imidazole salts with lipophilic or hydrophilic substituents on the imidazole and benzimidazole rings. **K.L. Shelton, P.O. Wagers, M.R. Southerland, M.A. DeBord, M.J. Panzner, N.K. Robishaw, C.A. Tessier, W.J. Youngs**

MEDI 123. Disrupting reactive oxygen species mediated pathways in human cancer models with ferrocenylated *N*-heterocyclic carbenes. **J.F. Arambula, K. Arumugam, D.J. Magda, C. Bielawski, J.L. Sessler**

MEDI 124. Targeting the hypoxia-adenosinerig pathway via A_{2A} antagonists; Toward cancer immunotherapeutics. **G. Yuan, S. Hatfield, M. Sitkovsky, M.J. Ondrechen, G. Jones**

MEDI 125. Triterpenoid derivatives and their biological activities. **M. Urban, J. Sarek, M. Hajdúch, J. Rehulka, P. Dzubak, L. Borkova**

MEDI 126. Development of a novel class of hydroxylated 2, 4-diphenyl indenopyridines as a selective non-intercalative topoisomerase II α catalytic inhibitor. **T.M. Kadayat, T. Thapa Magar, G. Bist, A. Shrestha, Y. Kwon, E. Lee**

MEDI 127. Preliminary structure-activity relationship studies of a fungal metabolite ophiobolin A – promising antiangioblastoma agent. **R. Dasari, V. Mathieu, R. Kiss, A. Evidente, A.V. Kornierko**

MEDI 128. Identification of the first selective small molecule GRPR (BB2) antagonists. **N.D. Harriott, S.B. Ravula, G. Beaton, N.J. Ashweek, J.P. Williams, S.R. Hoare, J. Fan**

MEDI 129. Withdrawn.

MEDI 130. Bishomiosoprenoid triazoles as inhibitors of geranylgeranyl diphosphate synthase. **V.S. Wills, J.I. Metzger, C. Allen, S.A. Holstein, D.F. Wiemer**

MEDI 131. Synthesis and structure-activity studies of drugs that affect a cancer causing mechanism and reduce cell growth. **A. Jelowicki, K.E. Tan, E.H. Li, C. Wen, C.M. Ott, N.V. Patel, P. De Lijser, C.A. Martindale**

MEDI 132. Click chemistry approach to diversification of novel base-modified thymidine analogs that exhibit anticancer activity. **P.R. Wolfkiel, K.M. Borland, E.J. Merino, M.C. Tranter, V.A. Litosh**

MEDI 133. Two-faced, biphenyl-based synthetic α -helix mimetics are effective inhibitors of the Mcl-1 oncoprotein. **M. Lanning, P. Wilder, S. Fletcher**

MEDI 135. Structure-based design of functionalized salicylates as potent Mcl-1 inhibitors. **L. Chen, J. Chauhan, J.L. Yap, P.T. Wilder, S. Fletcher**

MEDI 136. Design and synthesis of coumerin-aminoethylphenol hybrids as potential epigenetic modulators. **M. Branscum, T. Rowe, J. Brider, M.A. Alam**

MEDI 137. Design and chemoproteomic functional characterization of a chemical probe targeted to bromodomains of BET family proteins. **B.A. Lefker, K.F. Geoghegan, S.W. Wright, D.C. Limburg, J. Shin, C.M. Williams, P. Sahasrabudhe, P. Bonin, S. Ramsey**

MEDI 138. Identification and characterization of cellular histone deacetylase active site alterations Induced by deacetylase complex components. **T. Hanigan, I. Kastrati, J. Frasor, P.A. Petukhov**

MEDI 139. Comparison of local and tropical plants used as herbal remedies and their chemical make-up. **M.D. Mann**

MEDI 140. Transformations of allicin from garlic: The discovery of allylselenoalkylsulfonopyridazines and Its antitumor activity. **M. Park, C. Kim, D. Shin, M. Choi**

MEDI 141. Docking studies to develop GLL-associated oncogene inhibitors from natural products. **Y. Rifai**

MEDI 142. Discovery of novel hit molecules for Sphingosine kinase -1 inhibitory activity by structure based virtual screening. **C. Selvam, B.C. Jordan, S. Doshi**

MEDI 143. Novel method for targeting sphingosine kinase 2: Design, synthesis, and evaluation of bisubstrate inhibitors. **T.K. Dawson, R. Dyer, Y. Kharel, K. Lynch, T.L. Macdonald**

MEDI 144. Serotonin-linked NSAIDs as inhibitors of FAAH, TRPV1, and COX 2. **T.M. Rose, C.A. Reilly, C.E. Deering-Rice, C. Brewster, C. Brewster**

MEDI 145. Discovery of second generation P2X3 receptor antagonists for the treatment of chronic pain. **A. Ginnetti, D. Paone, S. Stauffer, C. Potteiger, A. Shaw, J.Z. Deng, D.N. Nguyen, C. Segerdell, C.S. Burgey, S. Graham, J. Anquandah, A. Calamaro, G. Cheng, S. Cook, S. Kane, M. Leiti, A. Liang, E. Moore, J. Panigel, C. Salvatore, M. Urban, J. Wang, K. Fillgrove, C. Tang**

MEDI 146. Design, synthesis, and in vitro evaluation of novel inhibitors of fatty acid amide hydrolase (FAAH). **S. Cramer, J. Johnson, A. El-Ally, J. Stec**

MEDI 147. Targeted far-red light activatable prodrugs: folate receptor-targeting, optical imaging, and a combination of photodynamic therapy and site-specific chemotherapy. **G.N. Nkekapang, M. Bio, P. Rajaputra, S.G. Awuah, Y. You**

MEDI 148. Synthesis of tripartite prodrugs via N \rightarrow C amidative-installation of the Katzenellenbogen-spacer: Application of the traceless Staudinger ligation. **T. Kirby, B.L. Barthel, T.H. Koch**

MEDI 149. Exploring CatSper channel openers and binding site interactions: Discovery of steroidal channel blockers. **E. Carlson, J. Hawkinson, G.I. Georg**

MEDI 150. Enzyme sensitive conjugates as a macromolecular delivery platform for siRNA. **J.C. Carlson, J. Benson, A. Sokoloff, D. Rozema, A.V. Blokhin**

MEDI 151. Development of a catalytic Mitsunobu reaction. **J.A. Buonomo, C.C. Aldrich**

MEDI 152. Flow hydrogenation: A tool for creating 3D shaped molecules from flat precursors. **L. Kocsis, S. Fekete, J. Gerencsér, G. Makara, F. Darvas**

MEDI 153. Discovery of potent α_{2A} -adrenoceptor agonists: Design and synthesis of bicyclic derivatives. **S. Suzuki**

MEDI 154. Density functional calculations of the structural, thermodynamic, and spectroscopic properties of tautomers of avigan. **F.L. Nesbitt**

MEDI 155. Novel 3-nitrotriazole-based amides and carbinals as bifunctional anti-chagasic agents. **M.V. Papadopoulou-Rosenzweig, W.D. Bloomer, G.I. Lepesheva, H.S. Rosenzweig, M. Kaiser, E. Chatelain, J. Ioset**

MEDI 156. Syntheses and binding studies of novel benzimidazole compounds targeting the hepatitis C virus internal ribosome entry site. **A. Karner, A. Cholewczynski, D. Schmit, U. Milewicz, R. Wolkowicz, M.A. Boerneke, T. Hermann, M.B. Bergdahl**

MEDI 157. Discovery of MK-8325: A silyl proline containing HCV NS5A inhibitor with pan-genotype activity. **A.G. Nair, Q. Zeng, S.B. Rosenblum, O. Selyutin, Y. Jiang, D. Yang, K. Keertikar, G. Zhou, M.P. Dwyer, S. Kim, S. Bandarpalle, W. Yu, L. Tong, R. Mazzola, J.P. Caldwell, H. Tang, R. Liu, E. Asante-Appiah, S. Agrawal, E. Xia, S. Curry, P. Ingravallo, J.A. Kozlowski**

MEDI 158. Discovery of silyl proline containing HCV NS5A inhibitors: SAR development. **J.A. Kozlowski, N. Anilkumar, O. Selyutin, S.B. Rosenblum, Y. Jiang, D. Yang, K. Keertikar, G. Zhou, M.P. Dwyer, S. Kim, B. Shankar, W. Yu, L. Tong, R. Mazzola, J.P. Caldwell, H. Tang, S. Agrawal, E. Asante-Appiah, S. Curry, P. McMonagle, S. Black, A. Nomeir**

MEDI 159. Design and synthesis of dual-tropic HIV entry inhibitors that utilize a homologous CCR5/ CXCR4 binding site. **S. Gupta, A.R. Prosser, B.D. Cox, L.J. Wilson, D. Liotta**

- MEDI 160.** Synthesis and biological evaluation of substituted pyrimidines. **B.S. Clark**, J. Kudrynsch, S.Q. Smith, V.E. Zottig
- MEDI 161.** Star-branched polymers with antioxidant activities. **U.G. Huynh**, C.Y. Lee, A. Sharma

MONDAY MORNING

Section A

Colorado Convention Center
Mile High Blrm 2A/2B

Innate Potential: Advances in Non-Biologic Modulation of Innate Immune Targets

A. J. Dyckman, J. Hynes, D. S. Weinstein, *Organizers, Presiding*

9:00 Introductory Remarks.

- 9:05 MEDI 162.** Structure-based design of small molecule modulators of TLR8. **S.A. David**
- 9:45 MEDI 163.** Development of novel IRAK4 inhibitors for the treatment of inflammation related disorders. **W.M. Seganish**, W.T. McElroy, S. Brumfield, G. Li, D. Tulshian, J. Tata, R. Herr, B.J. Lavey
- 10:15 MEDI 164.** Identification of highly potent and mono-selective RIP1 kinase inhibitors for the treatment of TNF-dependent diseases. **PA. Harris**
- 10:45 MEDI 165.** Designing RIP2 kinase inhibitors for innate immunity-driven indications. **L. Casillas**

- 11:15 MEDI 166.** Identification of selective TYK2 inhibitors and their role in IL12- and IL23-pathway signaling. **S. Magnuson**, J. Liang, V. Tsui, Y. Lai, B. Zhang, K. Williams, C. MacLeod, Y. Wenqian, S. Sohn, J. DeVoss, I. Peng, J. Lesch, M. Balazs, A. Van Abbema, K. Barrett, P. Bir Kohli, W. Blair, C. Chang, A. Johnson, L. Berezkhovskiy, J. Driscoll, P. Fan, A.N. Sambrope, P. Chiang, C. Eigenbrot, S. Shia, M. Ulsch, N. Ghilardi, L. Wu

- 11:45 MEDI 167.** Oligonucleotide inhibitors of endosomal toll-like receptors: Novel approach to treatment of autoimmune diseases. **S. Agrawal**

Section B

Colorado Convention Center
Mile High Blrm 1A/1B

Recent Advances in Targeting the Nav1.7 Sodium Channels

M. Chu-Moyer, *Organizer*
E. H. Harrington, *Organizer, Presiding*

- 9:00 MEDI 168.** Recent advances in therapeutic targeting of NaV channels. **D.C. Pryde**, B. Marron, N. Swain, C.W. West
- 9:30 MEDI 169.** Imaging pain generators in vivo using radiolabeled sodium channel toxin derivatives. **D. Behera**, A. Hoehne, W.H. Parsons, B. Shen, D.C. Yeomans, S. Biswal, F.T. Chin, J. Du Bois
- 10:00 MEDI 170.** Potent and selective Nav1.7 inhibitory peptides from tarantula venom. **K. Biswas**, J.K. Murray, B. Wu, J. Long, K. Sham, A. Zou, D. Liu, J.A. Ligutti, L. Poppe, J.B. Jordan, K.L. Andrews, S. McDonough, L.P. Miranda, B.D. Moyer

- 10:30 MEDI 171.** Identification of GNE-131: A potent and selective hNa_v1.7 inhibitor for the treatment of pain. **B.S. Safina**, G. Bankar, P. Bichler, C. Chabot, E. Chang, J. Chang, C. Chen, S. Chowdhury, C.J. Cohen, S. Decker, C.M. Dahnhardt, T. Fockan, M.E. Grimwood, D. Hackos, I. Hemeon, K. Khakh, C. Koth, R. Kwan, S. Lin, K. Nelkenbrecher, D.F. Ortwine, J. Pang, J. Payandeh, L. Robinette, T. Sheng, S. Sun, M. Waldbrook, A. White, M. Wilson, C. Xie, C. Young, A. Zenova, Y. Zhang, D. Sutherland
- 11:00 MEDI 172.** Design of subtype selective Na_v1.7 inhibitors for the treatment of pain. **N. Swain**

- 11:30 MEDI 173.** Development of oral Na_v1.7 inhibitors with excellent selectivity over Na_v1.5 for the treatment of pain. **M. Layton**, A.J. Roecker, J.E. Pero, M.S. Egbertson, B. Gomez, K. Jones, Z. Zhao, S. Wolkenberg, J. Mulhearn, M.J. Kelly, M.A. Rossi, H.D. Fjii, L. Zhao, P.J. De Leon, D. Li, K. Gilbert, A.K. Houghton, R. Kraus, B. Klein, M. Clements, C. Daley, J. Wang, T. Finger, J. Majercak, V. Santarelli, I. Gegan, M. Cato, T. Filzen, A. Jovanovska, Y. Wang, D. Wang, X. Peng, X. Wang

Section C

Colorado Convention Center
Mile High Blrm 2C

Approaches to Targeting RNA with Small Molecules

N. A. Meanwell, R. E. Olson, *Organizers, Presiding*

- 8:30 MEDI 174.** Rational design of small molecules to target the DNA/RNA of trinucleotide repeat (TNR) diseases. **S.C. Zimmerman**, L. Nguyen, L. Luu, J. Lee
- 9:05 MEDI 175.** New chemical and analytical tools for understanding RNA recognition. **B.L. Miller**
- 9:40 MEDI 176.** Identification of biologically active, RNA-binding small molecules using small molecule microarrays. **J. Schneckloth**
- 10:15 MEDI 177.** High-throughput platform assay technology for the discovery of pre-microRNA-selective small molecule probes. **A.L. Garner**
- 10:50 MEDI 178.** Giving SMN2 a push in the right direction: The discovery of small molecule splicing modulators. **M.G. Wolf**, H. Qi, A. Turpoff, N. Zhang, X. Zhang, G. Chen, N.A. Naryshkin, A. Dakka, J. Narasimhan, V. Gabbeta, M. Weetall, X. Zhao, N. Risher, J. Sheedy, G.M. Karp

- 11:25 MEDI 179.** Progress on the development of rational methods to target RNA with small molecules. **M.D. Disney**

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Sponsored by AGFD, Cosponsored by AGRO and MEDI

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Blrm 1A/1B

New Models for Drug Discovery: Public, Private, and Non-Profit

J. Crawford, A. A. Estrada, B. Shotwell, *Organizers, Presiding*

- 2:00 MEDI 180.** Investigation of highly optimized LRRK2 kinase inhibitors in preclinical safety studies via a Michael J. Fox Foundation-Genentech collaboration. **A.A. Estrada**
- 2:30 MEDI 181.** New collaborative ways of discovering and developing anti-malarial therapies. **P. Willis**
- 3:00 MEDI 182.** ENABLE(ing) drug discovery: A public private partnership addressing antimicrobial resistance in serious gram negative infections. **A.T. Price**
- 3:30 MEDI 183.** Development of antiviral agents to treat poliovirus infections. **M. McKinlay**
- 4:00 MEDI 184.** Foundation-directed therapeutic development: Pfizer collaboration on PDE inhibitors. **C. Dominguez**
- 4:30 MEDI 185.** First small molecule clinical candidate discovered in Africa. **K. Chibale**

Section B

Colorado Convention Center
Mile High Blrm 2A/2B

Modulators of the Nuclear Receptor ROR γ

B. P. Fauber, S. J. Taylor, *Organizers, Presiding*

- 2:00 MEDI 186.** Development of RORalpha/beta/gamma subtype selective ligands. **T.P. Burris**
- 2:25 MEDI 187.** Small molecule inhibitors of RORgamma: Their development to study the function of inflammatory immune cells. **J. Huh**
- 2:50 MEDI 188.** Structural basis for the inverse agonism of novel ROR γ inhibitors. **X. Li**
- 3:15 MEDI 189.** Optimization of quinoline tertiary alcohols as modulators of ROR γ . **K. Leonard**, A. Fourie, X. Xue, M.J. Urbanski, H. Venkatesan, K. Barbay, D.A. Kummer, R. Nishimura, R.L. Wolin, K.D. Kreutter, C.R. Woods, V.M. Tanis, A. Wang, W. Jones, K. McClure, S.D. Goldberg, E. Fennema, C. Martin, J. Pierce, G. Bacani, J. Spurlino, C. Schalk-Hihi, C. Milligan, P. Wilkinson, T. Cao, M.C. Abad, R. Luna, K. Herman, A. De Leon, E. Nulton, M. Nelen, J. Yu, M.D. Cummings, B. Scott, K. Sepassi, S. Nguyen, M. Sablad, N. Rozenkrants, Y. Zhang, T. Rao, A. Nidor, S. Branun, J. Spink, C.A. Teleha, D. Pippel, R. Russell, T. Schlueter, J.P. Edwards
- 3:40 MEDI 190.** Dealing with a highly lipophilic binding pocket: design and development of novel ROR γ inverse agonists with the consideration of ligand polarity and conformational diversity. **J. Chao**
- 4:05 MEDI 191.** Reversed sulfonamide series of selective ROR γ inverse agonists. **M.B. van Niel**, B.P. Fauber, M. Cartwright, S. Gaines, J.C. Killen, O. René, S.I. Ward, G.d. Boenig, Y. Deng, C. Eidschenck, C. Everett, E. Gancia, A. Ganguli, A. Gobbi, J. Hawkins, A.R. Johnson, J.R. Kiefer, H. La, P. Lockey, M. Norman, W. Ouyang, A. Qin, N. Wakes, B. Waszkowycz, H. Wong
- 4:30 MEDI 192.** Discovery of novel ROR γ antagonists. **M. Shiozaki**

Section C

Colorado Convention Center
Mile High Blrm 2C

Symposium in Honor of Richard Gibbs

B. Blagg, T. E. Prisinzano, *Organizers, Presiding*

- 2:00 MEDI 193.** Targeting indenoisouquinoline topoisomerase I inhibitors to cancer cells. **D.E. Beck**, T. Nguyen, W. Lv, P.N. Reddy, M. Abdelmalak, K. Agama, C. Marchand, Y. Pommier, J. Roy, A. Kanduluru, C. Venkatesh, P. Low, **M. Cushman**
- 2:35 MEDI 194.** Inhibition of geranylgeranyl diphosphate synthase by isoprenoid bisphosphonates. **D.F. Wiemer**
- 3:10 MEDI 195.** Small molecule epigenetic modulators for the treatment of cardiovascular disorders. **C.J. Kutz**, S.L. Holshouser, **P.M. Woster**
- 3:45 MEDI 196.** Protein prenylation: From enzymology to biotechnology and therapeutic application. **M.D. Distefano**, Y. Wang, C.C. Palsuledesai, J.K. Dozier
- 4:20 MEDI 197.** Biosynthesis of squalene: A new pathway in bacteria. **J. Pan**, **C.D. Poulter**

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Sponsored by AGFD, Cosponsored by AGRO and MEDI

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

Drug Discovery

ADME & Informatics

Sponsored by COMP, Cosponsored by CINF and MEDI

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

W. B. Young, *Organizer*

8:00 - 10:00

- 44, 53, 56, 68, 70, 78, 84, 96, 99, 128, 137.
See previous listings.
278, 286, 294, 298, 323, 331, 333, 338, 343.
See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Blrm 2A/2B

E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Symposium in Honor of Ruth R. Wexler

Cosponsored by WCC

W. B. Young, *Organizer*
J. E. Macor, *Presiding*

- 9:00 MEDI 198.** Lessons learned in the practice of medicinal chemistry. **P.S. Anderson**
- 9:35 MEDI 199.** In search of small molecule modulators for the treatment of autoimmune and inflammatory diseases. **J.C. Barrish**
- 10:10 MEDI 200.** Thrombin receptor antagonists for the prevention of arterial thrombosis: Discovery of vorapaxar (zontivity™). **W.J. Greenlee**

- 10:45 MEDI 201.** Structure-based design of serine protease inhibitors: The quest for safer and efficacious anticoagulants. **M.L. Quan**
- 11:20 MEDI 202. Award Address**
(E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances sponsored by Merck Research Laboratories). Adventures in cardiovascular drug discovery: New frontiers and lessons learned. **R.R. Wexler**

Section B

Colorado Convention Center
Mile High Blrm 1A/1B

Observations from Recent Drug Launches: The Rules of Today May Not Apply Tomorrow

J. B. Schwarz, *Organizer, Presiding*

- 9:00 MEDI 203.** Discovery of macitentan: Can we apply rules of yesterday tomorrow? **M.H. Bolli**
- 9:30 MEDI 204.** Discovery and development of covalent BTK inhibitors. **W. Chen**
- 10:00 MEDI 205.** Chiral, nonracemic hemiaminals to the rescue: The discovery of the HIV-1 integrase inhibitors dolutegravir and cabotegravir. **B.A. Johns**
- 10:30 Intermision.**
- 10:45 MEDI 206.** Discovery of thalidomide and amino substituted analogs as anticancer agents. **R. DAmato**
- 11:15 MEDI 207.** Ponatinib, a pan-Bcr-Abl kinase inhibitor approved for leukemia treatment, potently inhibits the T3151 mutant and overcomes mutation-based resistance. **W. Huang**
- 11:45 MEDI 208.** Pirfenidone and optimized pirfenidone analogs for antifibrotic indications. **J.Y. Ramphal**, L. Pan, C. Schaefer, S.D. Seiwert, B.O. Buckman, **J.B. Schwarz**

Section C

Colorado Convention Center
Mile High Blrm 2C

Why You Should Have Paid Attention in P-Chem: Thermodynamics in Drug Discovery

A. J. Peat, B. Shotwell, *Organizers, Presiding*

- 9:00 MEDI 209.** Thermodynamic-based approach to the inhibition of HIV-1 cell infection. **E. Freire**

9:30 MEDI 210. Thermodynamics guided lead discovery and optimization. G.M. Keseru
10:00 MEDI 211. Ligand-protein binding thermodynamics from fragments to drugs. G. Ferenczy

10:30 Intermission.

10:45 MEDI 212. Exploring applications and origins of binding kinetics in structure-based drug discovery. D. Meinhold

11:15 MEDI 213. Accelerating drug discovery: the role of free energy calculations. R. Abel, R. Friesner, R. Farid, T. Lin, L. Frye, J. Knight, G. Krilov, L. Wang

11:45 MEDI 214. Lipophilic efficiency as a tool for identifying and optimizing enthalpic interactions. M.D. Shultz

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

Phenolic & Polyphenolic Chemistry in Food Processing

Reactions/Properties

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

Drug Discovery

Methodology

Sponsored by COMP, Cosponsored by CINF and MEDI

TUESDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Blrm 1A/1B

Smisssman Award: Symposium in Honor of Dennis Liotta

W. B. Young, *Organizer*
J. E. Macor, *Presiding*

2:00 MEDI 215. Nucleoside analogs: Synthesis and medicinal chemistry. Y. Guindon, M. Prévost, S. Dostie, P. Mochirian, G. Tambutet

2:45 MEDI 216. Therapeutic opportunities of chemical targeting of mitochondria. P. Wipf

3:30 MEDI 217. Targeting protein-protein interactions for new cancer therapeutics. S. Wang

4:15 MEDI 218. Discovery of novel therapeutics for treating various types of viral diseases, cancers, and inflammatory disorders. D. Liotta

Section B

Colorado Convention Center

Mile High Blrm 2A/2B

The Role of Rings in Drug Design

N. A. Meanwell, P. M. Scola, *Organizers, Presiding*

2:00 MEDI 219. Rings in drugs. R. Taylor

2:35 MEDI 220. Small, medium, and large ring systems: Observations and examples of their roles in molecular recognition and drug design. D.L. Cheney

3:10 MEDI 221. Development of novel transition metal-catalyzed approaches toward heterocycles. V. Gevorgyan

3:45 MEDI 222. Rings in (candidate) drugs: Case stories. J. Boström

4:20 MEDI 223. Sulfur-containing heterocycles in drug design. M.D. Bartberger

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

Phenolic & Polyphenolic Chemistry in Food Processing

Sources

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

Drug Discovery

Methodology

Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY MORNING

Section A

Colorado Convention Center

Mile High Blrm 2A/2B

General Oral Session

W. B. Young, *Organizer*
J. Rudolph, *Presiding*

8:30 MEDI 224. Discovery and synthesis of first-generation single-drug "cocktails" to combat HIV. A.R. Prosser, B.D. Cox, S. Gupta, L.J. Wilson, D.C. Liotta

8:55 MEDI 225. B-DNA structure-based removal of genotoxicity from a series of inhibitors of the IκB-kinase IKK2. L. Borjesson, I. Shamovsky, M. Andersson, T. Brimert, C. Ekström, A.K. Ray, P. Zlatoidsky, P. Åberg

9:20 MEDI 226. Selective inhibition of group-II p-21-activated kinases (PAKs). S.T. Staben, J. Feng, W. Wang

9:45 MEDI 227. Discovery of novel indole derived mineralocorticoid receptor antagonists. A.K. Ogawa

10:10 MEDI 228. Discovery of phosphonic acid containing LpxC inhibitors as broad spectrum antibacterial agents. Q. Dang, P. McNicholas, D. Olsen, P.T. Meinke

10:35 MEDI 229. Discovery of novel anti-chagas agents targeting T. cruzi CYP51. J. Choi, D. Vieira, C. Claudia, J. Siqueira-Neto, D. Kellar, J. Gut, J. Johnston, M. Cameron, J. McKerrow, L. Podust, W.R. Roush

11:00 MEDI 230. Potent and selective pyridone BTK inhibitors with activity against mutant forms of BTK. J. Crawford

11:25 MEDI 231. Understanding our love affair with para-chlorophenyl: Scientific rationale or unsubstantiated bias? D.G. Brown, M. Gagnon, J. Boström

11:50 MEDI 232. Learning from experience: 15 years of protein-fragment X-ray crystal structures and the consequences for fragment library design. D. Norton

Section B

Colorado Convention Center

Mile High Blrm 1A/1B

Advances in the Treatment of Fibrotic Diseases

P. Devasthale, *Organizer*
W. B. Young, *Presiding*

8:30 MEDI 233. Organ and tissue fibrosis: Principles and prospects for therapy. S. Friedman

9:00 MEDI 234. Therapeutic targeting of Nox4 leads to reversal of age-associated persistent fibrosis. L. Hecker, N. Logsdon, L.H. Hurley, V. Thannickal, J. Garcia

9:30 MEDI 235. Development of a small molecule inhibitor of integrin αvβ1. W.F. Degradó

10:00 MEDI 236. Development of novel sGC activators that protect against the progression of diabetic nephropathy in ZSF-1 rats. C.R. Sarko, J. Breneman, T. Bosanac, C. Boustany, H. Chen, H. Clifford, R. Fryer, J. Ginn, P.C. Harrison, J.I. Levin, K. Lincoln, H. Qian, S. Pullen, G. Reinhart, J. Richman, H. Wang, D. Wong, K. Gueneva-Boucheva

10:30 MEDI 237. Galectin-3 antagonists with therapeutic implications in fibrosis. U.J. Nilsson, H. Leffler, H. Schambye, A. Mackinnon, T. Sethi

11:00 MEDI 238. Needs and challenges in anti-fibrosis drug discovery: Experience from JNK inhibitors. Y. Satoh

11:30 Discussion.

Section C

Colorado Convention Center

Mile High Blrm 2C

Small Molecule Approaches to Autism Spectrum Disorder Therapy

K. A. Emmitte, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 MEDI 239. Harnessing rodent models to develop new therapeutic targets in autism spectrum disorder. J. Veenstra-VanderWeele

9:40 MEDI 240. Therapeutic strategies for restoring excitatory/inhibitory balance in Rett syndrome: Focus on BDNF/TrkB signaling. D. Katz

10:15 MEDI 241. Utility of NMDA antagonists for the treatment of Rett syndrome. R.J. Mather

10:50 MEDI 242. Development of a highly selective and CNS penetrant mGlu₁, NAM: An in vivo tool for further elucidating the role of group II mGlu₁ in psychiatric disorders. J.L. Engers, L.C. Konkol, A.L. Rodriguez, R.D. Morrison, F.W. Byers, A.D. Thompson Gray, J.S. Daniels, C.M. Niswender, C.K. Jones, P.J. Conn, C.W. Lindsley, K.A. Emmitte

11:25 MEDI 243. Approaches toward the identification of rodent models of autism spectrum disorder suitable for use in lead optimization efforts. C.K. Jones

Drug Discovery

Ligand-Based

Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Blrm 1A/1B

First Time Disclosures

L. A. Thompson, *Organizer, Presiding*

1:30 MEDI 244. Discovery of JNJ-42847922, a selective orexin-2 antagonist for the treatment of insomnia disorder. M.A. Letavic, P. Bonaventure, K.S. Ly, Z. Aguilar, L. Aluisio, N.I. Carruthers, S. Chaplan, C. Dugovic, R. Halter, T. Koudriakova, B. Lord, T.W. Lovenberg, M. Kramer, K.L. Morton, A. Ndifor, M. Rizzolio, C. Shah, J. Shelton, J. Shoblock, S. Sutton

2:05 MEDI 245. Discovery and optimization of the human histamine H4 antagonist Toreforant (JNJ38518168) for the treatment of inflammatory diseases. J.D. Venable, D.E. Kindrachuk, D.J. Buzard, P.J. Dunford, L. Karlsson, R.L. Thurmond, J.P. Edwards

2:40 MEDI 246. Discovery of MK-8931: A BACE inhibitor in Phase 3 clinical development for Alzheimer's disease. J.N. Cumming, J.D. Scott, S.W. Li, M. Cartwright, X. Chen, K. Cox, M. Forman, E.J. Gilbert, R. Hodgson, L. Hyde, Y. Jin, I. Kazakevich, R. Kuvelkar, X. Liang, H. Mei, J. Misiaszek, P. Orth, J. Stone, C. Strickland, J.H. Voigt, H. Wang, B. Werner, J. Wong, E.M. Parker, W.J. Greenlee, M.E. Kennedy, A.W. Stamford

3:15 MEDI 247. Discovery of GSK2881078A: A selective androgen receptor modulator (SARM) for the treatment of muscle wasting disorders. P. Turnbull, R. Cadilla, Y. Shen, C. Poole, E. Stewart, R. Gampe, R. Clark, B.R. Henke, A. Russell

3:50 MEDI 248. Discovery of a next generation irreversible inhibitor targeting the resistance mutation T790M and activating mutations in NSCLC with a broad selectivity margin over EGFR wild type. S. Planken, B.W. Murray, J. Lafontaine, S. Weinrich, M. Hemkens, J.C. Kath, S.K. Nair, T.O. Johnson, H. Cheng, S.C. Sutton, M. Zientek, M. Yin, J. Solowiej, A. Nagata, K. Gajjwala

4:25 MEDI 249. Discovery and early development of vibegron (MK-4618): A potent and selective β₂-AR agonist for the treatment of overactive bladder. S. Edmondson, C. Zhu, N.F. Kar, R. Berger, S.D. Gobie, B. Harper, G. Morriello, C. Moyes, L. Wang, P.N. Brown, K.H. Dingley, J. DiSalvo, A. Fitzmaurice, T. Frenkl, S.A. Green, A.L. Hurlay, N. Jochnowitz, S. Khalilieh, R.R. Miller, H. Nagabukuro, J.D. Ormes, B. Sacre-Salem, G.M. Sallituro, D. Stickens, A.A. Kulick, A.T. Sanfiz, A. Stevenson, K. Villa, L.A. Wickham, B.A. Zamljnyy, M. Struthers, A.E. Weber

Section B

Colorado Convention Center

Mile High Blrm 2A/2B

MEDI Award Symposium

W. B. Young, *Organizer*

J. E. Macor, *Presiding*

2:00 MEDI 250. Phenylalkylamine: Scaffolding for drugs of abuse, with a focus on synthetic cathinones. R.A. Glennon

2:45 MEDI 251. Award Address (George and Christine Sosnovsky Award for Cancer Research sponsored by the George and Christine Sosnovsky Endowment Fund). Design and development of ligand-targeted therapies and imaging agents for multiple human diseases. P.S. Low, C.P. Leamon, J. Reddy, I.R. Vlahov

3:30 MEDI 252. Award Address (George and Christine Sosnovsky Award for Cancer Research sponsored by the George and Christine Sosnovsky Endowment Fund). Personalized medicine using targeted small molecule drug conjugates and companion imaging agents for cancer therapy. C.P. Leamon

4:15 MEDI 253. Award Address (Earle B. Barnes Award for Leadership in Chemical Research Management sponsored by the Dow Chemical Co. Foundation). Getting the chemistry right: Catalyzing translational innovation at NIH. C.P. Austin

Section C

Colorado Convention Center

Mile High Blrm 2C

General Oral Session

W. B. Young, *Organizer*

J. J. Bronson, *Presiding*

1:30 MEDI 254. Design, synthesis, and biological evaluation of manassantin analogues for HIF-1α inhibition. D. Kwon, K. Park, D. Weitzel, S. Lee, T. Stephenson, C. Lee, J. Chi, R. Mook, M. Dewhurst, Y. Lee, J. Hong

1:50 MEDI 255. First discovery of a single digit nanomolar small molecule protein-protein interaction blocker. L.K. Petersen, F. Sloek, P. Blaksjaer, L. Larsen, J. Holmkvist, A.B. Christensen, J. Rasmussen-Dietvorst, T. Hansen, N. Hansen

2:10 MEDI 256. Discovery of the mGlu₅ receptor NAM HTL14242 by fragment based drug discovery. M. Congreve, S.J. Aves, K.A. Bennett, J.A. Christopher, A.S. Doré, J.C. Patel, B. Tehan, F.H. Marshall

2:30 MEDI 257. Small molecules targeting XBP-1s expression in CLL. J.R. Del Valle, S. Ranatunga, C. Kang, C. Hu

2:50 MEDI 258. Stabilized cyclopropane analogs of the spliceosome Inhibitor FD-895. M.D. Burkart

3:10 MEDI 259. Investigating aromaticity effects in the tail region of sphingosine kinase 2 selective guanidine-based inhibitors. M.D. Congdon, Y. Kharel, K. Lynch, W. Santos

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.

[†] Cooperative Cosponsorship

- 3:30 MEDI 260.** Repurposing aspartic protease inhibitors as novel antimalarial agents. **M.J. Meyers**
- 3:50 MEDI 261.** Chemical optimization of novel inhibitor classes selectively targeting PI4KIIIb α : A host lipid kinase crucial for enterovirus replication. **A. Leivers**, A. Maynard, A.J. Peat, E. Nartey, J. Shotwell, J. Botyanszki, J. Gobet, J. Catalano, J.F. Miller, J. Seal, L. Want, L. Shewchuk-Chapman, P.Y. Chong, P. Xiong, S. Dickerson, S. You, V.W. Tai
- 4:10 MEDI 262.** Variation in ADC linker composition generated from aldehyde-tagged antibodies impacts both efficacy and PK. **A.W. Garofalo**
- 4:30 MEDI 263.** HIV microbicide development using a combination of Qsar and structure-based approaches. **L. Guasch**, A.V. Zakhharov, M.C. Nicklaus
- 4:50 MEDI 264.** Dihydroquinazolinones: A novel class of hOCT3 inhibitors. **M. Dukat**, X. Pan, M. Argade, K.A. Iyer, P.D. Mosier, D. Sweet
- Drug Discovery**
- Ligand-Based**
- Sponsored by COMP, Cosponsored by CINP and MEDI
- WEDNESDAY EVENING**
- Section A**
- Colorado Convention Center
Four Seasons Ballroom
- General Poster Session**
- W. B. Young, *Organizer*
- 7:00 - 9:00**
- MEDI 134.** Amphipathic α -helix mimetics based on a 1,4-disubstituted 2,3,4,5-tetrahydro-1H-benzo[e][1,4]diazepine: Inhibition of the Mcl-1 oncoprotein. **L. Chen**, K. Jeong, S. Fletcher
- MEDI 265.** Physical compatibility of co-solubilized vancomycin, piperacillin, and tazobactam in aqueous solution. **R.N. Mason**, S.C. Butler, H.N. Gray, H.S. Gray
- MEDI 266.** Development and validation of RP-HPLC method for simultaneous determination of guaifenesin impurities in multidrug combinations. **R. Grigoryan**
- MEDI 267.** Carbon monoxide releasing property of amine carboxyboranes. **N.N. Dingra**
- MEDI 268.** Use of Fc receptor affinity separation resin to obtain high potency glycoforms (nonfucosylated) of antiviral immunoglobulin. **A. Boesch**, G. Bolton
- MEDI 269.** Structure-activity relationships of prazole fragment inhibitors of *T. vaginalis* uridine nucleoside ribohydrolase using NMR-based activity and binding assays. **T.A. Shea**, M.A. VanAlstine-Parris, B.J. Stockman
- MEDI 270.** Aminomethyl spectinomycins as novel therapeutics for drug resistant respiratory tract and sexually transmitted bacterial infections. **S.L. Waidyarachchi**, D.F. Bruhn, J. Liu, D.B. Madhura, D. Shcherbakov, Z. Zhong, Y. Abdelrahman, A. Singh, C. Rathni, R. Belland, B. Meibohm, J. Rosch, E. Böttger, R.E. Lee
- MEDI 271.** Targeting *Mycobacterium tuberculosis* biotin protein ligase (MTBPL): Synthesis and evaluation of nucleoside-based bisubstrate adenylation inhibitors. **M.R. Bockman**, A. Kainda, D. Tiwari, T. De la Mora, B. Finzel, D. Schnappinger, C.C. Aldrich
- MEDI 272.** Hybridization of metronidazole with natural product tetramic acids improves its antifidicilic efficacy. **P.T. Cherian**, X. Wu, R.E. Lee, J. Hurdle
- MEDI 273.** Lipidated cyclic gamma-AA peptides display both antimicrobial and anti-inflammatory activities. **Y. Li**, C. Smith, H. Wu, S. Padhee, H.H. Yin, J. Cai
- MEDI 274.** Design and biological evaluation of novel Cdc42 inhibitors. **B.J. Aguilari**, B. Hincley, S. Huo, Y. Chen, Q. Lu
- MEDI 275.** Development of $\alpha_2\beta_2\gamma_2$ -subtype selective ligands for GABA_A receptors. **R.S. Verma**, C. Witzigmann, J.M. Cook
- MEDI 276.** Quantitative structure-activity relationship (QSAR) investigations of abuse-related neurochemical and behavioral effects of para-substituted methcathinone derivatives. **F. Sakloth**, R. Kolanos, M. Barnier, P.D. Mosier, J. Partilla, M.H. Baumann, R.A. Glennon
- MEDI 277.** Structure-activity studies on the α -modified analogs of the abused substance methylenedioxypyrovalerone (MDPV) as reuptake inhibitors at the dopamine transporter (DAT). **F. Sakloth**, R. Kolanos, A.D. Jain, J. Partilla, M.H. Baumann, R.A. Glennon
- MEDI 278.** Synthesis, SAR, and progress toward orally available, brain penetrant P2X7R antagonists for the treatment of neuroinflammatory disorders. **C. Chrovin**
- MEDI 279.** Structure-activity relationships of iminoheterocyclic BACE1 inhibitors: Discovery of MK-8931 for the treatment of Alzheimer's disease. **J.D. Scott**, S.W. Li, X. Chen, K. Cox, J. Cumming, M. Forman, E.J. Gilbert, W.J. Greenlee, R. Hodgson, C. Huang, L. Hyde, Y. Jin, U. Iserlohn, I. Kazakevich, R. Kuvelkar, G. Li, X. Liang, J. Misiaszek, P. Orth, E.M. Parker, C. Strickland, J.H. Voigt, H. Wang, B. Werner, J. Wong, M.E. Kennedy, A.W. Stamford
- MEDI 280.** Robust and efficient amination route toward the development of N-substituted piperazines as serotonergic ligands for autism spectrum disorder. **J. Dhuguru**, S.W. Goldstein, A. Khalil, O.M. Ghoneim
- MEDI 281.** Computational approach for performing medchem transformations within a 3D active site. **M.R. Goldsmith**
- MEDI 282.** Applying extended Huckel theory to pharmacophore modeling. **A. Deschenes**
- MEDI 283.** Exploring the role of solvation in drug design and optimization. **M.L. Drummond**, J. Truchon, C. Williams, P. Labute
- MEDI 284.** Performance of structure based and ligand based virtual screening methods for ten selected anticancer targets. **C. Selvam**, T. Ramasamy
- MEDI 285.** Scaffold hopping: Balancing novelty, accessibility, and physicochemical properties. **T. Cheeseright**, S. Tomásio, P. Tosco, M. Mackey
- MEDI 286.** Discovery of KSI-6666, a novel S1P1 antagonist for the treatment of autoimmune disease. **Y. Ohswa**, H. Inoue, T. Suzuki, Y. Maruyama, K. Ohno, N. Arisaka, S. Muto, Y. Okuhara, M. Hayashi, A. Yamamoto, K. Kaidoh, H. Mukaiyama, M. Hiratochi
- MEDI 287.** Discovery of a new indole-based group IVA cytosolic phospholipase A_2 inhibitor as a promising drug candidate for treatment of respiratory diseases. **T. Tomoo**, T. Nakatsuka, T. Katayama, Y. Hayashi, Y. Fujieda, M. Terakawa, K. Nagahira
- MEDI 288.** Controlled-release mechanism for sulfur mustard anti-inflammatory drugs based on polyamine platform. **C.J. Lacey**, J. Saxena, C.D. Guillon, G.M. Composto, L.B. Joseph, D.E. Heck, J.D. Laskin, N.D. Heindel
- MEDI 289.** Synthesis and anti-inflammatory activity of three nitro chalcones. **A. Gómez Rivera**, C.E. Lobato García, H. Aguilar Mariscal, N. Romero Ceronio
- MEDI 290.** Microwave assisted synthesis, pharmacological activities, and molecular docking studies of Ethyl 2-substituted-4-(2-thienyl) thiazole-5-acetates. **M. Attimarad**, M.A. Kheodr, B.E. AlDubai
- MEDI 291.** Toward a bioisosteric alkalest: Targeting the human dehydroorotate dehydrogenase (hDHODH) by a scaffold hopping bioisosteric approach using hydroxylated pentamantoic heterocycles. **M.L. Loli**, A.C. Pippione, S. Saines, S. Mensa, M. Giorgis, M. Piccinini, E. Lupino, S. Al-Kadaraghi, D. Boschi
- MEDI 292.** Discovery of thienopyrimidinones as a new series of potent phosphodiesterase 7 inhibitors. **Y. Endo**, K. Kawai, T. Asano, S. Amano, K. Sawada, K. Ogura, N. Ueo, N. Takahashi, Y. Sonoda, M. Nagai, N. Kamei
- MEDI 293.** Development of fluorescent affinity probes for the P2Y₄ G protein-coupled receptor. **E. Kiselev**, M. Barrett, E. Hammes, V. Kaitrich, R. Balasubramanian, A. Yin, S. Paolotta, C. Weitzner, Q. Zhao, R. Stevens, T. Harden, K. Jacobson
- MEDI 294.** Design, evolution, and in vivo profile of a novel series of GPBAR 1 agonists for the treatment of diabetes and metabolic syndrome. **R. Kurukulasuriya**, S.K. Shah, J. Dellufreccio, S. Fung, L. Guo, J. Szewczyk, M. Trujillo, R.P. Nargund, W.K. Hagmann, A. Poci, R.J. Devita
- MEDI 295.** Withdrawn.
- MEDI 296.** Benzothiazolyl substituted iminothiazolidinones and benzamido-oxothiazolidines as potent and partly selective aldose reductase inhibitors. **J. Iqbal**
- MEDI 297.** Design and bioevaluation of novel human 4-hydroxyphenylpyruvate dioxygenase inhibitors. **H. Lin**, G. Yang, W. Yang
- MEDI 298.** Targeting integrin $\alpha_v\beta_3$ receptors with multivalent RGD peptidomimetics. **J.L. Teh**, R.N. Hanson, S. Sridhar
- MEDI 299.** Design, synthesis, topoisomerase I and II inhibitory activity, cytotoxicity, and structure-activity relationship study of novel 2-phenyl-4-aryl indenopyridines. **G. Bist**, T.M. Kadayat, T. Thapa Magar, A. Shrestha, Y. Kwon, E. Lee
- MEDI 300.** Importance of side chain orientation on large macrocycles: Structure activity relationship of sanguinamide B analogs on colon cancer HCT-116 cells. **A. Pietkiewicz**, H. Wahyudi, J. McConnell, S. McAlpine
- MEDI 301.** Synthesis, characterization, and in vitro anticancer activity of quinoxalylmethyl- and naphthylmethyl-substituted imidazolium salts. **P.O. Wagers**, M. DeBord, M.J. Panzner, C. Tessier, W.J. Youngs
- MEDI 302.** Development of novel casein kinase 1 inhibitors. **R.L. Schroeder**, N.A. Pham, P. Tram, T. Stone, K. Nguyen, J. Geathers, D.Q. Nguyen, E. Skripnikova, M.R. Bratton, J. Sridhar
- MEDI 303.** Synthesis and biological evaluation of novel naphthoquinones as HER2 inhibitors for the treatment of trastuzumab resistant breast cancer. **R.L. Schroeder**, M.E. Sfondouris, M.R. Bratton, N.A. Pham, P. Tram, T. Stone, K. Nguyen, J. Geathers, D.Q. Nguyen, C.L. Stevens, F.E. Jones, J. Sridhar
- MEDI 304.** Anthracenyl isoxazole amides (AIMs) stabilize quadruplex DNA structures in telomeric and c-MYC promoter sequences. **S. Stump**, M.J. Weaver, N.S. Duncan, A.K. Kearns, N.R. Natale, H.D. Beall
- MEDI 305.** Design, synthesis, and biological screening of novel estrone analogs toward treatment of hepatocellular carcinoma. **M. Mahnashi**
- MEDI 306.** Synthesis, structure-activity relationship (SAR) study, and mode of action study of cationic triazole analogs of 1,4-naphthoquinone: A new class of highly potent anticancer agent. **J.P. Shrestha**, C.T. Chang
- MEDI 307.** ZMPSTE24 protease inhibitors as senescence agonists for cancer chemotherapy. **D. Xanthopoulos**, A. Matralis, H. de Vries, G. Huot, G. Ferbeyre, Y.S. Tzantrizos
- MEDI 308.** Thio-sugars can sensitize human cervixadenocarcinoma (Hela) cancer cells to Bleomycin and ROS generator. **J. Sarnik**, A. Czubatka, T. Poplawski, Z.J. Witzczak
- MEDI 309.** Low glucose level enhances the cytotoxicity of CARB-pharmacophore to cancer cells. **A. Czubatka**, J. Sarnik, T. Poplawski, Z.J. Witzczak
- MEDI 310.** N,N'-bisquinoxalylmethyl-2-alkyl and N-quinoxalylmethyl-N'-naphthylmethyl-2-alkyl substituted imidazolium salts as potential therapeutics for the treatment of lung cancer: Synthesis, characterization, and in vitro anticancer activity. **M. DeBord**, P.O. Wagers, M.J. Panzner, C. Tessier, W.J. Youngs
- MEDI 311.** 2,4-Diaryl-indenopyridine derivatives: Design, synthesis, topoisomerase I and II inhibition, cytotoxicity, and structure-activity relationship study. **T. Thapa Magar**, T.M. Kadayat, G. Bist, A. Shrestha, Y. Kwon, E. Lee
- MEDI 312.** Mechanistic studies of imidazolium salts as antitumor agents. **M.R. Southerland**, P.O. Wagers, M. DeBord, K.L. Shelton, L. Shriver, S.M. Paruchuri, C. Tessier, M.J. Panzner, W.J. Youngs
- MEDI 313.** Design, synthesis, and in vitro anticancer activities of the 7-chloro-6-fluoro-N-substituted-2-phenylquinoline-4-carboxamide derivatives. **A.P. Patel**, H.G. Bhatt
- MEDI 314.** Synthesis of pyrazole derivatives as potential cytotoxic agents. **T. Rowe**, **J. Bridger**, M. Branscum, M.A. Alam
- MEDI 315.** Synthesis of curcumin mimics with substituted triazolyl groups and their sensitization effect of TRAIL against brain cancer cells. **S. Lee**, S. Oh, D. Kwon, Y. Park, W. Shin
- MEDI 316.** 10-oxy-anthracenyl isoxazole amides (AIMs) as potential G-quadruplex stabilizing antitumor agents. **N.S. Duncan**, N.R. Natale, H.D. Beall
- MEDI 317.** Ferrocenyl derivatives as promising scaffolds for anticancer and antileishmanial agents. **S. Zaib**, J. Iqbal, M. Hassan, F. Maccava, A.K. Powell
- MEDI 318.** Improved efficacy for a novel class of G-quadruplex binding anti-tumor agents. **M.J. Weaver**, N.R. Natale
- MEDI 319.** Design, synthesis, and antineoplastic evaluation of isoform selective inhibitors of AKR1C3. **K. Verma**, T. Zhang, T.M. Penning, P.C. Trippier
- MEDI 320.** Discovery and development of a series of irreversible EGFR_T790M 7H-pyrrolo[2,3-d]pyrimidine inhibitors with high selectivity over EGFR wild type. **S. Plankens**, S.K. Nair, J.C. Kath, J. Lafontaine, S. Wehrich, H.K. Cheng, S.C. Sutton, T.O. Johnson, M. Zientek, A. Nagata, K. Gajiwala, J. Solowiej, B.W. Murray, M. Yin, M. Hemkens
- MEDI 321.** Synthesis of PF-06459988; a next generation irreversible EGFR_T790M inhibitor for resistant non-small cell lung cancer. **K.T. Tran**, D.C. Behenna, S. Cho-Schultz, S. Kephart, J.A. Matthews, S.K. Nair, M.A. Ornelas, S.T. Orr, M.A. Parrish, P. Richardson, D.T. Richter, N. Sach, H. Shen, S.C. Sutton, R. Zhou
- MEDI 322.** Synthesis of warhead containing scaffolds on irreversible 7H-pyrrolo[2,3-d]pyrimidine EGFR T790M inhibitors. **J.J. Matthews**, S.E. Kephart, R. Zhou, M.A. Parrish, D. Behenna, S. Cho-Schultz, S.K. Nair, M.A. Ornelas, S.T. Orr, D.T. Richter, H. Shen, S.C. Sutton, K.T. Tran
- MEDI 323.** Exploring EGFR kinase-ligand interactions for optimizing dual action inhibitors. **C. Williams**, A. Ajamian, P. Kamya, B. Jean-Claude, Z. Rachid
- MEDI 324.** Fully automated radiosynthesis of [11C]AZD8931 as a new PET agent for imaging of EGFR, HER2 and HER3 signaling. **M. Wang**, M. Gao, Q. Zheng
- MEDI 325.** Synthesis of carbon-11-labeled aminoalkylindole derivatives as new candidate CBR radioligands for PET imaging of alcohol abuse. **M. Gao**, A. Gao, M. Wang, Q. Zheng
- MEDI 326.** Development of isoform selective compounds for Grp94 inhibition. **S. Mishra**
- MEDI 327.** Targeting Hsp90: Development of C-terminal inhibitors. **M. Anyika**
- MEDI 328.** Deuterated dabrafenib (BRAF kinase inhibitor): Metabolism and pharmacokinetics. **J.M. Ralph**, L.E. Richards-Peterson, T. Wilde, D. Bershaw, E.A. Minthorn, A. Kaura, M. Bleam, S. Laquerre, M. Arnore, C. Manning, J.L. Adams
- MEDI 329.** Combination therapy with epothilone and aurora kinase inhibitors induces a novel form of cell death. **L. Woods**, R.E. Taylor, K.T. Vaughan

MEDI 330. Identification of 2-(4-benzamido-phenyl)-7-phenyl-5H-benzo[c]pyrimido[4,5-e]azepines as potent aurora kinase inhibitors. **R.E. Gershanm,** S.G. Stroud, D.A. Janowick, T.B. Sells, M. Rezaei, C.F. Claiborne, S.J. Critchley

MEDI 331. Rational design of ALK2 small molecule inhibitors for treatment of fibrodysplasia ossificans progressiva (FOP). **Y.L. Luo,** A. Alsamrah

MEDI 332. Discovery and SAR exploration of a novel series 8-oxo-8,9-dihydro-7H-purine-6-carboxamides as mTOR kinase inhibitors. **P. Papa**

MEDI 333. Discovery of substituted morpholinophene and morpholinothiazole carboxylic acids as selective inhibitors of PI3Kb kinase. **Z. Shi,** D. Cardin, J. Chouitar, J. Ecsedy, K. Galvin, R. Griffin, P. Hales, M. Hirose, T. Hu, N. Natasha Iartchouk, D.A. Janowick, Y. Kawakita, M. Rezaei, T. Sells, M. Smith, S. Stroud, L. Takaoka, S. Vyskocil, D. Deborah Wysong, T. Xu, W. Zhang

MEDI 334. Inhibition of the inositol phosphatase SHIP utilizing quinoline-based small molecules. **C.M. Russo,** A.A. Adhikari, D.R. Wallach, R. Brooks, F. Sandra, A.N. Balch, W.G. Kerr, J.D. Chisholm

MEDI 335. Disruption of STAT3 phosphorylation by novel pyrimidino-thiazinones, PI3K- α and δ inhibitors. **B. Akula,** D. Subbaiah, M.R. Mallireddigari, S. Cosenza, V. Bharathi, V. Pallala, G. Panda, . Reddy, M. Reddy

MEDI 336. Structure based design, synthesis, and anticancer evaluation of human neutrophil elastase inhibitors. **Q. Sun,** Y. Li, J. Li, W. Yang, G. Yang

MEDI 337. Synthesis and biological evaluation of potential isoform-selective benzimidazole-4-carboxamide inhibitors of poly(ADP-ribose)polymerases. **J. Pickles,** C. Cano, B. Golding, S. Hamor, S. Jackson, H. Newell, J. Travers, R. Griffin

MEDI 338. Novel strategies for improving the pharmacological properties of platinum-acridine anticancer agents. **S. Ding,** A. Pickard, G. Kucera, U. Bierbach

MEDI 339. Labeling of TSPO PET radioligands by [¹⁸F]fluorination of diarylsulfoxide precursors. **F.G. Simeon,** E. Barresi, S. Lu, S. Taliani, F. Da Settimo, V.W. Pike

MEDI 340. Red blood cell-mediated photodynamic therapy for improved cancer treatment. **W. Tang,** J. Xie, Z. Zhen

MEDI 341. Molecular modeling studies of choline acetyltransferase inhibitors as potential PET probes. **R. Kumar,** T. Darresh-Shori

MEDI 342. Target identification and mechanism elucidation of chalcones' cytotoxicity via photoaffinity probes. **B. Zhou,** X. Yu, C. Zhuang, P. Jiang, S.S. Wickramaratne, Y. Lin, J. Lü, C. Xing

MEDI 343. Activity-based probe for acyl protein thioesterases. **Y. Chen,** M. Zompa, R. Bisiewicz, C.T. Seto

MEDI 344. Design and application of lipid probes for proteomic characterization of protein binding partners. **S. Eni,** M. Best, S. Mattern-Schain, K. Tschersch

MEDI 345. Design and synthesis of novel fluorinated amines. **P. Mykhailiuk**

MEDI 346. Synthesis of conformationally restricted scaffolds by double-Mannich reaction of cyclic ketones. **P. Mykhailiuk**

MEDI 347. Synthesis of novel unique pyrrolidines by [3+2]-cycloaddition of azomethine ylides with electron-deficient alkenes. **P. Mykhailiuk**

MEDI 348. Affinity selection-mass spectrometry screening: Development and validation of a 384-well ultrafiltration format for drug discovery. **R.E. Williamson,** D. Terry, G. Roth

MEDI 349. Plasma treatment of dentin surfaces for improving dental composite restoration bonding. **X. Dong,** M. Cheng, Y. Wang, H. Li, Q. Yu

MEDI 350. Synthesis and evaluation of inhibitors of the salicylate synthase (Mbtl) involved in siderophore biosynthesis in *Mycobacterium tuberculosis*. **F. Liu,** Z. Liu

MEDI 351. Large scale storage stability analysis of molecules in the MLSMR. **C. Laggner,** Y. Shayo, C. Hendarto, C.R. Johnson, C.R. Loomis

MEDI 352. Development of novel nitrogen based heterocyclic antibiotic adjuvants. **R.E. Furlani,** C. Melander

NUCL

Division of Nuclear Chemistry and Technology

J. C. Braley and D. E. Hobart, Program Chairs

SOCIAL EVENTS:

Social Hour, 6:30 PM: Mon

BUSINESS MEETINGS:

NUCL Executive Business Meeting, 5:30 PM: Sun

NUCL Business Meeting, 5:30 PM: Mon

SUNDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, Organizers, Presiding

8:30 NUCL 1. Studies of the thermodynamics of actinide reactions: A tribute to Heino Nitsche. **K.L. Nash**

8:50 NUCL 2. Treatment of contaminated water at Fukushima. **D. Hobbs, R. Peterson, K. Yamaguchi, M. Yamamoto**

9:20 NUCL 3. Thermodynamics and predicting actinide behavior in repository science. **D.T. Reed**

9:40 NUCL 4. Spatially resolved characterization techniques for next generation nuclear forensics signature development. **J.M. Schwantes, L. Sweet, E. Buck, T.J. Johnson, D.D. Reilly, D. Abrecht, E. Mausolf**

10:10 Intermission.

10:30 NUCL 5. Investigation of silica-grafted CMPO-modified calix[4]arenes for radionuclide separations. **E.M. May, Y. Wanglee, A. Solovoyov, Y. Matvieiev, A.S. Katz, V. Kalchenko, H. Nitsche**

10:50 NUCL 6. Interactions of plutonium and ordered mesoporous materials. **T. Parsons-Moss, D. Olive, S. Jones, J. Wang, D. Zhao, Z. Dai, M. Zavarin, A. Kersting, H. Nitsche**

11:10 NUCL 7. FIONA: A new mass analyzer for superheavy elements. **N. Esker, J.M. Gates, G.K. Pang, K.E. Gregorich, H. Nitsche**

11:30 NUCL 8. Solid-phase extractants for sequestration and separation of actinides and lanthanides. **J. Shusterman, A. Bruchet, H. Mason, E.C. Uribe, H. Nitsche**

11:50 NUCL 9. DTRA basic research for combating weapons of mass destruction. **S. Wilk**

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG† and NUCL

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, Organizers, Presiding

1:20 NUCL 10. Scientific contributions of Heino Nitsche to actinide and transactinide chemistry. **C. Düllmann, R. Wilson**

1:40 NUCL 11. Heavy element studies at Berkeley. **K.E. Gregorich**

2:10 NUCL 12. Impact of [Ca, UO, (CO)₃] aq.-complex formation on environmental behavior of uranium. **G. Bernhard, G. Geipel, V. Brendler**

2:40 NUCL 13. Molecular scale investigations towards actinide retention at mineral surfaces. **H. Geckeis**

3:10 Intermission.

3:30 NUCL 14. Applications of molten salts in nuclear technology. **T. Fanghänel, O. Beneš, J. Glatz, R. Konings, R. Malmbeck, P. Souček**

4:00 NUCL 15. Advances in the production and chemistry of the heaviest elements. **A. Tuerler**

4:30 NUCL 16. Laser-induced spectroscopy of actinides: From simple metal systems to species in living cells. **G.C. Geipel**

5:00 NUCL 17. Toward A and Z identification of superheavy elements. **J.M. Gates**

5:30 NUCL 18. Chronology of 239/240Pu and of 236U in the Miaergou glacier from eastern Tien Shan, China. **H.W. Gaeggeler, S. Hou, C. Wang, M. Christl, S. Maxeiner, H. Snyal, C. Vockenhuber**

Section B

Embassy Suites Denver–Downtown Convention Center
Crestone Ballroom B

Nuclear Forensics

Fission Product Studies

A. Klingensmith, R. S. Rundberg, Organizers

1:00 NUCL 19. Energy dependence of fission product yields from 235U, 238U and 239Pu for incident neutron energies between 0.5 and 14.8 MeV. **M. Gooden, C. Arnold, T.A. Bredeweg, J. Wilhelmly, D. Vieira, A. Tonchev, M.A. Stoyer, W. Tornow**

1:25 NUCL 20. Measurement of fission product yields and nuclear reaction crossSections using mono-energetic neutrons from a dense plasma focus. **R.S. Rundberg**

1:50 NUCL 21. Fission product chain yields from fission spectrum irradiations at NCERC. **T.A. Bredeweg, K.R. Jackman, A.C. Olson, S.M. Bowen, A. Schake, S.A. Kozimor**

2:15 NUCL 22. SPIDER: New instrument for fission mass yield measurements. **K.C. Meierbachtol, F. Tovesson, C. Arnold, T.A. Bredeweg, M. Devlin, M. Jandel, J. Lestone, R. Nelson, A. Sierk, D. Shields, M. White, A. Hecht, R. Blakeley**

2:40 NUCL 23. Relative fission product yield determination in varying neutron environments. **M. Koehl, J. Braley**

Section B

Embassy Suites Denver–Downtown Convention Center
Crestone Ballroom B

Nuclear Forensics

Separations

T. A. Bredeweg, A. Klingensmith, Organizers

3:20 NUCL 24. Synthesis of rapid separation targets by hydrothermal methods. **J.M. Dorhout, K. Czerwinski**

3:45 NUCL 25. Thermochromatographic separations of volatile rare earth compounds for nuclear forensics analysis. **J.D. Auxier, S.A. Stratz, D.E. Hanson, M.L. Marsh, A.V. Jones, H.L. Hall**

4:10 NUCL 26. Synthesis and characterization of Ln[fojd]₃ and Ln[dpm]₃ compounds for the development of rapid gas-phase separation methods. **S.A. Stratz, J.D. Auxier, M.L. Marsh, D. Hanson, A.V. Jones, H.L. Hall**

4:35 NUCL 27. Determination of decontamination factor for various radioisotopes during the PUREX process of irradiated DUO₂. **T.K. Bhardwaj, P. Mendoza, R. Du, M. Bencomo, J. Allred, M. Swinney, C.M. Folden, S. Chirayath**

5:00 NUCL 28. Source facility determination based on PUREX process trace metal signatures. **A. Baldwin, J.C. Braley**

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG† and NUCL

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, Organizers, Presiding

8:10 NUCL 29. Actinide sorption to aluminum (hydr)oxides: Influence of sorption site acidity. **T. Baumer, P.E. Kay, A. Ko, A.E. Hixon**

8:30 NUCL 30. Pu transport mechanisms in the environment: Field evidence, conceptual models, and experimental data. **M. Zavarin, J. Beggs, C. Joseph, P. Zhao, A. Kersting**

8:50 NUCL 31. Separating uranyl nanostructures using ultrafiltration membranes. **M. Sharifirouzi, C.R. Andrews, J.E. Szymanski, G.E. Sigmor, W.A. Phillip, P.C. Burns**

9:10 NUCL 32. Superheavy element discovery and chemistry program at LLNL. **D.A. Shaughnessy, R. Henderson, K. Moody, N. Gharibyan, J. Despotopoulos**

9:30 Intermission.

9:50 NUCL 33. Biotransformation of plutonium. **T. Ohnuki, A.J. Francis**

10:10 NUCL 34. Plutonium hydrolysis and condensation. **L. Soderholm, S. Skanthakumar**

10:40 NUCL 35. Role of multinucleon transfer reactions in making neutron-rich transactinide nuclei. **W. Loveland, R. Yanez, S. Barrett**

11:00 NUCL 36. Relativistic quantum theory for chemical identification of the heaviest elements. **V. Pershina**

11:30 NUCL 37. Heino Nitsche's contributions to the understanding of Pu reactions at mineral-water interfaces and their implications on present reactive transport modeling. **B.A. Powell, D. Kaplan**

Section B

Embassy Suites Denver–Downtown Convention Center
Crestone Ballroom B

Nuclear Forensics

Surrogates

T. A. Bredeweg, R. S. Rundberg, Organizers

8:15 NUCL 38. Mass transport in aerodynamic fallout glass from a near-surface nuclear explosion. **D. Weisz, S.G. Prussin, K. Knight, B. Jacobsen, N.E. Marks, I.D. Hutcheon**

8:40 NUCL 39. Constraints on fallout melt glass formation from a near-surface nuclear test. **G.R. Eppich, K.B. Knight, G. Spriggs, I.D. Hutcheon**

9:05 NUCL 40. Production of activation species for use with realistic surrogate debris materials. **B.B. Bandong**

9:30 NUCL 41. Forensic analysis of urban nuclear melt glass surrogates. **A.V. Giminaro**, J.P. Auxier, J.A. Gill, S.A. Stratz, C.J. Oldham, H.L. Hall

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Surrogates

A. Klingensmith, R. S. Rundberg, *Organizers*
T. A. Bredeweg, *Organizer, Presiding*

10:10 NUCL 42. Controlled pore glass materials as use for a surrogate nuclear explosion debris (SNED) material. **A.J. Carman**, B. Valenzuela, M.V. Snyder, M. Endres, M. Liezers, A. Prinke, G.C. Eiden

10:35 NUCL 43. Surrogate nuclear explosion debris methods: ICP-fluoridized bed reactor and agglomerated laser melt material. **M. Endres**, M. Liezers, G. Eiden, A.J. Carman

11:00 NUCL 44. Radiochemistry for the production of a realistic post-det surrogate debris. **N. Gharibyan**, K. Moody, P. Grant, S. Tumey, T. Brown, K. Roberts, D. Shaughnessy

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG† and NUCL

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, *Organizers, Presiding*

1:20 NUCL 45. Behavior of U(VI) silicate minerals and Np(V)-doped U(VI) silicates. **N. Wall**, S.B. Clark

1:40 NUCL 46. Production and decay studies of ²⁶⁵Sg for chemical studies of seaborgium using the gas-filled recoil ion separator GARIS at RIKEN. **H. Haba**

2:10 NUCL 47. Recent advances in uranium cluster chemistry research. **P.C. Burns**

2:40 NUCL 48. Use of projectiles with $Z \geq 20$ to produce heavy and superheavy elements. **C.M. Folden**

3:10 Intermission.

3:30 NUCL 49. Second break in the actinide series occurs at californium. **T.E. Albrecht-Schmitt**

4:00 NUCL 50. Heavy element studies at the University of Nevada Las Vegas. **R. Sudowe**, J. Despotopulos, J. Rolles

4:20 NUCL 51. Plutonium speciation during interaction with argillaceous rocks. **T. Reich**

4:50 NUCL 52. X-ray spectroscopy characterisation of radionuclide-NOM interaction. **M.A. Denecke**

5:20 NUCL 53. Plutonium uptake by mammalian cells. **M.P. Jensen**, B. Aynal, T. Paunesku, G. Woloschak

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Spectroscopic Methods

T. A. Bredeweg, A. Klingensmith, *Organizers*
R. S. Rundberg, *Organizer, Presiding*

1:00 NUCL 54. Spectroscopic signatures for forensic sciences. **N. Wozniak**, S.M. Clegg, K. Czerwinski, G.L. Wagner, M.P. Wilkerson

1:25 NUCL 55. Calibration of femtosecond laser ablation inductively coupled plasma mass spectrometer using a thermal inkjet picofluidic system for sensitive isotopic nuclear material characterization. **G.J. Havrilla**, K.G. McIntosh, J. Gonzalez, D. Oropeza, R. Russo, M.S. Morey

1:50 NUCL 56. FIER: A method for forensic attribution of fission mixtures using beta-delayed gamma-ray signatures. **E. Matthews**, B.L. Goldblum, B.J. Quiter

2:15 NUCL 57. Considerations when using scanning electron microscopy for nuclear forensics. **A.L. Tamasi**, G.L. Wagner, B. Scott, J.R. Walensky, M.P. Wilkerson

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Other

T. A. Bredeweg, R. S. Rundberg, *Organizers*
A. Klingensmith, *Organizer, Presiding*

2:55 NUCL 58. Electrochemistry of a modified-hematite film electrode for the detection of rhenium as a technetium analog. **L. Gribat**, H. Beyenal, N. Wall

3:20 NUCL 59. Stability constants and total dissolution of Tc(IV) and DTPA complexes. **T. Omoto**, N.A. Wall

3:45 NUCL 60. Cathodoluminescent signatures of neutron irradiation. **G.F. Peaslee**, D.K. Silletti, S. Brokus, J. Buscajgia

4:10 NUCL 61. Applications for nuclear forensics at the National Ignition Facility. **D.A. Shaughnessy**, K. Moody, N. Gharibyan, P. Grant, C. Yeamans, K. Holliday, J. Despotopulos

4:35 NUCL 62. Boron-rich benzene and pyrene derivatives for the detection of thermal neutrons. **H. Yamam**, A. Mahl, U. Koldemir, U. Greife, A. Sellinger

5:00 NUCL 63. Plutonium speciation Influence on the ²²Na yield from the ¹⁹F[α ,n] reaction. **W.M. Kerlin**, J.D. Despotopulos, D.D. Reilly, R. Sudowe, K. Czerwinski

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

50th Anniversary of the NUCL Division

T. E. Albrecht-Schmitt, J. Auxier II, D. E. Hobart, D. S. Peterson, D. A. Shaughnessy, D. K. Shuh, *Organizers*

J. C. Bralley, *Organizer, Presiding*

8:00 NUCL 64. Division of Nuclear Chemistry and Technology 50th Anniversary celebration. **D.E. Hobart**

8:30 NUCL 65. Division of Nuclear Chemistry and Technology (1990-2015). **D.C. Hoffman**

9:00 NUCL 66. Heavy element chemistry at Berkeley: A distinguished history with a promising future. **D.K. Shuh**

9:20 NUCL 67. Heavy element chemistry and separations science at Argonne National Laboratory: A current perspective. **J.V. Beitz**, **L. Soderholm**

9:40 NUCL 68. Decades of progress in actinide solution chemistry in NUCL/DNCT. **K.L. Nash**

10:00 Intermission.

10:20 NUCL 69. Fifty years of heavy element science: Understanding their elemental states. **R. Haire**

10:50 NUCL 70. NUCL and the ACS/DOE summer school in nuclear chemistry: A historical perspective. **P.A. Baisden**

11:10 NUCL 71. Helping build a future nuclear forensics and radiochemistry workforce: Education efforts within the Seaborg Institute at Lawrence Livermore National Laboratory. **A. Kersting**

11:30 NUCL 72. Thirty years of bridging the gap: The ACS Summer Schools in Nuclear and Radiochemistry. **J.D. Robertson**

11:50 NUCL 73. NUCL Division strategic plan. **P.F. Mantica**

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG† and NUCL

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

50th Anniversary of the NUCL Division

J. Auxier II, D. S. Peterson, D. A. Shaughnessy, D. K. Shuh, *Organizers*

T. E. Albrecht-Schmitt, D. E. Hobart, *Organizers, Presiding*

1:00 NUCL 74. Thermodynamics of actinide solution chemistry: Complexation by alpha-hydroxy organic acids in mixed solvent systems. **S.B. Clark**

1:20 NUCL 75. EMSL radiochemistry annex: A new international user-facility for the study of radiological samples. **N.J. Hess**

1:40 NUCL 76. Radiochemistry at Los Alamos National Laboratory: Past, present, and future. **D.S. Peterson**

2:00 NUCL 77. The Radiochemistry Center of Excellence at the University of Tennessee. **H.L. Hall**

2:20 NUCL 78. Molecular electronic structure theory applied to heavy-element chemistry: Some past accomplishments, present challenges, and future opportunities. **B.E. Bursten**

2:40 NUCL 79. Savannah River National Laboratory and [NUCL] a joint history. **M.G. Bronikowski**

3:00 Intermission.

3:20 NUCL 80. Online chemistry research at Texas A&M University. **C.M. Folden**

3:40 NUCL 81. Protactinium: Chemistry at the intersection of the 5f and 6d elements. **R. Wilson**, S. De Sio, V. Vallet

4:00 NUCL 82. Radiotracers for biological, environmental, and medical applications. **S.S. Jurisson**

4:20 NUCL 83. Recent advances in molecular f-element chemistry centered on TRU elements. **J.L. McDonald**, A. Gaunt

4:40 NUCL 84. High field and high frequency EPR study of isotopic heterobimetallics. **K. Diefenbach**, T.E. Albrecht-Schmitt

5:00 NUCL 85. Microstructural characterization of structural alloys for nuclear energy applications. **M. Li**

5:20 NUCL 86. Optimization and characterization of a molecular plating technique for homogenous thin film samples. **A. Roman**, R.S. Rundberg

WEDNESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

50th Anniversary of the NUCL Division

T. E. Albrecht-Schmitt, J. Auxier II, J. C. Bralley, D. E. Hobart, D. S. Peterson, *Organizers*

D. A. Shaughnessy, D. K. Shuh, *Organizers, Presiding*

8:00 NUCL 87. Fission and the DNCT. **W. Loveland**

8:20 NUCL 88. Nuclear shape triaxiality in neutron-rich niobium isotopes. **J.O. Rasmussen**, Y.X. Luo, Y. Liu

8:40 NUCL 89. Exploiting fast neutrons: From nuclear structure to neutrinoless double-beta decay. **S.W. Yates**

9:00 NUCL 90. New opportunity: Coincident spectroscopy in neutron-deficient actinides. **O.R. Gothe**, K.E. Gregorich, B. Baartman, P. Fallon, N. Esker, J.T. Kwarisick, A. Machiavelli, P. Mudder, D. Olive, G.K. Pang, J. Rissanen, H. Nitsche

9:20 NUCL 91. Comparing nuclear counting statistics with the network statistics. **S.E. Beach**, **T.M. Semkow**, D.J. Remling

9:40 NUCL 92. Working toward measurement of nuclear structure in superheavy elements. **K.E. Gregorich**

10:00 Intermission.

10:20 NUCL 93. Response of actinide materials to highly ionizing radiation. **R.C. Ewing**

10:40 NUCL 94. Reductive routes to low-oxidation states actinide materials. **T.E. Albrecht-Schmitt**

11:00 NUCL 95. Determination of Pu in spent nuclear fuel: Results from field testing of high resolution X-ray (hiRX). **G.J. Havrilla**, K.G. McIntosh, R. Gilmore, D. Missimer, M. Holland

11:20 NUCL 96. Accumulation of specific nuclides by fish bodies in Fukushima-Ken (Prefecture) EEZ (Exclusive Economic Zone), Japan in November 2012. **H. Katsura**

11:40 NUCL 97. Cost effective tank waste characterization at the Savannah River site. **S.H. Rebound**, D.P. Diprete, J.M. Pareizis, F.G. Smith, R.H. Young

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Convergence of Theory & Experiment in Heavy Element Chemistry

A. P. Sattelberger, D. K. Shuh, L. Soderholm, *Organizers, Presiding*

8:20 NUCL 98. Elucidation of redox properties, structures, and bonding for cerium and uranium complexes through DFT and experiment. **E.J. Schelter**

8:40 NUCL 99. Water adsorption on AnO₂ (An = U, Np, Pu) surfaces. **J.P. Wellington**, A. Kerridge, **N. Kaltsayannis**

9:00 NUCL 100. Evaluation of the coordination chemistry and reactivity of trimethylsilylani- lido and phosphinimide complexes of U and Th. **R.K. Thomson**

9:20 NUCL 101. Structure and stability of uranyl(VI) and uranium(VI) imido complexes with high-nitrogen ligands. **K.A. Maerzke**, N. Henson, J. Veauthier, J.L. Kiplinger

9:40 NUCL 102. Bonding and magnetism in tris-cyclopentadienyl neodymium and uranium complexes and their isocyanide adduct. **W.W. Lukens**, R.A. Andersen, N.M. Edelstein, P. Yang, M. Speldrich

10:00 Intermission.

10:20 NUCL 103. Experimental and theoretical determinations of covalency in d- and f-block metal oxides. **S.G. Minasian**, E.R. Batista, C. Booth, J.M. Keith, W.W. Lukens, S.A. Kozimor, R.L. Martin, D. Nordlund, D.K. Shuh, D. Sokaras, T. Tylliszczak, X. Wen, T. Wang

10:40 NUCL 104. Strong correlations and covalency in actinide materials. **R.L. Martin**

11:00 NUCL 105. Toward controlling the formation of cation-cation interactions in neptunyl(V) compounds. **G. Jin**, S. Skanthakumar

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at:

www.acs.org/denver2015

11:20 NUCL 106. Combined structural characterization, raman spectroscopy, and theory to promote an enhanced understanding of aqueous speciation. T. Forbes, M.C. Basile, J. de Groot

11:40 NUCL 107. Characterisation of actinide selective N-donor extractants using spectroscopic and quantum theoretical methods. M.A. Denecke

WEDNESDAY AFTERNOON

Section A

Embassy Suites Denver—Downtown Convention Center

Crestone Ballroom A

50th Anniversary of the NUCL Division

T. A. Albrecht, J. C. Braley, D. E. Hobart, D. A. Shaughnessy, D. K. Shuh, *Organizers*
J. Auxier II, D. S. Peterson, *Organizers, Presiding*

1:00 NUCL 108. Actinide interactions with aminopolycarboxylates: Heavy element curiosities. J. Braley

1:20 NUCL 109. Advances in organometallic chemistry at the bottom of the periodic table. J.L. Kiplinger

1:40 NUCL 110. Use of molecular dynamics to evaluate tributyl phosphate and diamylmethyl phosphonate containing systems. M. Servis, J.C. Braley, D. Wu

2:00 NUCL 111. Historical overview of radioisotope thermolectric generators. C.E. Whiting

2:20 NUCL 112. Characterization of actinide reactivity and speciation at mineral:water interfaces. B.A. Powell, S.L. Estes, D. Kaplan, A. Kersting, M. Zavarrin

2:40 NUCL 113. Enhanced immobilization of iodine by biochar in soil-water system. D. Zhang, L. Wang, H. Zhao

3:00 NUCL 114. Studies on the thermodynamics of trivalent lanthanide/actinide extraction by tri-*n*-octylphosphine oxide and bis(2-ethylhexyl) phosphoric acid. T.S. Grimes, P.R. Zalupski, L.R. Martin

3:20 Intermission.

3:40 NUCL 115. Specific recognition and enhanced luminescence sensitization of trivalent actinides. R.J. Abergel, B.E. Allred, M. Sturzbecher-Hoehne, A. Dalo

4:00 NUCL 116. Minor actinide separations using a combination of a dithiophosphinic acid and a synergist. D.R. Peterman, P.R. Zalupski, J.R. Kleahn

4:20 NUCL 117. Probing for differences in the electronic properties of actinides and lanthanides using 1,10-phenanthroline-2,9-dicarboxylic acid. S.K. Cary, T.E. Albrecht-Schmitt

4:40 NUCL 118. Structural and electronic variations in *f*-block containing plumbite clusters. J.T. Stritzinger, K. Pace, T.E. Albrecht-Schmitt

5:00 NUCL 119. Supramolecular coordination polymers of lanthanide and actinide metals featuring the 1,8-naphthalimide tecton. A. Leitner, D.L. Reger, M.D. Smith

5:20 NUCL 120. Ionothermal flux syntheses of isomorphous metalborate clusters. G. Parker, A.L. Chown, T.E. Albrecht-Schmitt

Section B

Embassy Suites Denver—Downtown Convention Center

Crestone Ballroom B

Convergence of Theory & Experiment in Heavy Element Chemistry

D. L. Clark, A. P. Sattelberger, D. K. Shuh, L. Soderholm, *Organizers, Presiding*

1:20 NUCL 121. Correlation between single-atom adsorption enthalpies and solid-state properties. H.W. Gaeggeler

1:40 NUCL 122. Predicting the redox potentials of actinide complexes (An=U, Np, Pu) using first-principles. W. Huang, J. Li, P. Yang

2:00 NUCL 123. Actinide chemistry in the gas phase: A fruitful interplay between experiment and theory. J.K. Gibson

2:20 NUCL 124. Exploring the highest oxidation state in actinide compounds. J. Li

2:40 NUCL 125. Spectroscopy and structure of the simplest actinide bonds. M.C. Heaven, J. Bartlett, R. VanGundy

3:00 NUCL 126. Experimental and quantum chemical studies of alkali-ion promoted formation of uranyl(VI) peroxide rings and a comparison with similar reactions in 12-crown-5 and 15-crown-5 systems. V. Vallet, P. Zanonato, P. Di Bernardo, Z. Szabo, I. Grenthe

3:20 Intermission.

3:40 NUCL 127. Integration of computational modeling and experiments in actinide chemistry. W. Dejong, S. Odoh, Y. Gong, J.K. Gibson

4:00 NUCL 128. Toward accurate ab initio thermochemistry for molecules containing *f*-block elements. K.A. Peterson, D.A. Dixon

4:20 NUCL 129. Reactivity of aqueous thorium(IV) and plutonium(IV) clusters. M. Vasiliu, K. Knope, L. Soderholm, D.A. Dixon

4:40 NUCL 130. Tetravalent actinide-small organic molecule containing compounds. K.E. Knope

5:00 NUCL 131. Theoretical study of the electronic spectrum of the UO and UO⁺ molecules. R. Tyagi, Z. Zhang, R.M. Pitzer

5:20 NUCL 132. Solution and gas phase solvation of *f*-element ions in binary water/methanol solutions. M. Kelley, A.E. Clark, S.B. Clark

THURSDAY MORNING

Section B

Embassy Suites Denver—Downtown Convention Center

Crestone Ballroom B

Convergence of Theory & Experiment in Heavy Element Chemistry

D. L. Clark, A. P. Sattelberger, D. K. Shuh, L. Soderholm, *Organizers, Presiding*

8:20 NUCL 133. Computational studies of actinide and metal oxides, fluorides, and chlorides. D.A. Dixon, K.A. Peterson

8:40 NUCL 134. Combining theory with experiment to understand aggregation in solvent extraction systems for heavy element separations. R.J. Ellis, B. Qiao, T. Demars

9:00 NUCL 135. Role of ionic solute vs. amphiphilic solute on local interfacial properties. Y. Ghadar

9:20 NUCL 136. Examining covalency in actinide complexes with soft donor ligands and metal-ligand multiple bonding. J.R. Walensky, A. Behre

9:40 NUCL 137. Revealing the hydration of thorium(IV) with combined techniques involving EXAFS, HEXS and molecular dynamics simulations. F. Réal, V. Vallet, M. Masella, Y. Hu, S. Skanthakumar, L. Soderholm

10:00 Intermission.

10:20 NUCL 138. Effects of strong π -donors on actinides: bent uranyl(VI) and molecular Pu(IV). M. Silver

10:40 NUCL 139. Covalency in *f*-element materials probed with ligand K-edge X-ray absorption spectroscopy. E.R. Batista

11:00 NUCL 140. Solvation thermodynamics of trivalent actinide (An=U, Np and Pu) ions using polarizable force field. P. Pamar, Y. Ghadar, A.E. Clark

11:20 NUCL 141. Divergence between plutonium and americium in oxoanion materials. T.E. Albrecht-Schmitt

11:40 NUCL 142. Combined theoretical and experimental study of the binding features of the super uranyl-binding protein.

L. Gagliardi, S. Odoh, G. Bondarevsky, J. Karpus, C. He, Q. Cui, R. Spezia

ORGN

Division of Organic Chemistry

M. C. McIntosh and R. D. Broene, *Program Chairs*

SUNDAY MORNING

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*

P. Willoughby, *Presiding*

8:00 ORGN 1. New synthetic approaches to biologically active amino containing natural products: Total synthesis of oxybenzophenanthridines. E.D. Calder, Fl. McGonagle, A.H. Harkiss, G.A. McGonagle, S.A. Sharif, A. Sutherland

8:20 ORGN 2. Development of complexity generating and stereoselective carbon carbon bond forming reactions. B.J. Cowen

8:40 ORGN 3. Rh(III)-catalyzed C-H activation of *N*-enoxyphthalimides. T. Piau, T. Rovis

9:00 ORGN 4. Regioselective C-H activation of azine *N*-oxides in arylation and dimerization. D.E. Stephens, J. Lakey-Beitia, A.C. Atesin, T. Atesin, G. Chavez, H. Arman, O. Larionov

9:20 ORGN 5. Butyrolactone synthesis via polar radical crossover cycloaddition reactions: Diastereoselective synthesis of methyl-lactocin and protolichsterinic acid. M. Zeller, M. Riener, D.A. Nicewicz

9:40 ORGN 6. A K₂CO₃ mediated regioselective synthesis of indole/pyrrole-fused 1,4-oxazines: An unexpected indole-fused azlactone synthesis. J. Vandavasi, W. Hu, J. Wang

10:00 ORGN 7. Metal- and reagent-free highly selective anodic cross-coupling reaction. D.R. Waldvogel, B. Elsler, D. Schollmeyer, K. Dyballa, R. Franke

10:20 ORGN 8. Surprising organic synthesis: Serendipitous discovery of a novel cascade process. J.A. Simanis, E.L. Woodall, C.M. Law, C.G. Hamaker, J.R. Goodell, T.A. Mitchell

10:40 ORGN 9. Near-IR uncaging chemistry: discovery, and applications. M.J. Schnermann

11:00 ORGN 10. Synthesis of *N*-phthalimido-*O*-acyl-*N,O*-acetals from aldehydes and their conversion into β -branched phthalimides. P.H. Willoughby, R.N. Enright, L.T. Henningsen, L.I. Wurtz, E.R. Cliff, J.L. Grinde

11:20 ORGN 11. Pentadehydro-Diels-Alder (PDDA) reaction Part 2: Cycloadditions of allenynes with nitriles to give pyridine derivatives. R. Naredla, T. Wang, T.R. Hoye

Section D

Colorado Convention Center
Room 708

Asymmetric Reactions and Syntheses

M. C. McIntosh, *Organizer*

E. S. Spahn, *Presiding*

8:00 ORGN 12. Insights into the enantioselectivity of monoprotected amino acid assisted C-H activation reaction. G. Cheng, P. Chen, T. Sun, J. Yu, X. Zhang, Y. Wu

8:20 ORGN 13. Enantiodivergent hydrovinylation reaction. S. Biswas, J.P. Page, T. RajanBabu

8:40 ORGN 14. Asymmetric hydrovinylation of siloxydienes: Making enantio-pure nucleophilic synthons. S. Biswas, J.P. Page, T. RajanBabu

9:00 ORGN 15. Expedient synthesis of chiral polysubstituted 1,4-oxazepanes. M. Bezanson, J. Pottel, N. Moitessier

9:20 ORGN 16. New strategy for the asymmetric conjugate addition of acetylenes to activated olefins via sequential palladium and copper catalysis. B.M. Trost, J.T. Masters, B.R. Taft, J.G. Lumb

9:40 ORGN 17. Development of an enantio- and diastereoselective Simmons-Smith bromocyclopropanation reaction and mechanistic considerations. S. Taillemaud, N. Diercxsens, A. Gagnon, A.B. Charette

10:00 ORGN 18. Kinetic resolution of 2-aryl cyclohexanols via asymmetric silylation. L. Wang, R. Akhani, S.L. Wiskur

10:20 ORGN 19. Efficient synthesis of enantio-pure lignin models and their catalytic oxidation using cobalt-Schiff base complexes. C. Nijjob, J.J. Bozell, B.K. Long

10:40 ORGN 20. Development of an asymmetric synthesis of Letermovir exploiting a novel PTC-catalyzed aza-Michael reaction. G.R. Humphrey, Z. Song, S. Dalby, B. Xiang, T. Andreani, K.M. Belyk, A. Tschaen

11:00 ORGN 21. Phosphonate-directed catalytic asymmetric hydroboration. S. Chakraborty, R. Carr, J.M. Takacs

11:20 ORGN 22. Toward the reproducibility of Cu(PHET) hydrosilylations. E.S. Spahn, M.C. McIntosh, R.E. Gawley

Section E

Colorado Convention Center
Room 702

Materials, Devices and Switches

M. C. McIntosh, *Organizer*

D. J. Dibble, *Presiding*

8:00 ORGN 23. Multiscale simulations of morphology and charge-transport in oligothiophenes. S.A. Lopez, I. Yavuz, L. Zhang, B.P. Cherniawski, A.L. Briseno, K.N. Houk

8:20 ORGN 24. Withdrawn.

8:40 ORGN 25. New organic conjugated molecules toward semiconducting and light-emitting materials. D. Zhang

9:00 ORGN 26. Graphene oxide coupled metal oxide nanosheets incorporating small organic molecules for *n*-type and *p*-type field effect transistors (FETs). M. Samal, N. Barange, K. Yun

9:20 ORGN 27. Tunable electronic and spin-tropic properties in highly conjugated multi-[(porphinato)metal] oligomers. R.C. Bruce, R. Wang, M.J. Therien, W. You

9:40 ORGN 28. Protein-based protonic transistors. D.D. Ordinario, L. Phan, J. Jocsos, T. Nguyen, A.A. Gorodetsky

10:00 ORGN 29. Synthesis and electrochemical characterization of oligonucleotide-inspired organic nanowires. A. Mazaheripour, N. Hüsken, J. Jocsos, A.M. Burke, A.A. Gorodetsky

10:20 ORGN 30. Better than metals: Cyanostar macrocycles stabilize and switch organic anion radicals. C. Benson, A.H. Flood

10:40 ORGN 31. Withdrawn.

11:00 ORGN 32. Chemistry of boron-doped graphene flakes. S. Yamaguchi

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

Ronald Breslow Award for Achievement in Biomimetic Chemistry: Symposium in Honor of Eric T. Kool

K. Walker, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 33. Mimicry of protein tertiary structures by expanding beyond natural constraints of covalent connectivity in biological sequences. W.S. Horne

1:50 ORGN 34. Carbene and nitrene transfer reactions catalyzed by engineered hemoproteins. R. Fasan

2:35 ORGN 35. Looking beneath the surface to determine what makes DNA damage deleterious. M.M. Greenberg

3:20 Introduction of Awardee.

3:25 ORGN 36. Award Address (Ronald Breslow Award for Achievement in Biomimetic Chemistry sponsored by the Ronald Breslow Award Endowment). Designer DNA bases: Probing molecules and mechanisms in biology. E.T. Kool

Section B

Colorado Convention Center
Four Seasons Ballroom 1

Development of Direct C-H Functionalization Processes towards the Synthesis of Biologically Active Compounds

J. Mousseau, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 37. C–H functionalization: Can we leverage cutting-edge synthetic methods to enhance drug discovery? A.F. Stepan

1:35 ORGN 38. C–H bond functionalization cascades for the synthesis of complex heterocycles. J.A. Ellman

2:25 ORGN 39. Selective functionalization of alkyl and aryl C–H bonds — installation of temporary functional groups. J.F. Hartwig

3:15 ORGN 40. High-throughput experimentation methods in the development of direct functionalization reactions. L. Campeau

4:05 ORGN 41. Studies in natural product synthesis. P.S. Baran

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
S. Blakey, *Presiding*

1:20 ORGN 42. Development of Corey-Seebach *umpolung* reagents in palladium-catalyzed cross-coupling reactions. S. Baker Dockrey, J.R. Schmink

1:40 ORGN 43. Palladium-catalyzed decarboxylative C–C bond formation of secondary benzyl electrophiles. S.N. Mendis, J.A. Tunge

2:00 ORGN 44. Withdrawn.

2:20 ORGN 45. Catalyst development for enantioselective atom transfer C–H functionalization reactions. S. Blakey

2:40 ORGN 46. Triphenylphosphine promoted hydroalkoxylation of divinyl sulfone: An *ol-ene* “Click” reaction? S. Strasser, C. Slugovc, I. Hanghofer, A. Eder

3:00 ORGN 47. *N*-Boc amines to oxazolidones via Pd(II)/Bis-sulfide/Bronsted acid co-catalyzed allylic C–H oxidation. T.J. Osberger, M.C. White

3:20 ORGN 48. Photoredox catalysis in a complex pharmaceutical setting. J. Douglas, K.P. Cole, C. Stephenson

3:40 ORGN 49. Rhodium (I) catalyzed carbon-carbon bond activation: Decarbonylation of ynones. R. Whittaker, G. Dong

4:00 ORGN 50. New dehydrative glycosylation with phosphonium anhydrides. L. Dockery, R. Dyapa, M.A. Walczak

4:20 ORGN 51. Epoxide approach towards the synthesis of the polypropionate acid moiety of dolabriferol. K. Morales, J.A. Prieto

4:40 ORGN 52. One-pot tandem cyclization of alkynes to generate polycyclic products. R.A. Carmichael, A. O’Loughlin, W.A. Chalfoux

Section D

Colorado Convention Center
Room 708

Asymmetric Reactions and Syntheses

M. C. McIntosh, *Organizer*
D. Coltart, *Presiding*

1:00 ORGN 53. Methodological study of a proposed, asymmetric Rauhut–Currier reaction/aldol condensation and current efforts to synthesize the anticancer agent xenitorin A. J.E. Dander, B. Chandler

1:20 ORGN 54. Catalytic, stereoselective vicinal difunctionalization of alkenes. S.T. Eey, A.J. Cresswell, S.E. Denmark

1:40 ORGN 55. Lewis base catalyzed, enantioselective, intramolecular sulfenamination of olefins. H. Chi, S.E. Denmark

2:00 ORGN 56. Progress and efforts toward the asymmetric total synthesis of antascomycin B. B. Walker, M.C. McIntosh

2:20 ORGN 57. Enantioselective [2+2] cycloadditions using visible light photocatalysis. K.L. Skubi, J. Du, D.M. Schultz, T.P. Yoon

2:40 ORGN 58. Pd(II)/Bronsted acid catalyzed enantioselective oxidative carbocyclization-borylation of enallenes. T. Jiang, T. Bartholomeyzyk, J. Mazuela, J. Willersinn, J. Bäckvall

3:00 ORGN 59. Asymmetric synthesis of piperidines by zinc-catalyzed [4+2] cycloaddition of 1-azadienes and nitro-alkenes. C. Chu, D. Dalton, T. Rovis

3:20 ORGN 60. Organocatalyzed enantioselective conjugate addition of heteroaryl and aryl trifluoroborates and application to the synthesis of discopipryrole D. J. Shih, T.S. Nguyen, J. May

3:40 ORGN 61. Highly enantioselective preparation of chiral amines by direct asymmetric hydrogenation of ketoximes and by direct asymmetric reductive amination of ketones. P. Ryberg

4:00 ORGN 62. Highly efficient enantioselective hydrogenation of *N*-alkyl-pyridinium salts with an iridium-phosphate catalyst. Y. Chen, M. Chang, Y. Huang, S. Liu, S.W. Kraska, I.W. Davies, X. Zhang

4:20 ORGN 63. Development of iridium (III) bis(imidazolyl)phenyl complexes for enantioselective atom transfer C–H functionalization with acceptor-only metallocarbenes. N.M. Weldy, C. Owens, A. Schaefer, C. Herting, S. Blakey

4:40 ORGN 64. Umpolung approach to the asymmetric α -alkylation of aldehydes and ketones. D.M. Coltart

Section E

Colorado Convention Center
Room 702

Nanomaterials
Chemistry of Fullerenes

M. C. McIntosh, *Organizer*
C. C. Kirkpatrick, *Presiding*

1:30 ORGN 65. Chemical sensing with porous molecular crystals. C.H. Hendon, A. Walsh

1:50 ORGN 66. Shape-persistent macrocycles conjugated with biomacromolecules and nanoparticles. K.D. Okochi, D. Domaille, J. Cha, W. Zhang

2:10 ORGN 67. Extension of air stability in organic light-emitting diodes using MoS₂ and WS₂ synthesized by chemical vapor deposition. K. Kwon, C. Kim, L. Quyet, S. Kim, H. Jang

2:30 ORGN 68. How to get selective organo(hydro)fullerenes through Rh/organoboron combination. A. Poater, J. Martinez, M. Solà

2:50 ORGN 69. Exploiting the unique properties of carbon nanotubes for unprecedented biological applications. C.J. Serpell, B.G. Davis

3:10 ORGN 70. High level computational study of C60-*X*- systems (*X*=F-, Cl-, Br-) using LPNO-CEPA/1/CBS and MP2/CBS variants. B. Welch, C.C. Kirkpatrick

3:30 ORGN 71. Computational studies of the interaction between carbon nanotubes and aromatic species: Energy components and SAPT methods. C.C. Kirkpatrick, P. Bruce-Vanderpuije

SUNDAY EVENING
Section A

Colorado Convention Center
Hall C

Asymmetric Reactions and Syntheses; Chemistry of Fullerenes, Carbon Nanotubes, and Graphene; Materials, Devices and Switches; Nanomaterials; Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species; Total Synthesis of Complex Molecules

R. D. Broene, *Organizer*

8:00 - 10:00

ORGN 72. Chiral transfer in nucleophilic reactions using chiral ionic liquids. H.M. Thorfinnson, M.D. Mosher **ORGN 73.** Asymmetric synthesis of β -amino nitriles via Mannich reactions of silyl ketene imines. J. Zhao, X. Feng

ORGN 74. Asymmetric synthesis of spiro-epoxyindoles by the catalytic Darzens reaction of isatins with phenacyl bromides. Y. Kuang, X. Feng

ORGN 75. Asymmetric synthesis of 2,3-dihydroquinolin-4-one derivatives catalyzed by a chiral bisguanidium salt. X. Xiao, X. Feng

ORGN 76. Stereoselective preparation of 3, 5-disubstituted pyrrolidine-3-carboxylic acids as catalysts in asymmetric Aldol and Mannich reactions. H. Kotapati, J. Robinson, D.S. Masterson

ORGN 77. Catalytic asymmetric synthesis of tetrahydroquinolines via tandem 1,5-hydride transfer/Ring closure. W. Cao, L. Lin, X. Feng

ORGN 78. Catalytic asymmetric [3 + 2] cycloadditions about oxiranes by C–C bond cleavage of epoxides. L. Lin, W. Chen, X. Feng

ORGN 79. Reactions of KPPh₃ with cyclopalladated complexes containing an (sp)²C–Pd bond. G.C. Dickmu, I.P. Smoliakova

ORGN 80. Synthesis of a transition state analog for mechanistic study of catalytic enantioselective reactions. X. Wang, L. Morrill, D.G. Alberg, G.E. Hofmeister

ORGN 81. Silylation-based kinetic resolution of 2-aryl cyclohexanols. L. Wang, R. Aghani, S.L. Wiskur

ORGN 82. Synthesis of all carbon quaternary aldehydes by palladium catalyzed asymmetric allylic alkylation (Pd-AAA): Toward the synthesis of Horsfiline. M. Asad, M. Hossain

ORGN 83. Withdrawn.

ORGN 84. β -D-carbafuropyranosyl-1,2-diamine-derived salen emerges as a promising new chiral ligand from a miniaturized enzymatic screen (ISES). K.R. Karukurichi, X. Fei, R.A. Swyka, S. Broussy, W. Shen, S. Dey, S.K. Roy, D.B. Berkowitz

ORGN 85. *N,N'*-dioxide-scandium(III)-catalyzed asymmetric Friedel–Crafts reactions of phenol derivatives. S. Bai, X. Feng

ORGN 86. Synthesis and reaction of silyloxy vinylketene iron complexes. O. Kool, Y. Guo

ORGN 87. Hydrogen bond mediated enantioselective catalysis by Werner complexes. S.K. Ghosh, J.A. Gladysz

ORGN 88. Synthesis of chiral sultines and derivatives: Investigation of the effect of sulfur atom in the helicity of phenyl rings. D.R. Viemes, C.S. Jungong, V.S. Kandula, C.K. Wach, A.G. Goos, D.J. Kerwood, D.C. Dittmer

ORGN 89. Asymmetric isomerization of alkynyl to allenyl aldehydes bearing a traceless organo-manganese η^2 -auxiliary. A. Roy, B. Bhat

ORGN 90. Catalytic asymmetric intermolecular Stetter reaction of aldehydes and α,β -unsaturated ketones. D. Flanigan, T. Rovis

ORGN 91. Construction of trifluoromethylated all carbon quaternary stereocenters using Friedel–Crafts alkylation of arenes. H. Subramanian, M.P. Sibi

ORGN 92. Development of novel carboxylate-containing N-heterocyclic carbenes and their application towards new and enhanced chemical transformations. A. Munoz, T. Rovis

ORGN 93. Effect of added acid on the diastereoselective synthesis of chiral β -substituted [3.3.0]-bicyclic lactams. P.T. Buonora, H. Abriam, L. Ung, D. Nugyen

ORGN 94. Studies on the synthesis of terpene-derived chiral ketone and iminium salt catalysts for asymmetric olefin epoxidation. K.R. Overly, C. Williams, J. Bouchard, A. Trainor

ORGN 95. Catalytic enantioselective synthesis of 2-aryl chromenes. B. Zeng, K. Scheidt

ORGN 96. Rapid synthesis of 3,3'-bis-arylated BINOL derivatives using a C–H borylation in situ Suzuki–Miyaura coupling sequence. I. Ahmed, D.A. Clark

ORGN 97. Dynamic kinetic resolution (DKR) of atropisomers by fluxional DMAP catalysts. G. Ma, M.P. Sibi

ORGN 98. Aza-MIRC reactions. Asymmetric synthesis of trifluoromethyl substituted aziridines. R. Moorthy, M.P. Sibi

ORGN 99. Stereodynamic catalysts: Bidirectional enantioselectivity controlled by temperature. G. Storch, O. Trapp

ORGN 100. Synthesis of arylamine tribenzopentaphenes and investigation of their hole mobility. B.A. Alameddine, C.K. Luscombe, T. Jenny

ORGN 101. Synthetic tuning of the electronic properties of fused-ring oligothiophenes. M.J. Kleinsasser, C.B. McCausland, E.J. Uzalac, S.C. Rasmussen

ORGN 102. Bent-core 6-oxoverdazyls — a new class of mesogens. S. Ciastek, M. Jasinski, D. Pocięcha, H. Monobe, J. Szczytko, P. Kaszynski

ORGN 103. Polar liquid crystals based on pyridinium zwitterions of the [*clos*-1-CB_nH₁₀] and [*clos*-1-CB_nH₉] anions. J.G. Pecyna, B. Ringstrand, P. Kaszynski

ORGN 104. Synthesis of photoreleasable protecting groups. M.L. Hunsley, S.M. Reed

ORGN 105. Colorimetric investigation of responsive catechol-based coatings inspired by melanin. S.L. Lewandowski, L.M. Choban, S.A. Flatt, J.M. Belitsky

ORGN 106. Hydrogen peroxide sensing for reproductive health. R.S. Purdey, E.P. Scharfner, T.M. Monro, R.J. Aitken, J.G. Thompson, A.D. Abell

ORGN 107. Reversible switching of chiral DNA-templated metalloporphyrin nanoassemblies. S. Tannir, G. Sargsyan, M. Balaz

ORGN 108. Design and synthesis of a new switchable [2]rotaxane with a rhodamine B and pyrene as two fluorescent stoppers. J. Shi, X. Bao

ORGN 109. Synthesis of crosslinked membranes based on polyvinyl alcohol and naphthalene diimides. R. Altamimi

ORGN 110. Formulation of conductive carbon aerogels from polysaccharide-based sources. A.A. Jauregui, B.R. Luginbuhl, B.D. Cutler, C.C. Browder

ORGN 111. Electrical optimization of agar-derived carbon aerogels for use in structural electric double-layer capacitors. B.R. Luginbuhl, B.D. Cutler, A. Jauregui, C.C. Browder

ORGN 112. Naphthalene diimide based materials with adjustable redox potentials for organic lithium ion batteries. G. Vadehra, R.P. Maloney, B. Dunn, M.A. Garcia-Garibay

ORGN 113. Thermoluminescent boron compounds: Synthesis, characterization, and photophysical properties. A.A. Molina Paredes, B. Muñoz

ORGN 114. Small molecular donor-acceptor dyads as additives for organic photovoltaics. D. Chavis, J. Strain, H.P. Rathnayake

ORGN 115. Fused arenes-based molecular systems as additives for organic photovoltaics. D. Patel, R. Nees, H.P. Rathnayake

ORGN 116. Mechanochromic luminescent heteroaromatic difluoroboron β -diketonate complexes. M. Kolpaczynska, W. Morris, C.A. DeRosa, C.L. Fraser

ORGN 117. Novel route to synthesize polymers containing single mechanical bond.
U. Choudhary, B.H. Northrop

ORGN 118. Synthesis and photochemical properties of bis (4'-azo-4" (5)substituted dibenzo-18-crown-6) carboxylic acid derivatives. **R. Khatmullin**

ORGN 119. Poly(1,4-phenylene vinylene) derivatives with ether substituents to improve polymer solubility for use in organic light-emitting diode (OLED) devices.
C.A. Young, T. Lee

ORGN 120. Novel ionic liquid crystals based on nitrile functionalized imidazolium.
T.A. Sanders, L. Douce, B. Heinrich

ORGN 121. Preparations and self-assembly study of gold nanoparticles composed with discotic organic molecules. **Y. Mi**, P. Liang, D. Wang, Z. Yang

ORGN 122. Proton-electron dual responsive system of ferrocene-bound nickeladithiolene. **A. Tanushi**, T. Kusamoto, Y. Hattori, K. Takada, H. Nishihara

ORGN 123. Substituent and solvent effects: Examining acidity via infrared spectroscopy.
J.E. Buhle, M. Samet, S.R. Kass

ORGN 124. Mechanism and stereoselectivity of an isothiourea-catalyzed [2,3]-rearrangement: Control via electrostatics and orbital interactions. **D.M. Walden**, T.H. West, R.C. Johnston, A.D. Smith, P.H. Cheong

ORGN 125. Computational study of diaryliodonium reagents for heteroatom arylation reactions. **J. Buchanan**, S.K. Sundaram, D.R. Stuart, P.H. Cheong

ORGN 126. Highly efficient and selective epoxidation catalyzed by iron corrole complexes and iodobenzene diacetate. **T. Chen**, K. Kwong, W. Luo, A.C. Carver, R. Zhang

ORGN 127. Visible light-promoted selective sulfoxidations catalyzed by ruthenium porphyrins with iodobenzene diacetate. **W. Luo**, T. Chen, Z. Yuan, A.C. Carver, R. Zhang

ORGN 128. Synthetic and mechanistic studies of catalytic oxidations by manganese(III) porphyrins and iodobenzene diacetate. **K. Kwong**, T. Chen, W. Luo, R. Zhang

ORGN 129. Synthesis and photophysical studies of two lophine derivatives with electron-donating groups on the aryl ring in the 2-position. **T. Le**, T. Hamada, J. Rimby, R.A. Isovitsch

ORGN 130. Kinetics of retro-hetero-Diels-Alder reactions to model controlled release from novel sulfonamide drug-polymer conjugates. **C.S. Erkkila**, N.A. Yakelis

ORGN 131. Phenylchlorocarbene additions to diarylcyclooctenes and diarylcyclooctenes. **E. Dalchand**, S. Tsuno, A. Scoresse, K. Francisco, C. Buzard, D.C. Merrer

ORGN 132. Getting beyond frontier molecular orbital theory to predict regioselectivity of nucleophilic aromatic photosubstitution reactions. **G.G. Wubbels**

ORGN 133. Computational investigations into stereoselective alkylation reactions: Evidence for torsional and Curtin-Hammett control. **A.M. Harned**

ORGN 134. Radical viologen organic spin cross over materials. **M.J. Juetten**, A. Winter

ORGN 135. Density functional theory treatment of substituent effects on the amide-acetal Claisen rearrangement. **M. Hartley**, G.W. Daub, R.J. Cave

ORGN 136. Computational mechanistic study on hexadecylo-Diels-Alder reactions.
L.R. Furan, K.T. Kuwata

ORGN 137. Fluoro-amide and fluoro-sulfonamide gauche effects: An experimental study. **B.U. Emenike**

ORGN 138. Abnormal substrates give "abnormal" products: Competition between classical Diels-Alder vs. hexadecylo-Diels-Alder (HDDA) reactions. **Q. Luu Nguyen**, B. Baire, T.R. Hoyer

ORGN 139. Sterically demanding bis-(o-bi-phenyl)-phosfine ligands in gold(I) catalysis. **C. Griebel**, D.D. Hodges, A.C. Jones

ORGN 140. Investigation of spin coated pristine and blended organic semiconductor films containing perylene dimides: The role of molecular structure and crystal formation in blended film composition. **J.M. Szarko**, A. Austin, E. Xhakaj, S. Liu

ORGN 141. DFT study of phosphine-borane bonds: Exploring electronic effects.
PA. Sibbald

ORGN 142. Expeditious, radical pathway for sonication assisted Mitsunobu reaction of hindered secondary alcohols. **R. Florre**, R. Heckler, P. Cohn, S. Rajaraman

ORGN 143. Mechanistic studies on the catalytic oxidative cyclization reactions of 2'-arylbenezaldehyde oxime ethers. **N.R. Amada**, J. Hofstra, B. Grassbaugh, Q. Tran, P. De Lijser

ORGN 144. Solution photophysics of α -carborane carrying one or two singlet-fission chromophores (1,3-diphenylisobenzofuran). **Y. Hervault**, J. Schrauben, M. Schreiber, J.C. Johnson, J. Michl

ORGN 145. (f-Bu)₂P(O-dimethylaminophenyl): The role of P, N ligands in gold(I) catalysis.
J. Piedad, A.C. Jones

ORGN 146. Experimental study of solution Ag(I)- π interactions using molecular balances. **J. Maier**, K.D. Shimizu

ORGN 147. Revealing the carbon centered radical reactivity towards oxygen by DFT calculations. **D.M. Sriyaratne**, A.D. Gudmundsdottir

ORGN 148. Synthesis of tetra(benzyloxy) benzenes for mass spectrometry studies.
R. Brumbaugh, R. Taylor, R. Hark, D. Kuck, W.M. Ames, P. Schettler

ORGN 149. Source of the puzzling effect of the primary isotope on secondary kinetic isotope effects in alcohol dehydrogenases. **J. Lefton**, J. Eilers, Y. Lu

ORGN 150. Primary isotope dependence of secondary kinetic isotope effects in NADH/NAD⁺ model reactions. **M. Boroujeni**, Y. Lu

ORGN 151. Progress toward the total synthesis of tetarimycin A. **E. Jones-Mensah**, S.H. Lusk, J. Magolan

ORGN 152. Withdrawn.

ORGN 153. Synthesizing and trialing tries-terified monosaccharides for protected culture pest control. **H. Cavender**, M.W. Fultz, M. Guetzloff, B. Liedl

ORGN 154. Studies into the total synthesis of the drimentine alkaloids. **S.M. Pound**, C.J. Douglas

ORGN 155. Catalytic approach to the MH-031 lactone: Application to the synthesis of geraldine analogs. **R. Tello-Aburto**, A.N. Lucero, S. Rogelji

ORGN 156. Progress towards the total synthesis of (-)-gilbertine. **T. Folda**, K.S. Feldman

ORGN 157. Progress towards the synthesis of 7,20-diisocyanoadociane. **PC. Roosen**, C.D. Vanderwal

ORGN 158. 2,5-Cyclohexadienones as a useful launching point for the synthesis of the brianene diterpenoids. **N.G. Moon**, A.M. Harned

ORGN 159. Total synthesis of cyanolide A.
T. Lek, R.W. Bates

ORGN 160. Work toward the synthesis of aspodospermine via a ring fragmentation and 1,3-dipolar cycloaddition sequence.
G. Giampa, M. Brewer

ORGN 161. Synthesis and biological activity of 1-aryl and 1-heteroaryl analogs of eudistomin U. **C.M. Roggero**, J. Giuletto, P. Tate, S.P. Mulcahy

ORGN 162. Highly stereoselective total synthesis of Lagunamide A. **A. Kanner**, N. Kohnen, B. Banasik, L. Wang, M.B. Bergdahl

ORGN 163. Preparation of isogemichalcone analogs, potential inhibitors of aromatase. **A. Angelbello**, M. Morales, S. Longson, E.G. Casillas

ORGN 164. First enantiospecific total synthesis of macrosalidine chloride (4) and progress toward the synthesis of macrolone-related indole alkaloids macrocarpine A, B, and C will be presented. **M. Rahman**, R. Jahan, R.V. Edwankar, J.R. Deschamps, J.M. Cook

ORGN 165. Progress toward the enantioselective total syntheses of leodomycins A and B via an asymmetric vinyllogous aldol strategy. **A. Chin**, J.D. Carrick

ORGN 166. Configuration-encoded 1,5-polyol synthesis: Access to the anti,syn-1,5,7-triol within the C15-C25 fragment of tetrafratricin. **R. Friedrich**, G.K. Friestad

ORGN 167. Progress toward the total synthesis of hippolachnin A. **M.E. McCallum**, J.L. Wood

ORGN 168. Efficient synthesis of polycyclic skeletons of *Aspidosperma* and *Corynanthe* indole alkaloids. **Z. Angel**, E.K. Leggans

ORGN 169. Synthesis of carbazole alkaloids via an HDDA-based strategy. **T. Wang**, D. Niu, T.R. Hoyer

ORGN 170. Synthesis of unnatural enantiomers of morphinan derivatives as toll-like receptor 4 inhibitors. **W.T. Hartwig**, T. Sannakia

ORGN 171. Toward the total synthesis of phomoidride D. **J. Leung**, A.A. Bedermann, N. Hama, G. Murphy, C. Schneider, P. Dong, J.L. Wood

ORGN 172. New and facile synthesis of brazilin via intramolecular alkyne-aldehyde metathesis. **Y. Jung**, I. Kim

ORGN 173. Progress toward the total synthesis of tetrapetalone A. **H. Dhanjee**, Y. Kobayashi, T.C. McMahon, J.F. Buegler, M. Haley, J.M. Howell, J.L. Wood

ORGN 174. Assessing the need for a trityl group as a steric buttress to initiate a Diels-Alder reaction. **C.D. Choony**

ORGN 175. Ongoing work to prepare the anticancer agent xenitorin A. **S.M. Soars**, B. Chandler

ORGN 176. Total synthesis of Herbarin A and B and determination of their anti-oxidant properties and toxicity in Zebra fish model.
J. Heimberger, H. Cade, M.A. Lnu

MONDAY MORNING

Section A

Colorado Convention Center
 Four Seasons Ballroom 2&3

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in Honor of Jin-Quan Yu

B. B. Snider, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **ORGN 177.** Innovative methodology introduced in the total synthesis and subsequent diversification of vinblastine.
D.L. Boger

9:20 **ORGN 178.** Metal-catalyzed cross-coupling reactions of alkyl electrophiles.
G.C. Fu

10:05 **ORGN 179.** Catalytic activation of nucleophiles for selective reactions. **L. Deng**

10:50 Introduction of Awardee.

11:00 **ORGN 180.** Award Address (Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator sponsored by the Pfizer Endowment Fund). Ligand-accelerated C-H activation reactions: Near and far. **J. Yu**

Section B

Colorado Convention Center
 Four Seasons Ballroom 1

Miniaturization in Chemistry: (sub)-Nanoscale Synthesis, Analysis & Application
S. Dreher, Organizer, Presiding

8:00 Introductory Remarks.

8:05 **ORGN 181.** From synthesis in flow to integrated dose-response screening in flow. **R.E. Martin**, M. Werner, C. Kuratli, R. Hochstrasser, T. Enderle, H. Vogel

8:50 **ORGN 182.** From screening of (enantioselective) catalysts by integration of analysis and synthesis to the application in a pilot plant. **O. Trapp**

9:35 **ORGN 183.** High-throughput high-content screening using model organisms enabled by automated microfluidics. **H. Lu**

10:20 **ORGN 184.** Nanomolar scale high throughput chemistry for complex molecules synthesis. **S. Dreher**, A. Buitrago Santanilla, T. Cernak, C.J. Welch, R.M. Helmy, I.W. Davies, E. Regalado, a. pereira, P. Vachal, Z. Shi, P.G. Nantermet, M. Shevlin

11:05 **ORGN 185.** Flow chemistry miniaturization and optimization. **K.F. Jensen**

Section C

Colorado Convention Center
 Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, Organizer
 S. Luesse, Presiding

8:00 **ORGN 186.** Enantioselective cycloadditions of aminoazoxylenes photogenerated via proton transfer in aromatic imines and oxazolines offer expedited access to diverse polyheterocyclic molecular architectures. **O. Mukhina**, N.N. Bhuvan Kumar, D. Kuznetsov, A.G. Kutateladze

8:20 **ORGN 187.** Stereoselective homoallylation with cyclopropanated allylation reagents.
I.J. Krauss

8:40 **ORGN 188.** Efficient assembly of epoxyisoindoline derivatives through a tandem Diels-Alder-Ugi-Smiles process. **S.B. Luesse**, B. Richey, K. Mason, M. Meyers, R. Poornotamed

9:00 **ORGN 189.** Protodecarboxylation of unstabilized carboxylic acids and malonic acid derivatives through photoredox catalysis. **J. Griffin**, M. Zeller, D.A. Nicewicz

9:20 **ORGN 190.** C-H activation and C-C bond formation through cross-coupling reaction by using potassium organotrifluoroborates. **M. Al-Masum**, W. Shaban

9:40 **ORGN 191.** Chiral anti-diols from alpha-oxaldehydes. **G.A. Abeykoon**, S. Chatterjee, J.S. Chen

10:00 **ORGN 192.** Multicomponent reactions in deep eutectic solvents. **S.T. Handy**

10:20 **ORGN 193.** Efficient synthesis of N-alkylated amides from nitriles and alcohols catalyzed by the combination of gold and iridium complexes. **F. Li**, J. Ma, L. Lu, X. Bao

10:40 **ORGN 194.** Mechanistic studies and applications of tertiary amine trapping of HDDA-generated benzynes. **S.P. Ross**, T. Hoyer

11:00 **ORGN 195.** Synthesis of highly functionalized aryl sulfides from HDDA-generated benzynes: Scope and mechanisms.
J. Chen, V. Palani, T.R. Hoyer

11:20 **ORGN 196.** Withdrawn.

11:40 **ORGN 197.** Synthesis of 6-hydroxyquinoline starting from glycerol via improved microwave-assisted modified Skraup reaction and Bamberg rearrangement.
C. Len, N. Thiebault, H. Saggadi, D. Luart, I. Poluert, L. Estel

Section D

Colorado Convention Center
 Room 708

Molecular Recognition and Self-Assembly
 M. C. McIntosh, Organizer
 J. J. Reczek, Presiding

9:00 **ORGN 198.** Isothermal titration calorimetric analyses of the hydrophobic and Hofmeister effects. **P. Sikkalingam**, B.C. Gibb

9:20 **ORGN 199.** Studies of statistically patterned two-component self-assembled monolayers. **Y. Yang**, M.B. Zimmt

9:40 **ORGN 200.** Development of a molecular Turing machine. **S. Varghese**, J.A. Elemans, A.E. Rowan, R. Nolte

10:00 **ORGN 201.** Rapid threading of a long polyethylene glycol chain through a macrocycle in water. **E. Peck**, W. Liu, G. Spence, B. Smith

10:20 **ORGN 202.** Chemosensors for redox-active biomolecules. **J. Hong**, D. Lee, J. Oh

10:40 **ORGN 203.** Self-assembly of collagen mimetic nanofibers through triple-helical hybridization. **B. Sarkar**, J.D. Hartgerink

[†] Cooperative Cosponsorship

- 11:00 ORGN 204.** C-alkylpyrogallo[4]arenes: Robust building blocks for supramolecular organic frameworks (SOFs). R. Patil, H. Kumari, J.L. Atwood
- 11:20 ORGN 205.** Highly substituted anthracenes as self-assembly components of new donor-acceptor columnar liquid crystalline materials. J.J. Reczek

Section E

Colorado Convention Center
Room 702

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*
C. Hamann, *Presiding*

- 8:30 ORGN 206.** Comparison of high spin nitrene isomers with low-temperature matrix isolation spectroscopy. K. Long, M. Maehara, E. Mendez-Vega, D. Sander
- 8:50 ORGN 207.** Synthesis and characterization of di- and tri-aryl pentanes as model for conducting organic polymers. A. Agrahari, J. Masnovi
- 9:10 ORGN 208.** Experimental studies on how *meta*- and *para*-substituents influence the strength of the off-set aromatic stacking interaction. J. Hwang, K.D. Shimizu
- 9:30 ORGN 209.** Degradation of thiophenes by singlet oxygen: Insights from theoretical photochemistry. M. Wykes, J. Gierschner, D. Roca-Sanjuán
- 9:50 ORGN 210.** Withdrawn.
- 10:10 ORGN 211.** Do *aza-ortho*-quinone-methide mediated transformations involve *aza-ortho*-quinone-methides? P.H. Cheong, R.C. Johnston, M.T. Hovey, K. Scheidt
- 10:30 ORGN 212.** De novo catalyst design of scaffolding bifunctional catalysts for the site-selective functionalization of *trans*-1,2 diols. R.C. Johnston, O.M. Ogba, M.F. El Mansy, H. Yao, R.G. Carter, P.H. Cheong
- 10:50 ORGN 213.** Light-induced radical trapping (LIRT): A new approach to molecular photomagnetism from old principles of organic photochemistry. H. Phan, A. Dragulescu-Andrasi, K. Lakin, S.M. Winter, R.T. Oakley, M. Shatruk
- 11:10 ORGN 214.** Exploring the conformational isomerization of the humulyl cation using computational methods. C.S. Hamann, D.J. Tantillo
- 11:30 ORGN 215.** Carbenic, allenic, and propargylic nitrile imines. C. Wentrup

MONDAY AFTERNOON

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

Herbert C. Brown Award for Creative Research in Synthetic Methods: Symposium in Honor of Gary A. Molander

C. White, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05 ORGN 216.** New allylic alkylation reactions: Asymmetric construction of acyclic quaternary carbon stereogenic centers. P. Evans
- 1:50 ORGN 217.** Straightforward strategies to access N-containing structure: Organocatalysis for the benefit of natural products. G. Masson
- 2:35 ORGN 218.** Catalysis in light and shadow. K. Zettler
- 3:20 ORGN 219.** From alkaloids to terpenoids: New strategies and tactics for the synthesis of polycyclic natural products. S.E. Reisman
- 4:05** Introduction of Awardee.
- 4:10 ORGN 220. 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). Novel mechanistic paradigm for organoboron cross-coupling. G.A. Molander

Section B

Colorado Convention Center
Four Seasons Ballroom 1

Synthetic Biology Applied to Natural and Unnatural Product Pathways

B. Bachmann, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05 ORGN 221.** Microbial natural product discovery and diversification: New tools and applications. J.S. Thorson
- 1:55 ORGN 222.** New recipes for biocatalysis: Expanding the cytochrome P450 reaction landscape for non-natural chemistry. E. Brustad
- 2:45** Intermission.
- 3:00 ORGN 223.** Introduction of noncanonical amino acids into a lasso peptide, microcin J25. F.J. Piscotta, A. Link
- 3:20 ORGN 224.** Engineered biosynthesis of antimycin-type depsipeptides. W. Zhang
- 4:10 ORGN 225.** Adapting the retrograde evolution hypothesis to build new biosynthetic pathways for unnatural molecules. B.O. Bachmann

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
D. Bandyopadhyay, *Presiding*

- 1:20 ORGN 226.** Unusual rearrangement of 3-acyl-2-alkoxyfurans enabling appendage of a carbon substituent at C-2: Application to the synthesis of furanulabdanes. C. Thibault, J. Boukouvalas
- 1:40 ORGN 227.** Photochemistry of *o*-nitroarenes: Trifluoromethylated *o*-nitrobenzyl systems as efficient photosynths for selective trifluoromethylated arenes and heteroarenes. G. Prakash, K. Belligund, T. Mathew, G.A. Olah
- 2:00 ORGN 228.** Regioselective synthesis of chloro/bromostyrenes: Chloro/bromotrimethylsilane-nitrate salt as efficient reagent system. G. Prakash, L. Gurung, T. Mathew, G.A. Olah
- 2:20 ORGN 229.** Examining the scope of ISES hits: Pd-catalyzed halo- and pseudohalometalation/carbocyclization transformations. G.G. Malik, R.A. Swyka, G.A. Applegate, X. Fei, D.B. Berkowitz
- 2:40 ORGN 230.** Copper (I) catalyzed synthesis of enamines from thioamides and α -diazocarbonyl compounds. A. Pal, N. Koduri, S.R. Hussaini
- 3:00 ORGN 231.** Site-selective aliphatic C-H halogenation using N-haloamides. R.K. Quinn, V.A. Schmidt, A. Brusoe, E.J. Alexanian
- 3:20 ORGN 232.** Transition metal catalyzed redox-triggered C-C couplings of alcohols via transfer hydrogenation. B.Y. Park, T.P. Montgomery, T. Luong, V. Garza, M.J. Krische
- 3:40 ORGN 233.** Intramolecular [3 + 2] cyclocondensations of alkenes with indolidenes and indolidenium cations. I.Y. Gonzalez, C.M. Glinkerman, K.S. Feldman
- 4:00 ORGN 234.** Metal-free methodology for the preparation of sterically hindered ynones and its application to the synthesis of natural products. C. Taylor, Y. Bolshan
- 4:20 ORGN 235.** Dramatic kinetic isotope effects (kie), solvent effects, and tunneling in directed ortho metallation (DOM). M.G. Organ, J. Farmer, E. Leeruff, R. Froese
- 4:40 ORGN 236.** Radical decarboxylation in micellar media for the formulation of new surfactants. C. Len, F. Mangin, E. Banaszak-Leonard
- 5:00 ORGN 237.** Microwave-assisted dehydration of polyols in aqueous media. C. Len, S. Le Guenic, C. Ceballos

Section D

Colorado Convention Center
Room 708

Molecular Recognition and Self-Assembly

M. C. McIntosh, *Organizer*
I. Vargas-Baca, *Presiding*

- 1:30 ORGN 238.** CH- π Interactions of methyl ethers as a model for carbohydrate-N-heteroarene interactions. P. Li, T.M. Parker, J. Hwang, M.D. Smith, P.J. Pellechia, D. Sherrill, K.D. Shimizu
- 1:50 ORGN 239.** Design and self-assembly of metallo-supramolecular structures guided by density of coordination sites. M. Wang, B. Sun, A. Cisneros, X. Li
- 2:10 ORGN 240.** Molecular dynamics simulations of stacked DNA base surrogates. C. Markegard, A. Mazaheripour, J. Jocson, A.M. Burke, A.A. Gorodetsky, H. Nguyen
- 2:30 ORGN 241.** Supramolecular polymers for active layer organization in photovoltaics. L. Barreda, T. Aytun, A. Ruiz-Carretero, J. Lehman, S.I. Stupp
- 2:50 ORGN 242.** Overcoming static disorder within photoreactive co-crystals by vortex grinding. R.H. Groeneman, K.A. Kummer
- 3:10 ORGN 243.** Racemic hydrogels from self-assembling enantiomeric peptides: Predictions from Linus Pauling. J.P. Schneider
- 3:30 ORGN 244.** Supramolecular macrocycles self-assembled by iso-tellurazole N-oxides. P.C. Ho, J. Sinclair, L. Lee, I. Vargas-Baca
- 3:50 ORGN 245.** Regulating molecular recognition in synthetic supercontainers. Z. Wang, F. Dai, U. Sambasivam, Y. Qiao, A. Corbett
- 4:10 ORGN 246.** Peptide-based functional molecular gels. B. Escuder Gil, J. Miravet, M. Tena-Solsona, C. Berdugo, S. Diaz-Oltra

Section E

Colorado Convention Center
Room 702

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*
K. M. Miller, *Presiding*

- 1:30 ORGN 247.** Molecular origin of color tuning of deepwater Lake Baikal cottoid fish visual pigments. H. Luk, F. Montisci, F. Melaccio, N. Bhattacharyya, J. Morrow, B. Chang, F. Fanelli, M. Olivucci
- 1:50 ORGN 248.** On the mechanism of silver-catalyzed decarboxylative fluorination. N.R. Patel, R.A. Flowers
- 2:10 ORGN 249.** Physicochemical and thermal properties of 1,2,4-triazolium ionic liquids. K.M. Miller
- 2:30 ORGN 250.** Luminescent properties of an open-shell organic radical with high photostability. T. Kusamoto, Y. Hattori, H. Nishihara
- 2:50 ORGN 251.** Autocatalytic self-replicating micelles. K. Bukhriakov, S. Almahdali, V. Rodionov
- 3:10 ORGN 252.** Computational mechanistic investigation of a Cu(I)-catalyzed 1,3-halogen migration. B.M. Hudson, H. Wedler, R. Van Hoven, D. Bates, D.J. Tantillo, J.M. Schomaker
- 3:30 ORGN 253.** Intramolecular reactions of polysubstituted cyclobutenones: An in silico investigation of product specificity. F.E. Jernigan, L. Sun
- 3:50 ORGN 254.** 9-Imino-pyrone analogs: Rationally designed small-molecule fluorophores with large Stokes shifts. P. Sebej, P. Horvath, T. Solomek, P. Klan
- 4:10 ORGN 255.** Transition state *Gauche* effect controls the torquoselectivities of the electrocyclizations of Chiral 1-azatrienes. A. Patel, Z. Ma, J. Vella, R. Hsung, K.N. Houk
- 4:30 ORGN 256.** Semiempirical and QM/MM calculations of the noncovalent interactions between ATP and RecA DNA-repairing proteins. J.H. Rodriguez, M. Palenik, L. Beard

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

R. D. Broene, M. C. McIntosh, *Organizers*

8:00 - 10:00

- 77, 81, 87, 99, 108, 116, 133, 135, 146, 162, 171.** See previous listings.
330, 333, 335, 337, 377-378, 381, 394, 399, 405, 412, 418, 524, 539, 546, 555, 588, 594, 600. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

ACS Award for Creative Work in Synthetic Organic Chemistry: Symposium in Honor of F. Dean Toste

C. A. Maryanoff, *Organizer, Presiding*

8:20 Introductory Remarks.

- 8:25 ORGN 257.** Synthetic studies of complex natural products. T.J. Maimone
- 9:05 ORGN 258.** C-H bond aminations. M. White
- 9:45 ORGN 259.** Synthetic methods based on catalytic P(III)/P(V) cycling. A.T. Radosevich
- 10:25 ORGN 260.** Catalyst discovery with base metal heterobimetallic complexes. N.P. Mankad
- 11:05 ORGN 261. Award Address** (ACS Award for Creative Work in Synthetic Organic Chemistry sponsored by Aldrich Chemical Co., LLC). Concepts and catalysts for enantioselective reactions of carbon-carbon multiple bonds. F. Toste

Section B

Colorado Convention Center
Four Seasons Ballroom 1

ACS Award for Creative Invention: Symposium in Honor of Jotham W. Coe

P. L. Feldman, *Organizer, Presiding*

8:30 Introductory Remarks.

- 8:35 ORGN 468.** Chemical synthesis of secondary metabolites. R.A. Shenvi
- 9:25 ORGN 469.** Alcohol C-H functionalization via redox-triggered Carbonyl Addition: Borrowing hydrogen, returning carbon. M.J. Krische
- 10:15 ORGN 470.** Strategy for selective halogenation. N.Z. Burns
- 11:05** Introduction of Awardee.
- 11:10 ORGN 471. Award Address** (ACS Award for Creative Invention sponsored by ACS Corporation Associates). Discovery of Chantix (varenicline tartrate), an aid to smoking cessation. J.W. Coe

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
M. Emmert, *Presiding*

- 8:00 ORGN 262.** Rh(III)-catalyzed C(sp³)H allylic functionalization of *N*-tosylamides: An unexpected formation of azabicyclic compounds. A. Archambeau, T. Rovis
- 8:20 ORGN 263.** Synthetic clays as new catalysts for aerobic oxidation. J. Magolan, M. Karki, H.C. Araujo, J.J. Dalton, S.D. Holmbo, L. Baker
- 8:40 ORGN 264.** Cerium-free Luche reduction in the presence of alumina. E. Jones-Mensah, L.A. Nickerson, H.J. Knox, J. Magolan
- 9:00 ORGN 265.** New applications of dimethylsulfoxide as a terminal oxidant. J. Magolan, E. Jones-Mensah, M. Karki, J.T. Schmalz

- 9:20 **ORGN 266.** Iron catalyzed α -C-H oxidation of tertiary amines mimicking cytochrome P450 activity. M. Emmert
- 9:40 **ORGN 267.** Tetrabutylammonium bromide: Catalytic abilities in C-O activation. M. Emmert
- 10:00 **ORGN 268.** Catalytic olefin hydroamination with aminium radical cations: A photoredox method for direct C-N bond formation. A. Musacchio, R.R. Knowles
- 10:20 **ORGN 269.** Accessing triplet nitrenes by visible light triplet sensitization of azides. S. Scholz, E. Farney, T.P. Yoon
- 10:40 **ORGN 270.** 2,2,2-Trichloroethyl aryldiazacetates as robust reagents for site-selective C-H functionalization. D.M. Gupstll, H.M. Davies
- 11:00 **ORGN 271.** Synthesis of bridged bicycles via additional steps of metal carbene cascade reaction. Y. Kuo, J. May
- 11:20 **ORGN 272.** HOF-CH₃CN Probably the best oxygen transfer agent organic chemistry has to offer. S. Rozen, I. Vints, S. Potash

Section D

Colorado Convention Center
Room 708

Biologically-Related Molecules and Processes

M. C. McIntosh, *Organizer*
Y. Aye, *Presiding*

- 8:00 **ORGN 273.** Synthesis of novel carbon monoxide releasing molecules. T. Israsenanayudhya, C. Raymond, N.N. Dingra
- 8:20 **ORGN 274.** Determination of the absolute configuration of a single enantiomer of deoxyArbutin. A.M. Kornilov, M.A. Delong, A.J. Stein, J.B. Williams, D.K. Van Strien, M.C. Ammerman
- 8:40 **ORGN 275.** Synthesis and inhibition studies of a transition-state inhibitor for *Mycobacterium tuberculosis* GlgE. S. Veletti, J. Lindenberger, S. Thanna, D. Ronning, S.J. Sucheck
- 9:00 **ORGN 276.** Chemical modulation of lipid bilayer membranes via copper(II)-catalyzed azide alkyne cycloaddition. J.M. Beveridge, M.M. Baksh, M. Finn
- 9:20 **ORGN 277.** Syntheses of heteroatom-activated β -lactams and their evaluation as potential antibiotics and enzyme inhibitors. K.D. Watson, M.W. Majewski, P.L. Barker, M.J. Miller
- 9:40 **ORGN 278.** Cell death imaging using fluorescent probes for phosphatidylserine. K.J. Clear, K.M. Harmatys, D.R. Rice, B.D. Smith
- 10:00 **ORGN 279.** Generalizable platform for target- and signal-specific perturbation of a single signaling target in cells. Y. Aye
- 10:20 **ORGN 280.** Selective fluorescence detection of homocysteine over cysteine using aldehyde bearing fluorophores. A. Barve, R.M. Strongin
- 10:40 **ORGN 281.** Syntheses and evaluation of highly functionalized monobactams and cephalosporins as medicinally useful agents. M.W. Majewski, K.D. Watson, S. Cho, P.A. Miller, S.G. Franzblau, M.J. Miller
- 11:00 **ORGN 282.** Near infrared activated cobalamin-drug conjugates for light targeted delivery. W. Smith, N. Oien, R.M. Hughes, C. Marvin, Z. Rodgers, J. Lee, D.S. Lawrence
- 11:20 **ORGN 283.** Synthetic chemists to aid the community for open antimicrobial drug discovery. M.A. Blaskovich, J. Zuegg, A.G. Elliott, M.A. Cooper
- 11:40 **ORGN 284.** Tropane alkaloids from the Australian proteaceous plant *Floydia praealta*. F. Yang, A.R. Carroll, H. Zhao

Section E

Colorado Convention Center
Room 702

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*
D. B. Lawson, *Presiding*

- 8:30 **ORGN 285.** Intramolecular Diels-Alder reactions between aromatic dienes and a benzyne dienophile: Relative reactivities of the dienes. V. Poggala, T. Wang, T.R. Hoye
- 8:50 **ORGN 286.** Mechanism for reversible photodegradation of 1-substituted aminoanthraquinones doped in poly(methyl methacrylate). S. Hung, K. Schaedeman, M.D. McCluskey, K. Clays, M. Kuzym
- 9:10 **ORGN 287.** Synthesis and gas phase reactivity of charged σ, σ, π -tri- and $\sigma, \sigma, \sigma, \pi$ -tetra-radicals toward small organic substrates in a linear quadrupole ion trap (LQIT) mass spectrometer. R. Kothe, H.I. Kenttamaa
- 9:30 **ORGN 288.** Substituent effects on the [N-X-N]⁺ halogen bonds. A. Carlsson, A. Karim, M. Bedin, J. Grafenstein, M. Erdelyi
- 9:50 **ORGN 289.** Elucidating the role of Sml₂-water and glycol in reductions: Mechanistic studies of anthracene reduction. T.V. Chciuk, R.A. Flowers
- 10:10 **ORGN 290.** Radical arylation of epoxides by low-valent titanocene complexes: Mechanistic studies and methodology development. G. Fianu, R.A. Flowers
- 10:30 **ORGN 291.** Irreversible formation of high energy intermediates to achieve high yield photorelease of alcohol. K.R. Thenna Hewa, A.D. Gudmundsdottir, D.L. Phillips, M. Li
- 10:50 **ORGN 292.** Two-color fluorescent dyes for "click" labeling: Design and characterization. R.K. Meka, M.D. Heagy
- 11:10 **ORGN 293.** Computational studies of fluorinated biomimetic molecules. J.J. Urban, G.S. Kedziora, M. Hastings, N. Exleben, R.M. Crutcher, R. Atwood
- 11:30 **ORGN 294.** Evidence supporting a revised mechanism for the traceless Staudinger ligation of phosphino phenyl esters and aryl azides. T.P. Kirby, T.H. Koch
- 11:50 **ORGN 295.** DFT density and difference density volumes of transition states. D.B. Lawson

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

Ernest Guenther Award in the Chemistry of Natural Products: Symposium in Honor of Thomas R. Hoye

P. R. Hanson, *Organizer, Presiding*

- 1:00 **ORGN 296.** Recent studies toward the synthesis of rocaglamide and related natural products. J.A. Porco, Jr
- 1:40 **ORGN 297.** Worm language: A natural combinatorial library and a xylopyranose-based nucleoside. F.C. Schroeder
- 2:20 **ORGN 298.** Strategies and tactics for chemical synthesis inspired by complex alkaloids. R. Sarpong
- 3:00 **ORGN 299.** Evolution of anion relay chemistry (ARC) leading to Negishi cross-coupling without ZnCl₂. A.B. Smith
- 3:40 **Introduction of Awardee.**
- 3:45 **ORGN 300. Award Address** (Ernest Guenther Award in the Chemistry of Natural Products sponsored by Givaudan). Natural products as drivers of discovery. T.R. Hoye

Section B

Colorado Convention Center
Four Seasons Ballroom 1

James Flack Norris Award in Physical Organic Chemistry: Symposium in Honor of Charles L. Perrin

L. T. Scott, *Organizer, Presiding*

- 1:00 **Introductory Remarks.**
- 1:05 **ORGN 301.** In search of kinetically stable aryltrifluoroborates: B-18F bond formation for one-step 18F-labeling of peptides for PET imaging. D.M. Perrin, Z. Liu, Y. Li, R. Ting
- 1:45 **ORGN 302.** From host-guest chemistry to the nucleosome: Studies in biomolecular recognition. M. Waters
- 2:25 **ORGN 303.** Adventures in physical organic chemistry with Pd and Zn. P.J. Walsh
- 3:05 **ORGN 304.** Myths and models in aromatic chemistry. J.S. Siegel
- 3:45 **Introduction of Awardee.**
- 3:50 **ORGN 305. Award Address** (James Flack Norris Award in Physical Organic Chemistry sponsored by the ACS NortheasternSection). Logic behind a physical-organic chemist's research topics. C.L. Perrin

Section C

Colorado Convention Center
Rooms 704/706

Green Chemistry: Reactions in Alternative Media

B. H. Lipshutz, *Organizer, Presiding*

- 1:00 **Introductory Remarks.**
- 1:01 **ORGN 306.** Fluorous chemistry meets green chemistry. J.A. Gladysz
- 1:31 **ORGN 307.** Practical overview of organic synthesis in ionic liquids. R.D. Rogers, S.P. Kelley
- 2:01 **ORGN 308.** Biocatalysis and biomass conversion in alternative reaction media. R.A. Sheldon
- 2:31 **Intermission.**
- 2:46 **ORGN 309.** Switchable hydrophilicity solvents and switchable water: Design for applications and the environment. P.G. Jessop
- 3:16 **ORGN 310.** Transitioning organic synthesis from organic solvents to water. B.H. Lipshutz
- 3:45 **Intermission.**
- 4:00 **Panel Discussion.**

Section D

Colorado Convention Center
Room 708

Biologically-Related Molecules and Processes

M. C. McIntosh, *Organizer*
A. T. Koppisch, *Presiding*

- 1:30 **ORGN 311.** Discovery and synthesis of new crop protection solutions. B.A. Lorsbach, Z.L. Benko, T.A. Boebel, N. Breaux, K. Bryan, G. Davis, J. Epp, K.G. Meyer, J. Owen, M. Pobanz, J.M. Ruiz, M. Sullenberger, J.D. Webster, C. Yao, D. Young
- 1:50 **ORGN 312.** Profluorogenic activatable-substrate-probes for detection and imaging of disease markers. S.U. Hettiarachchi, B. Prasai, R.L. McCauley
- 2:10 **ORGN 313.** Synthesis of a novel class of proline-containing 2,5-diketopiperazine. S. Hamedzadeh, K. Ha, C. Hall, A. Katritzky
- 2:30 **ORGN 314.** De novo designed peptides from a sugar amino acid are permeable to neuronal and HeLa cells. A. Monreal, J.P. Saludes, H. Aguilar, G. Wayman
- 2:50 **ORGN 315.** Azasulfurylpeptide solid-phase synthesis, conformational analysis, and application as modulators of toll-like receptor inflammatory response in macrophages. S. Turcotte, K. Mellal, H. Ong, W.D. Lubell
- 3:10 **ORGN 316.** Indocyanine dye cancer targeting agents. C. Dietz, I. Mohammad, M. Smith, Q. Zhu, A. Abuteen, F. Zhou

- 3:30 **ORGN 317.** Synthesis and structure proof for a bioactive lipid associated with multiple sclerosis, isolated from *Porphyromons gingivalis*. C. Dietz, I. Mohammad, M. Smith, F. Nichols, P. Bhatt, T. Hart, I. Popiv
- 3:50 **ORGN 318.** Dehydroshikimate dehydratase from pathogenic *Bacillus* strains: Antibiotic target and catalyst for heterologous biosynthesis of polymer precursors. K.B. Finney, I.A. Simon, A.J. Rodin, G.M. Canales, P.A. Netz, K. Hotta, C.C. Browder, D.T. Fox, A.T. Koppisch
- 4:10 **ORGN 319.** Synthesis of intermediates of loline biosynthesis pathway. M. Bhardwaj, J. Pan, R.B. Grossman, C.L. Schardl

Section E

Colorado Convention Center
Room 702

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*
M. G. Organ, *Presiding*

- 1:30 **ORGN 320.** Selective carbamates synthesis by copper catalyzed oxidative coupling of formamides with silylaldaldehydes. B.D. Barve, Y. Wu, M. El-Shazly, D. Chuang, Y. Cheng, J. Wang, F. Chang
- 1:50 **ORGN 321.** Copper(II) ladder complexes and their use in organic synthesis. B. Buckley
- 2:10 **ORGN 322.** Development of copper catalysts for photoredox reactions. K.H. Jensen
- 2:30 **ORGN 323.** Synthesis of diaryl sulfones at room temperature: Cu-catalyzed cross-couplings of arylsulfonfyl chlorides with arylboronic acids. X. Lei, F. Hu
- 2:50 **ORGN 324.** Soft propargylic deprotonation: Designed ligand enables Au-catalyzed isomerization of alkynes to 1,3-dienes. Z. Wang, Y. Wang, L. Zhang
- 3:10 **ORGN 325.** Key mechanistic features of Ni-catalyzed C-H/C-O biaryl coupling of azoles and naphthalen-2-yl pivatalates. H. Xu, K. Muto, J. Yamaguchi, C. Zhao, K. Itami, J. Musaeu
- 3:30 **ORGN 326.** New co-catalyst strategy: Cobalt and nickel-catalyzed cross-electrophile coupling of biphenyl mesylates and aryl halides. L.K. Ackerman, L. Anka-Lufford, M. Naodovic
- 3:50 **ORGN 327.** Selective Negishi coupling of secondary alkynyl reagents to aromatics: Solving the 5-membered ring heterocycle problem. M.G. Organ, B. Atwater, M. Pompeo, J. Farmer, D. Mitchell, M.J. Rodriguez, R. Froese
- 4:10 **ORGN 328.** Mono arylation of primary amines and ammonia using specially designed Pd-NHC complexes. M.G. Organ, R. Rucker, S. Sharif, C. Lombardi, N. Chandrasoma, D. Mitchell, M.J. Rodriguez, R. Froese

TUESDAY EVENING

Section A

Colorado Convention Center
Hall C

Biologically-Related Molecules and Processes; Chemistry of Natural Resources; Metal-Mediated Reactions and Syntheses; Molecular Recognition and Self-Assembly; Peptides, Proteins, and Amino Acids

R. D. Broene, *Organizer*

8:00 - 10:00

- ORGN 329.** Synthesis and antibacterial study of Schiff bases from 2,2'-bipyridyl-5,5'-dialdehyde. M.R. Hoq, M.R. Karim
- ORGN 330.** Fluorescent triazaborolopyridinium dyes for cross metathesis labeling. R.R. Sapkota, M. Garcia, K.P. Dandamudi, T.M. Schaub, J.B. Arterburn
- ORGN 331.** Synthesis and kinetic investigation of differently substituted chalcones. I. Janser, R. Gopagani
- ORGN 332.** Platinum (IV) prodrugs: A simultaneous release of cisplatin and a glutathione S-transferase inhibitor. N. Pilli, I. Janser

- ORGN 333.** Proposed revision of the absolute structure of mandelamide B based on computational methods. **K.M. Snyder**, R.G. Carter, K.L. McPhail, P.H. Cheong
- ORGN 334.** Efficient synthesis of *l*-sirenin and its evaluation as CatSper channel agonist in human sperm. **S. Syeda**, E.J. Carlson, R. Francis, J. Hawkinson, G.I. Georg
- ORGN 335.** Improved syntheses of BET inhibitor JQ1. **S. Syeda**, S.R. Jakkiraj, G.I. Georg
- ORGN 336.** Allenic Pauson-Khand approach to bicyclo[5.3.0]decadienones and novel guaianolides. **S.M. Wells**, K.M. Brummond
- ORGN 337.** Withdrawn.
- ORGN 338.** Synthesis of modified nucleosides for the preparation of ribonucleic guanidine. **R. Van Ostrand**, A. Awad
- ORGN 339.** Synthesis, cytotoxicity, and DNA-binding studies of the natural product eudistomin U. **J. Giulietti**, P. Tate, C.M. Roggero, S.P. Mulcahy
- ORGN 340.** Modulating the reactivity of guaianolide analogs through modifications to the lactone ring. **PA. Jackson**, K.M. Brummond
- ORGN 341.** Progress on the design and synthesis of alternate substrates and inhibitors of indole-3-glycerol phosphate synthase. **R. Barrows**, D. Konas
- ORGN 342.** Synthesis of derivatives of the natural product radicinin that inhibit the plant pathogen *Xylella fastidiosa*. **M.J. Steinhilber**, J.M. Reader, M.J. Rouffet, T.J. Aldrich, P. Rolschhausen, M.C. Roper, K.N. Maloney
- ORGN 343.** Development of a photochromic drug delivery system: Storage and release of nitroxyl. **K.P. Schultz**, D. Spivey, E.K. Loya, J. Kellon, L. Taylor
- ORGN 344.** 9-Phenylethynyl pyronin analogs: Near infrared emitting fluorophores for imaging. **P. Sebej**, T. Pastierik, J. Medalova, P. Stacko, P. Klan
- ORGN 345.** Design and synthesis of dopamine analogs for analysis in SULT1A3. **J.C. Rote**, G.E. Bailey, M. Cañero, L.W. Peterson
- ORGN 346.** Conformational analysis of aplyronine A. **D. McKenzie**, C. Nicholson
- ORGN 347.** Conformational analysis of FD-895: Measuring flexibility and rigidity of different dihedral angles in the ring. **S. Jackson**, C. Nicholson
- ORGN 348.** Development of inhibitors of petrobactin biosynthesis: Dehydroshikimate dehydratase as a target for anti-anthrax therapeutics. **I.A. Simon**, A. Rodin, P.A. Netz, D. Fox, A.T. Koppisch, C.C. Browder
- ORGN 349.** Testing two conformational search methods of Aplyronine C. **T. Hutchinson**, C. Nicholson
- ORGN 350.** Development of nonhydrolyzable inositol pyrophosphate analogs and their application in the identification of inositol pyrophosphate binding partners. **A. Hager**, D. Fiedler
- ORGN 351.** Stereocontrolled total synthesis of pro-resolving lipid mediators derived from docosahexaenoic acid. **S.J. Glynn**, J.W. Winkler, C.N. Serhan, N.A. Petasis
- ORGN 352.** Incorporation of 3β-modified fluorescent cholesterol into liposomal and mycobacterial membranes. **A.N. Wercholkuk**, J.L. Stanley, E.S. Anderson, W.E. Allen
- ORGN 353.** Recognition of bacterial lipid head-groups by fluorescent crown ether-naphthalimides. **S.R. Marshall**, J.L. Stanley, W.E. Allen
- ORGN 354.** Installation of metal-binding functionality at lysine residues via azide-alkyne "click chemistry". **M.R. Baum**, D.P. Farrell, A.L. Sargent, W.E. Allen
- ORGN 355.** Improving the metal-binding efficiency of heterocyclic compounds targeting metal ion-dependent enzyme of hepatitis C virus. **A.M. Naanaa**, R. Chen, B. Smith, R. Wong, D.N. Ward
- ORGN 356.** Synthetic strategies to control bacterial virulence. **S.R. Dunbar**, K. March, M.A. Bertucci
- ORGN 357.** Effects of exposure of phthalates to chlorinated drinking water. **M. Neyrat**, H. Kim, T. Corbet, L. Li, K. Yeung
- ORGN 358.** Direct carbon-carbon bond formation from diaryl-1,3-iodanes and (hetero) aryl borates: Redefining formal S_NAr reactivity with carbon nucleophiles. **K. Jayatissa**, D.R. Stuart
- ORGN 359.** Kinetic analysis of the transesterification of soybean oil and methanol catalyzed by N-heterocyclic carbenes. **H. Palencia**, D.L. Broxterman
- ORGN 360.** From glycerol to gasoline: A new approach for the utilization of a renewable source. **J. Gmeiner**, V. Tran, O. Trapp
- ORGN 361.** Use of polarimetry in studying the isomerization of bittering agents in beer: The effects of temperature, pH, ultra-violet light, and solvents on the conversion of humulone to isohumulone. **S. Johnson**, M.D. Mosher
- ORGN 362.** Palladium-mediated tandem cyclization-coupling reactions of β,γ-unsaturated oximes. **J. Mikesell**, M.D. Mosher
- ORGN 363.** New diastereoselective synthesis of (E)-trisubstituted alkenes containing trimethylsilyl methyl and p-methoxyphenyl moieties via organoboranes. **N.G. Bhat**
- ORGN 364.** Reaction of (Z)-1-bromo-1-alkenylboronate esters with allylmagnesium bromide followed by Suzuki coupling with p-methylbromobenzene. **N.G. Bhat**
- ORGN 365.** Thiourea hydrogen-bond donors to promote the reductive Heck reaction. **C. Anderson**, T.M. Locascio, J.A. Tunge
- ORGN 366.** Solution and X-ray crystal structures of lithium pinacolone enolate solvated by HMPA. **J. Guang**, P.G. Williard
- ORGN 367.** 1,2-Boryl migration empowers regio-divergent synthesis of borylated furans. **R. Kazem Shiroodi**, O. Koleida, V. Gevorgyan
- ORGN 368.** Tetrahedral oxo-Sn catalyst. **E.V. Beletskiy**, Z. Shen, M.V. Rofskiy, X. Hou, J. Gallagher, J.T. Miller, Y. Wu, M.C. Kung, H.H. Kung
- ORGN 369.** Rhodium(I)-catalyzed enantioselective intramolecular hydroacylation of 4-alleans. **Y. Oonishi**, A. Hosotani, T. Yokoe, Y. Sato
- ORGN 370.** Magnetic-metal nanocatalysts for sustainable organic transformations. **A. Rathi**, M. Gawande, R.S. Varma, R. Zboril
- ORGN 371.** Recyclable soluble palladium N-heterocyclic carbene star polymer. **K. Bukhriakov**, C. Mugemana, V. Rodionov
- ORGN 372.** Electronic effects of intramolecular [2+2+2] cyclizations toward β-carbolines. **M. O'Donnell**, J.G. Varelas, S. Khanal, S.P. Mulcahy
- ORGN 373.** Palladium-catalyzed one-pot reactions towards β-carbolines. **J.G. Varelas**, M. O'Donnell, S. Khanal, S.P. Mulcahy
- ORGN 375.** Oxygen-mediated coupling of silicon and boron compounds. **E. Costello**, P. Kirby, C. Lindsey, C. McNamara, J. Hershberger
- ORGN 376.** C-H insertions in oxidative gold catalysis: Expedient synthesis of bicyclic dihydropyran-3-ones from in situ-generated α-oxo gold carbenes through the relay of vinyl cation intermediates. **Z. Zheng**, L. Zhang
- ORGN 380.** Effect of ligand structure in cycloisomerization reactions of enynes catalyzed by heterobimetallic Ti-Pt complexes. **R. Stokes**, M. Talley, W. Walker, D. Michaelis
- ORGN 381.** Negishi-type cross-coupling arylation of selected carbamates. **B.K. Sharp**, R.E. Gawley
- ORGN 382.** Enyne cycloisomerization reactions catalyzed by heterobimetallic Ti-Pt complexes. **M. Talley**, R. Stokes, W. Walker, D. Michaelis
- ORGN 384.** Gold-catalyzed synthesis of cyclic ethers and lactones. **J. Dotson**, R.D. Lyski, J.R. Vvyvan
- ORGN 385.** Influence of Biphenylphosphine Stabilization on Catalyst Structure and Reactivity. **W. Zhou**, A.C. Jones
- ORGN 386.** Ruthenium catalyzed CN bond formation from alcohols and various nitrogen sources. **S. Hong**
- ORGN 387.** Phosphine-free palladium-catalyzed direct double arylation of pyrroles with aryl iodides on water. **Y.K. Chung**, H. Bae, B. Cho
- ORGN 388.** Kinetic and thermodynamic solubility of pyrazinamide cocrystals. **E.J. Johnson**, H. Abourahma
- ORGN 389.** Progress in the synthesis and characterization of a resorcin[4]arene-based heterodimer. **E.G. Morado**, L.M. Tunstad
- ORGN 390.** Phosphate-coordination directed assemblies: From modeling to laboratory validation. **C. Jia**, B.P. Hay, R. Custelcean
- ORGN 391.** Synthesis and characterization of a covalently assembled molecular capsule for guest encapsulation. **E.S. Garcia**, L.M. Tunstad
- ORGN 392.** Divalent peptide recognition mediated by an auxiliary guest. **H. Lee**, N. Petukhov, Z.T. Ball, A.R. Urbach
- ORGN 393.** Covalent modification of a calixarene-capped azobenzene for increased solubility in polar media. **PA. Bonvallet**, V.C. Lungenich, A. Steiger, T.J. Horst
- ORGN 394.** Selective modification of emission intensity in a rhodamine-anthraquinone macrocycle. **M. Hoffman**, P.N. Basa, K. Mariappan, O. Schmidt, A.G. Sykes
- ORGN 395.** Investigation of the cleavage of Si-O bond in trimethylsilyl ether for quantitative measurement of fluoride. **G. Kim**, H. Cao
- ORGN 396.** Chiral channels in molecular co-crystals: Unexpected structures that arise from the co-crystallization of 2,4,6-tris(4-X-phenyl)arenes. **R. Wiscons**, H. Lai, M. Zeller, J. Rowsell
- ORGN 397.** Carboxylated polyphenylarenes: A new family of tunable porous organic crystal. **H.W. Lai**, R.A. Wiscons, M. Zeller, J.L. Rowsell
- ORGN 398.** 2,2'-Linked sulfonated dicalix[4]arene as a component in supramolecular species. **J.L. Fantini**, E.D. Cosco
- ORGN 399.** Depolymerization as an amplification method for analyze-triggered gelation. **D.M. Zurcher**, A.J. McNeil
- ORGN 400.** Supermolecular catalysis via metal-organic supercontainers (MOSCs). **Y. Qiao**, Z. Wang
- ORGN 401.** Chiral auxiliary/organocatalyst porphyrin hybrids: Modular hosts for chiral recognition. **J.G. Naizer**, M. Atyah Alqurafi, P. Battles, L. Mwangi, K. Truong, S.D. Starnes
- ORGN 402.** Novel electron-rich anthracene components in modular donor-acceptor columnar liquid crystals. **A. Gray Be**, J.J. Reczek
- ORGN 403.** Synthesis of a dual fluorescence probe for the G4 quadruplex. **T. Werner**, A. Do, M.D. Heagy
- ORGN 404.** Aromatic guests for cubic M8L6 metallocages. **H. Castillo**, J.D. Thoburn
- ORGN 405.** Dibrigehead diphosphine dioxide cages: Syntheses and unusual structural features. **S. Kharel**, J. Bluemel, J.A. Gladysz
- ORGN 406.** Impact of H-bonding and chirality on the self-assembly (and morphology) of mono and disubstituted ferrocenyl-peptide-conjugates. **B. Adhikari**, C. Singh, H. Kraatz
- ORGN 407.** Modulating rhodamine B isomerization in metal-organic supercontainers. **A. Corbett**, Z. Wang, F. Dai, U. Sambasivam
- ORGN 408.** Synthesis of a 1-aza-9-crown-3-substituted coumarin for fluorescence sensing of metal ions. **X. Zhang**, C.J. Forsythe, D.L. Nutbrown
- ORGN 409.** Quinoline-based turn-on sensors for fluoride. **X. Zhou**, C. Stains
- ORGN 410.** Synthesis of enantiomeric enriched disubstituted C₂-methyl-γ and δ-unnatural amino acids analogs. **E.R. Vogel**, D.S. Masterson
- ORGN 411.** Photodynamics of azobenzene-dipeptide (Pz-dipeptide) conjugates. **C.T. Brown**, S.K. Rastogi, W.J. Brittain
- ORGN 412.** Mechanism and stereocontrol models in peptide-catalyzed acylations. **O.M. Ogba**, P.H. Cheong
- ORGN 413.** Synthesis and conformational studies of hybrid α-aminoxy/cyclic β₂,3-aminoxy peptides. **K. An**, S. Dai, D. Yang
- ORGN 414.** Circular dichroism studies of hybrid cell penetrating – collagen peptides. **C. Hu**, K. Slowinska
- ORGN 415.** New coupling and cyclization strategy for peptide synthesis via chemoselective three-fragment hydroxyproline ligation. **J.W. McDaniel**, K. Ha, C. Hall
- ORGN 416.** Synthesis of four isomers of 5-hydroxypipercolic acid by intramolecular cyclization of epoxides derived from 2-amino-5-hexenoic acid. **S. Krishna Murthy**, T. Moriguchi, A. Tsuge
- ORGN 417.** Synthesis of ortho-fluorine derivatives of phenylazobenzoyloxycarbonyl(pz)-Pro-Leu for photodynamic study. **S.K. Rastogi**, C.T. Brown, W.J. Brittain
- ORGN 418.** Pyrophosphorylation of peptides and proteins using phosphorimidazolides. **A.M. Marmelstein**
- ORGN 419.** Characterization of a hydrophobic peptide which interacts with beta-sheet proteins. **T.M. Lutz-Rechtin**, J.P. Turner, S.L. Servoss
- ORGN 420.** Development of a highly regioselective *N*-2 arylation of indazole carboxamides: Application toward the synthesis of MK-4827 (Niraparib). **M.E. Scott**

WEDNESDAY MORNING

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

National Fresenius Award: Symposium in Honor of Abigail G. Doyle

Cosponsored by WCC

J. Aube, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **ORGN 421.** New approaches to the analysis of asymmetric catalytic processes. **M.S. Sigman**

9:25 **ORGN 422.** Proton-coupled electron transfer in organic synthesis and asymmetric catalysis. **R.R. Knowles**

10:15 **ORGN 423.** Functionalization of C–H bonds. **M. White**

11:05 Introduction of Awardee.

11:10 **ORGN 424. Award Address** (National Fresenius Award sponsored by Phi Lambda Upsilon, the National Chemistry Honor Society). New Csp³-electrophiles for Ni-catalyzed cross coupling. **A.G. Doyle**

Section B

Colorado Convention Center
Four Seasons Ballroom 1

Total Synthesis of Complex Molecules

M. C. McIntosh, K. Walker, Organizers
N. Choony, Presiding

8:20 **ORGN 425.** Expedient approach to bicyclic nucleosides: Precursors to nucleic acid modifications for antisense technology. **N.K. Narayanan**, A.M. Dmytrchuk, B.L. Merner

8:40 **ORGN 426.** Organocatalytic and protecting-group-free synthesis of (+)-artemone. **S.P. Wetzler**, B.C. Fielder, D.A. Vosburg

9:00 **ORGN 427.** Use of triphenylchloromethane (trityl chloride) as a steric buttress to enhance Diels Alder cycloaddition reactions. **N. Choony**

9:20 **ORGN 428.** Synthesis of bis(indole) alkaloids from *Arundo donax*. **A. Ferreira**, C. Beaudry

9:40 **ORGN 429.** Syntheses of acyclic polyhalogenated *Plocamium* monoterpene and evaluation of activity for solid tumors. **C.V. Vogel**, H. Pietraszkiewicz, O.M. Sabry, W.H. Gerwick, F.A. Valeriote, C.D. Vanderwal

10:00 ORGN 430. Case for a spontaneous, Diels-Alderase-free dimerization as the key step in the biosynthesis of (+)-paracaseo- lide A. **T. Wang**, T.R. Hoye

10:20 ORGN 431. Total synthesis of leider- matolide. **S. Williams**, K. Ng, I. Paterson

10:40 ORGN 432. Withdrawn.

11:00 ORGN 433. Total synthesis of aflastatin A. **D.A. Evans**, J.J. **Beiger**, E. Kattinig, P.H. Fuller, J.M. Young, J.D. Burch, F. Glorius, J. Zhang, W.C. Trenkle, D.A. Thaisrivongs

11:20 ORGN 434. Efficient and concise syntheses of spiroisoxazolines: Progress toward first total synthesis of 11-deoxyfistularin-3. **P. Das**, A.T. Hamme II

11:40 ORGN 435. Phytochemical study of the genus *Piper*: Synthesis and photoreactivity of chromene natural products. **T.T. Nguyen**, C.S. Jeffrey

12:00 ORGN 436. Total synthesis of 6-deoxy- pladienolide D and assessment of splicing inhibitory activity in a mutant SF3B1 cancer cell line. **K. Arai**, S. Buonomi, B. Chan, K. Corson, A. Endo, B. Gerard, M. Hao, C. Karr, K. Kira, L. Lee, X. Liu, J.T. Lowe, T. Luo, L.A. Marcaurella, Y. Mizui, M. Nevalainen, M.W. O'Shea, E. Park, S. Perino, S. Prajapati, M. Shari, P.G. Smith, P. Tivimhaisoon, J.Y. Wang, M. Warmuth, K. Wu, L. Yu, H. Zhang, G. Zheng, G.F. Keane

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
B. L. Ashfeld, *Presiding*

8:00 ORGN 437. Synthesis of 5, 6, 7, and 8-membered oxacycles by silver and gold catalysis. **R. Tata**, M. Harmata

8:20 ORGN 438. From carbon to cancer: The impact of reaction development on natural products and designed materials syntheses. **B.L. Ashfeld**, A. Chavannavar, E. White

8:40 ORGN 439. Transition metal catalyzed reactions for the functionalization of cubane and triptycene scaffolds. **M.O. Senge**

9:00 ORGN 440. Enantioselective N-heterocyclic carbene-catalyzed β -hydroxylation of enals using nitroarenes: An atom transfer reaction that proceeds via single electron transfer. **N.A. White**, T. Rovic

9:20 ORGN 441. Rh(III)-catalyzed synthesis of 2,3-dihydropyridines initiated by C-H activation. **F. Romanov Michailidis**, T. Rovic

9:40 ORGN 442. Highly active multidentate molybdenum (VI) catalysts for alkyne metathesis. **H. Yang**, C. Zhu, W. Zhang

10:00 ORGN 443. Chemo-enzymatic synthesis of key intermediates (S)- γ -hydroxymethyl- α,β -butenolide and (S)- γ -hydroxymethyl- γ -butyrolactone via lipase-mediated Baeyer-Villiger oxidation of levoglucosone. **A.L. Flourat**, A.A. Peru, A.R. Teixeira, F. Brunissen, F. Allais

10:20 ORGN 444. Synthesis of functionalized benzenoid macrocycles: Templates for carbon nanotube synthesis. **B.L. Memer**, N.K. Mitra, R. Meudom, S. Iqbal

10:40 ORGN 445. Pentadehydro-Diels-Alder (PDDA) reaction.Part 1: Cycloisomerization of tryenes to $\alpha,3$ -dehydrotoluene derivatives and their trapping reactions. **T. Wang**, R. Naredla, T.R. Hoye

11:00 ORGN 446. Automated simultaneous catalyst screening and cross-coupling reaction optimization in a continuous-flow microreactor system. **B.J. Reizman**, K.F. Jensen

11:20 ORGN 447. Flow chemistry for sustainable chemical manufacturing. **M.G. Organ**, D. Mallik, M. Tilley, K. Somerville, G. Li, A. Khadra, M.A. McGuire, K. Nalivela, D. Daly

Section D

Colorado Convention Center
Room 708

Heterocycles and Aromatics

M. C. McIntosh, *Organizer*
L. Silverberg, *Presiding*

8:00 ORGN 448. Pd-catalyzed iterative bis-amination of functionalized dihalo-1,2,4-triazinyl substituted heterocycles. **S. Tai**, S.V. Marchi, E.J. Dover, J.D. Carrick

8:20 ORGN 449. Development of an expedient process for the multikilogram synthesis of CHK1 inhibitor GDC-0425. **A. Stumpf**

8:40 ORGN 450. Benzo[ajimidazo[2,1,5-cd]indolizines as tunable heterocyclic fluorophores: Synthesis and applications. **E. Levesque**, L. Constantineau-Forget, G. Pelletier, W.S. Bechara, A.B. Charette

9:20 ORGN 451. Accessing diverse poly-heterocycle-fused diketopiperazines via cycloadditions of photogenerated azaxoxylenes. **N.N. Bhuvan Kumar**, D.M. Kuznetsov, A.G. Kutateladze*

9:40 ORGN 452. Prospective energetic materials derived from 4, 4'-bi[5-nitro-1, 2, 3-2H-thiazole]. **C. He**, J.M. Shreeve

10:00 ORGN 453. Synthesis, photochemical, and electrochemical characterization of N,N'-dimethyl-5,10-diaza[5]helicene bistetrafluoroborate and other helical viologens. **X. Zhang**, E.L. Ciennan

10:20 ORGN 454. Highly efficient synthesis of HIV NNRTI doravirine. **D.R. Gauthier**, Jr

10:40 ORGN 455. Synthesis of organo nitrogen compounds and heterocycles via catalytic allylic C-H amination. **S. Murru**, R. Srivastava

11:00 ORGN 456. Studies on cyclic six- and seven-membered 2, 3-dialkyl-1, 3-thiaza-4-ones. **L.J. Silverberg**, H.P. Yennawar, J. Tierney, C.N. Pacheco, K.C. Cannon, A.F. Lagalante, J.T. Bachert, L.M. Baker, J. Bayliff, R.V. Bendinsky, A.S. Cali, L. Chen, A.D. Cooper, D.J. Coyle, J.R. Dahl, M.J. Minehan, C.R. Mroz, H. Singh, Y. Xie

11:20 ORGN 457. Thiazole chemistry toward a second generation EML4-ALK inhibitor. **G. Smith**

11:40 ORGN 458. Withdrawn.

Section E

Colorado Convention Center
Room 702

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*
S. P. Mulcahy, *Presiding*

8:30 ORGN 459. Stereospecific nickel-catalyzed cross-coupling of benzylic ethers with Grignard reagents. **A. Johnson**, I.M. Yanova, L.W. Erickson, M.A. Greene, C.A. Osborne, E.R. Jarvo

8:50 ORGN 460. Efficient catalytic system for Ru-catalyzed C-H arylation: A practical synthesis of a pharmaceutical. **M. Seki**

9:10 ORGN 461. Terminal olefins to chromans, isochromans, and pyrans via allylic C-H oxidation. **S. Ammann**, G. Rice, M.C. White

9:30 ORGN 462. Intramolecular metal-coordinations of N,N'-dimethylhydrazinoalkenes. **A. Smith**, B. Sundahl, T. Livinghouse

9:50 ORGN 463. Mechanistic study of gold(I)-catalyzed alkene addition reaction. **Y. Zhu**, E.M. Petryna, A.C. Jones

10:10 ORGN 464. Efficient palladium-catalyzed reactions toward complex nitrogen-containing heterocycles. **S.P. Mulcahy**

10:30 ORGN 465. Catalyst-transfer direct arylation: Selectivity and potential initiators. **H. Johnson**, T. Schwochert, J. Enders, A. Olivares, T. Hougen, K. Woods, L. Lawrence, J.F. Tannaci

10:50 ORGN 466. Efficient synthesis of poly-substituted cyclopentadienyl ligands for Rh(III) catalysis. **N. Semakul**, T. Rovic

11:10 ORGN 467. BINAP-based metal-organic framework catalysts for asymmetric reactions. **T. Sawano**, J. Falkowski, T. Zhang, G. Tsun, Y. Chen, N.C. Thacker, A.R. Mclsaac, J.V. Lockard, W. Lin

WEDNESDAY AFTERNOON

Section C

Colorado Convention Center
Rooms 704/706

Peptides, Proteins, and Amino Acids

M. C. McIntosh, *Organizer*
J. Haseltine, *Presiding*

1:00 ORGN 472. Remodeling of bacterial cell surfaces using unnatural D-amino acids. **M.M. Pires**

1:20 ORGN 473. N-terminal modification for traceless expressed protein ligations. **E.J. Pettersson**

1:40 ORGN 474. Lanthipeptides with diverse ring topologies are generated by Procm through kinetic control. **S. Mukherjee**, Y. Yu, W.A. van der Donk

2:00 ORGN 475. Synthesis and responsive self-assembly of boronic acid-functionalized peptides. **B.H. Jones**, A. Martinez, J. Wheeler, D.R. Wheeler, E. Spoerke

2:20 ORGN 476. Orally bioavailable cyclic peptides. **D.S. Nielsen**, H.N. Hoang, R. Lohman, D.P. Fairlie

2:40 ORGN 477. Bioinspired strategy for the ribosomal synthesis of thioether-bridged macrocyclic peptides in bacteria. **N. Bionda**, R. Fasan

3:00 ORGN 478. Comparing methods for the solution-state synthesis of dipeptide and tripeptide esters. **O. Sugahara**, I.L. Beltran, J.T. Bauer, J.N. Haseltine

3:20 ORGN 479. Synthesis and applications of peptides with C-terminal esters to studies of protein prenylation. **M.D. Distefano**, V. Diaz-Rodriguez, J.S. Verveacke

3:40 ORGN 480. Development of 4-hydroxyproline ligation for coupling of peptide fragments. **K. Ha**

4:00 ORGN 481. Constrained N-amino peptide derivatives for conformational scanning applications. **J.R. Del Valle**, C. Kang, S. Ranatunga

Section D

Colorado Convention Center
Room 708

Heterocycles and Aromatics

M. C. McIntosh, *Organizer*
C. Santini, *Presiding*

1:00 ORGN 482. Porphyrin synthesis by grinding. **T.D. Hamilton**, D. Cordero, V.S. Hoelscher, T. Sabol, Q. Su

1:20 ORGN 483. Synthesis and reactions of 2-oxo-p-tert-butyltetramethoxyoxalyl[4]arene. **J.L. Fantini**, I.M. Delahunty, K.P. Klatt

1:40 ORGN 484. Dearomative (3+2) cycloadditions of aza-oxyallyl cation intermediates and indoles. **A. Acharya**, C.S. Jeffrey

2:20 ORGN 485. Trifluoromethyl heterocyclic compounds: Synthesis and characterization. **K.P. Castro**, A.M. Plunze, I.V. Kuvychko, E. Bukovsky, T. Cilkeman, Y. Chen, S.H. Strauss, O.V. Boltalina

2:40 ORGN 486. Modular approach to crowded benzoquinolines. **A. Mazaheripour**, D.E. Laidlaw, R. Lopez, D.J. Dibble, M. Umerani, Y. Park, A.A. Gorodetsky

3:00 ORGN 487. Gram scale total synthesis of veranamine. **J. Magolan**, H.C. Araujo, S.D. Holmbo, R. Gautam

3:20 ORGN 488. Gold-catalyzed cyclizations of cis-enediynes: Insights into the nature of gold-aryne interactions. **Y. Wang**, A. Yepremyan, S. Ghorai, R. Todd, D.H. Aue, L. Zhang

3:40 ORGN 489. Analysis of PAH(CF)_nPAH charge transfer complexes. **E.V. Bukovsky**, K.P. Castro, L. San, T. Cilkeman, I.V. Kuvychko, O. Boltalina, S.H. Strauss, Y. Chen

4:00 ORGN 490. New approaches in N-heterocycle construction and applications toward industrially relevant materials. **D. Pena**, A. Chavannavar, B.L. Ashfeld

4:20 ORGN 491. Oxidative 1,2 and 1,4-diamination of olefins using simple urea derivatives. **D. Anumandla**, C.S. Jeffrey

4:40 ORGN 492. Transition-metal mediated cycloaddition reactions of chiral diaziridines for the diastereoselective synthesis of N-containing heterocycles. **G. Moura-Letts**

Section E

Colorado Convention Center
Room 702

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*
B. Michel, *Presiding*

1:30 ORGN 493. Palladium-catalyzed intramolecular oxidative coupling of nitrogen heteroaromatics with unactivated arenes in the synthesis of fused N-heterocycles. **J. Laha**, N. Dayal, K. Jethava

1:50 ORGN 494. Stereoselective synthesis of allenyl alcohols using an organo-manganese η^2 -auxiliary: A new entry to furfuranone natural products. **A. Roy**, B. Bhat

2:10 ORGN 495. Mechanistic studies of isocyanide promoted Buchner insertion reactions with Ruthenium-based metathesis catalysts. **J.R. Griffiths**, E.J. Hofman, J.B. Keister, S.T. Diver

2:30 ORGN 496. Gold-catalyzed 1,3-transposition of ynones. **R. Kazem Shiroodi**, M. Soltani, V. Gevorgyan

2:50 ORGN 497. Withdrawn.

3:10 ORGN 498. Novel catalytic reactivities of PN3-pincer complexes. **K. Huang**

3:30 ORGN 499. Rhodium-catalyst controlled carbonyl and vinyllogous reactions of vinyldiazoacetates and silyl ketene acetals. **S. Negretti**, H.M. Davies

3:50 ORGN 500. Overcome inherent regioselectivity in oxidative gold catalysis: A desulfonylation approach. **H. Chen**, L. Zhang

4:10 ORGN 501. Powerful fluoroalkoxy molybdenum(V) reagent for the selective oxidative arene coupling reaction. **M. Schubert**, J. Leppin, K.M. Wehmig, D. Schollmeyer, D. Heinze, D.R. Waldvogel

WEDNESDAY EVENING

Section A

Colorado Convention Center
Four Seasons Ballroom

Heterocycles and Aromatics; New Reactions and Methodology

R. D. Broene, *Organizer*

7:00 - 9:00

ORGN 374. Air-stable palladium precatalyst for arylation of arylhalides with HBpin and experimental evidences on cationic metathesis mechanism. **X. Pu**, T. Colacot

ORGN 377. Iridium precatalysts for the C-H borylation of heterocycles. **P. Gildner**, C. Seechurn, S. Vivanathan, T. Colacot

ORGN 378. In depth understanding of palladium acetate. **W.A. Carole**, A. DeAngelis, T. Colacot

ORGN 379. Highly active pi-allyl Pd-precatalysts for challenging cross-coupling reactions. **A. DeAngelis**, R. Chow, C. Seechurn, T. Colacot

ORGN 383. Heck and Sonogashira coupling of aryl and heteroaryl chlorides using L2Pd(0) and L2Pd(II) catalysts: Understanding the structure-activity relationships. **H. Li**, X. Pu, T. Colacot

- ORGN 502.** High-load, hybrid ROMP reagents/scavengers/ligands immobilized on silica and Co/C magnetic nanoparticles for their application in sequestration and parallel synthesis. **S. Faisal**, P.K. Maity, A. Brandhofer, P.C. Kearney, D.S. Stoianova, O. Reiser, R.N. Grass, P.R. Hanson
- ORGN 503.** Synthesis of Tröger's base-derived ligands. **C.S. Hampton**, M. Harmata
- ORGN 504.** Synthesis of dibenz[c,h]acridines as potential G-quadruplex ligands. **K. Eckelman**, **K. Jara**, M.D. Mosher
- ORGN 505.** 9-Arylacridine atropisomers. **B. Redlinger**, M.D. Mosher
- ORGN 506.** Synthesis of 3,4,5-trisubstituted isoxazolines. **T.N. Leighton**, **K. Henson**, M.D. Mosher
- ORGN 507.** QSAR analysis of O-substituted 9-hydroxyflaminoacridines. **A. Carlson**, A. Lavianetskaya, M.D. Mosher
- ORGN 508.** Photocyclohydrofluorination. **K.E. Ivey**, Z. Li, R.J. Twieg
- ORGN 509.** Benzimidazol-2-one scaffolds derived from unique domino processes centered upon elegant benzodiazepine ring rearrangements. **G. Martinez-Ariza**, Z. Xu, A.P. Cappelli, C. Hulme
- ORGN 510.** Inverse-demand Diels-Alder of bis-(4-pyridyl)-1,2,4,5-tetrazine with alkenes and carbonyl under catalytic and non-catalytic conditions. **M.A. Max**, J. Wilson
- ORGN 511.** Cross coupling of iodo-substituted aurones. **Z.E. Taylor**, S.T. Handy
- ORGN 512.** Direct C-H functionalization of arenes in reactions with nitroalkanes and nitroalkenes in polyphosphoric acids. **A. Aksenov**, A.N. Smirnov, **N.A. Aksenov**, I.V. Aksenova, **M.A. Rubin**
- ORGN 513.** Heterocycles: An enhancement in the ferrocenyl derivatives pharmacophores. **J.C. Aponte-Santini**, I. Montes Gonzalez, S. Abdul-Hadi-Martinez, F.J. Correa-Delgado, D.J. Sanabria Rios, M.D. García Maldonado, A.R. Guadalupe Quiñones, F.T. Halawish, **A.E. Serrano Buzuela**, **E.E. Colón Lorenzo**
- ORGN 514.** Approaches to the synthesis of C1-substituted carbenepems. **T.Q. Nguyen**, W. Chai, J. Gu, K. Cook, E. Kim, S.E. Goetz, M. Chepur, M. Cox, P. Nguyen, H. Raja, P. Magistrado, F. Michael, P. Oelschlaeger, J.W. Janc, J.D. Buynak
- ORGN 515.** Copper(I) catalyzed reaction of 1-bromo-2-iodobenzene with 1,2-cyclohexanedione as a potential route to 2,3-dihydrodibenz[b,d]furan-4(1H)-one. **D.A. Hunt**, J. Bocanegra
- ORGN 516.** Synthesis, photochemical and electrochemical characterization of a series of new phenanthrenyl viologens. **T. Bakupog**, **E.L. Clennan**
- ORGN 517.** Air stable polycyclic aromatic hydrocarbons with strong electron accepting properties. **L.K. San**, E.V. Bukovsky, T.T. Cikeman, S. Deng, X. Wang, Y. Chen, O.V. Boltalina, S.H. Strauss
- ORGN 518.** Alternative routes to phenanthroline-based diones. **K.A. Pacheco**, **D.J. Covelli**, C.M. Bresch
- ORGN 519.** Optimization of the synthesis of 2,4,6-trimethylphenyl-1,10-phenanthroline and its derivatives. **K.A. Pacheco**, **D.B. Burgess**
- ORGN 520.** Synthesis of neo-confused porphyrins. **A.S. Almejel**, T.D. Lash
- ORGN 521.** Efficient methods of synthesizing benzyl azetidines. **C. Ochoa**, L.M. Bradley
- ORGN 522.** Synthesis of pyrazol-1-yl-benzenesulfonamides. **M. Belcher**, **B. Torok**, **R. Dembinski**
- ORGN 523.** Mono- and bis- phenylpropargyl imidazolium cations: Structure and reduction behavior. **G. Soper**, B.M. Barry, W.L. McClennan, K. Robertson, J. Huralmainen, T. Roemmel, H. Tuononen, R.T. Boore, J.D. Masuda, J.A. Clyburne
- ORGN 524.** Perfluoroalkyl and cyano derivatives of perylene diimides as novel electron acceptors for advanced electronics. **T. Cikeman**, E.V. Bukovsky, G. Rumbles, O. Boltalina, S.H. Strauss
- ORGN 525.** Synthesis of carba porphyrinoid systems using a carbatripyrin methodology. **L.M. Steteman**, T.D. Lash
- ORGN 526.** Photoinduced oxidative cyclizations of o-aryalkynyloximes. **M. Ko**, W. Kim, P. De Lijser
- ORGN 527.** Synthesis and characterization of ferrocenyl chalcones salts derivatives as potential antibacterial agents. **S.M. Delgado-Rivera**, R.E. Colón-Morillo, I.D. Montes-González, M.D. García Maldonado, A.R. Guadalupe Quiñones, D.J. Sanabria Rios, Y. Rivera-Tores, R. Gutiérrez
- ORGN 528.** Methods for N-alkylation of benzylidene oxindoles. **A.M. Lock**, K.W. Cox, K.J. Knisley, D.M. Ketcha
- ORGN 529.** New phenothiazinium derivatives for potential use in photodynamic therapy (PDT) and dye-sensitized solar cells (DSSC). **I. Kady**, N. Mehraban, S. Fanah
- ORGN 530.** C-Arylation of triazoles: Synthesis of novel vinyl triazole-fused sultams. **A.J. Cassidy**, J. Jun, N. Asad, N. Windmon, A. Diepenbrock, P.R. Hanson
- ORGN 531.** Efforts toward decorated azepine derivatives through a photochemical formal [5+2] cycloaddition. **S.M. Thullen**, D.M. Rubush, T. Rovis
- ORGN 532.** Synthesis of 1*H*-1,2,3-triazole esters and acids. **C.R. Butler**, A. Arroyave, K. McGee, A.M. Schoffstall
- ORGN 533.** Ultrasound-assisted green synthesis of diversely substituted oxindoles. **D. Bandyopadhyay**, O.M. Rodriguez, I.M. Chapa, A. Zavala, B.K. Banik
- ORGN 534.** Organocatalyzed green synthesis of bis-benzopyrazines: An entry to novel heteroaromatics. **D. Bandyopadhyay**, J.A. Perez, H.R. Gardenas, B.K. Banik
- ORGN 535.** Proxy-PET building blocks as a design element for library synthesis. **L.J. Mallin**, H. de Kraker, S.S. Huthmacher, D.M. Ketcha
- ORGN 536.** Efficient synthesis of 1,3,4-oxadiazoles promoted by NH₄Cl. **K.K. Gnanasekaran**, B. Nammalwar, M. Murie, R.A. Bunce
- ORGN 537.** Ring size and substitution effects in the tandem reduction-lactamization of ortho-substituted nitroarenes. **R.A. Bunce**, B. Nammalwar, J.T. Hiett
- ORGN 538.** Efficient synthesis of substituted 3-oxindoline-1-carbonitriles using mesoporous silica MCM-41. **B. Nammalwar**, **N.P. Muddala**, M. Murie, R.A. Bunce
- ORGN 539.** Synthetic studies on guaiipyridine alkaloids: Intramolecular Heck approach. **B. Woldehaimanot**, P.M. Shelton, J.R. Vyvyan
- ORGN 540.** Mechanistic studies on the Pechmann condensation reaction with fluorine-substituted reactants. **M.A. Vanalstine-Parris**, J. DeGrote, S. Tyndall, K. Wong
- ORGN 541.** Withdrawn.
- ORGN 542.** One-pot synthesis of indole-4,9-diones from naphthoquinone. **J.D. Guerra**, Q.H. Liu, C.M. Castaneda, M.A. Martinez, S. Mito
- ORGN 543.** Efficient preparation of pyridinyl-1,2,4-triazines via telescoped condensation with diversely functionalized 1,2-dicarbonyls. **S.V. Marchi**, J.D. Carrick
- ORGN 544.** Study on the palladium-catalyzed Friedel-Crafts-type allylic arylations and aryl etherifications of phenols. **C.A. Discolo**, A.G. Graves, D.R. Deardorff
- ORGN 545.** Progress on the preparation of 3,5-disubstituted 2-isoxazolines. **N. Schiltz**, E. Van Meter, M.D. Mosher
- ORGN 546.** Hypoiodite mediated stoichiometric or catalytic cyclopropanation of alkenes with malononitrile. **A. Yoshimura**, J. Fuchs, T.N. Jones, V.V. Zhdankin
- ORGN 547.** Development of an alternative energy synthetic pathway to ibuprofen through the use of solar irradiation as the sole heat source. **B. Agee**, G. Mullins, D.J. Swartling
- ORGN 548.** Visible-light mediated synthesis of constrained cyclic-peptides from phenacyl protected cysteine residues. **R.C. McAtee**, T.M. Monos, C.R. Stephenson
- ORGN 549.** Cycloaddition reactions of *N*-vinyl nitrones with ketenes and ketenimines. **K. Chando**, R.E. Michael, T. Sannakia
- ORGN 550.** Synthesis and base-mediated rearrangement of cis-1-hydroxy-2-(2-oxoethanyl)cyclopropanes: Approach to hydroxycyclopropane peptidomimetics. **C.K. Zercher**, I. Taschner, M. Mower, P. Moran, Y.M. Bhogadi, R. Chhetri, K. Bala
- ORGN 551.** Stereoselective samarium diiodide organotrifluoroborate carbon bond forming reactions. **C. Aretz**, H. Escobedo, B.J. Cowen
- ORGN 552.** Diversity oriented synthesis of quinoline scaffolds employing acetal substrates in the Doebner-Miller reaction. **G. Rahman**, S.D. Pegan, B.J. Cowen
- ORGN 553.** Sulfonic acids as catalysts for carbon carbon bond forming reactions. **B.J. Cowen**, **J. Miao**
- ORGN 554.** Iodination of potassium organotrifluoroborates and tributyl(aryl) stannanes using iron(III) chloride/sodium iodide. **D.W. Blevins**, **G.W. Kabalka**, M. Yao, L. Yong
- ORGN 555.** Catalytic functionalization of unactivated sp³ C-H bonds through intramolecular oxygen nucleophiles affording cyclic ethers. **S.J. Thompson**, G. Dong
- ORGN 556.** Ligand- and proton-source effects in samarium(II)-mediated elimination/isomerization reactions of allylic benzoates. **A.M. Wright**, G.W. O'Neil
- ORGN 557.** Ring-closing metathesis reactions of acyloxysulfones: Synthesis of γ -alkylidene butenolides. **I. Phan**, G. Gilbert, G.W. O'Neil
- ORGN 558.** Regiocontrolled palladium-catalyzed domino synthesis of *N*-sulfonyl dihydrophenanthridines and dihydrodibenz[e,h]azepines. **N. Dayal**, R. Jain, K. Patel, J.K. Laha
- ORGN 559.** New quinazolin-2-yl-guanidines for medicinal chemistry approaches to neuropsychiatric disorders. **S. Ibrahim**, G. Obenauf, J.K. Britt, A. Pieper, G.K. Friestad
- ORGN 560.** Photogenerated diketopiperazine-spiro-oxiranes as versatile synthons for accessing diverse polyheterocyclic scaffolds. **D.M. Kuznetsov**, N.N. Bhuvan Kumar, A.G. Kutateladze
- ORGN 561.** Practical, scalable synthesis of carbohydrate based oxepines. **R Vannam**, M.W. Peczuh
- ORGN 562.** Reaction of 1,2-cyclohexanedione with diols. An unexpected aromatization reaction. **A.E. Solinski**, **D.A. Hunt**
- ORGN 563.** Mechanistic studies into the reaction of aldehydes with *N*-acylphthalimides. **R.N. Enright**, L.T. Henningsen, P.H. Willoughby
- ORGN 564.** Investigation of oxidopyrylium [5+2] cycloaddition conjugate-addition cascade sequences. **C. Law**, C.R. Zwick, J. Simanis, E.L. Woodall, J.R. Goodell, T.A. Mitchell
- ORGN 565.** Lithium-promoted reaction of aldehydes with *N*-acylphthalimides. **L.T. Henningsen**, R.J. Enright, P.H. Willoughby
- ORGN 566.** Intramolecular cycloadditions of photogenerated Azaxylylanes as key steps in the diversity-oriented synthesis of novel N,O,S-polyheterocycles. **W. Umstead**, O. Mukhina, A.G. Kutateladze
- ORGN 567.** Development of palladium-catalyzed directed alkene functionalization reactions. **S.L. Moss**, L. Xu, B.W. Michel
- ORGN 568.** Formation and reactions of benzyl azetidide compounds. **S.C. Allen**, L.M. Bradley
- ORGN 569.** Toward the development of greener synthetic methods involving modified Knoevenagel-Doebner reaction. **K. Banerjee**, M. Collins
- ORGN 570.** Mechanistic studies on selective monohydrolysis of symmetric diesters with the use of dynamic light scattering. **S. Niwayama**, Y. Hiraga
- ORGN 571.** Regio- and stereoselective additions to enynes containing an organo-manganese auxiliary leading to highly substituted allenyl aldehyde products. **E. Nagy**, A. Roy, S.D. Lepore
- ORGN 572.** Palladium-catalyzed microwave heated cross-coupling of organotrifluoroborates and metal fluoride. **R.L. Welch**, M. Al-Masum
- ORGN 573.** Pd-catalyzed cross-coupling reaction of styryltrifluoroborates with activated alkynes and alkanes. **W. Shaban**, M. Al-Masum
- ORGN 574.** Cu-catalyzed one-pot electrophilic amination with heteroarylaluminum reagents. **H. Yoon**, Y. Lee
- ORGN 575.** Synthesis of fluorinated homoallylic compounds via ring-opening nucleophilic fluorination of methylene cyclopropanes (MCP). **A. Boateng**, O. Okoromoba, G.B. Hammond
- ORGN 576.** Exploring the reactivity of hexadehydro-Diels-Alder (HDDA)-generated benzenes with acids. **M.K. Haj**, P. Willoughby, T.R. Hoye
- ORGN 577.** Synthesis of 2F-HAT discotic liquid crystal via PCDHF approach. **Z. Li**, R.J. Twieg
- ORGN 578.** Green and scalable synthesis of γ -hydroxybutenolides via aerobic oxidation of 2-silyloxyfurans. **M. Jean**, N. Bruneau-Latour, J. Boukouvalas
- ORGN 579.** Photochemistry of trifluoromethylated 2-nitrobenzyl alcohols. **G. Prakash**, **K. Belligund**, T. Mathew, G.A. Olah
- ORGN 580.** Development and deployment of a new methoxyvinyl cation equivalent. **C.D. McCune**, **M.L. Beio**, J.A. Friest, S. Ginotra, D.B. Berkowitz
- ORGN 581.** Amine conjugate addition to α,β -unsaturated olefins promoted by NHC-Cu catalyzed. **S. Kim**, Y. Lee
- ORGN 582.** Alkyl-substituted nitrophenols in the Passerini-Smiles reaction. **C. Summers**, K. Hausman, S.B. Luesse
- ORGN 583.** Peroxide electrophiles for C-O bond formation. **A. Horn**
- ORGN 584.** Phosphorus-based tether methods in the synthesis of complex polyols. **J.L. Markley**, P.R. Hanson
- ORGN 585.** Amine and isocyanide variation in the Ugi-Smiles Diels-Alder tandem process. **K. Mason**, M. Meyers, B. Richey, S.B. Luesse
- ORGN 586.** Examining the use of conjugated, heterocyclic aldehydes in the Ugi-Smiles reaction. **M. Meyers**, K. Mason, B. Richey, S.B. Luesse
- ORGN 587.** N-heterocyclic carbene catalyzed synthesis of 2-aryl-Indoles. **M.T. Hovey**, C. Check, A.F. Sipher, K. Scheidt
- ORGN 588.** Synthesis of novel β -keto-sultams: Tetramic acid analogs and their derivatives. **J. Jun**, M. Hur, P.R. Hanson, T. Atkinson
- ORGN 589.** Synthesis of pyrazolopyranopyrimidines under controlled microwave exposure: An eco-friendly approach. **D. Bandyopadhyay**, C.L. Gibbs
- ORGN 590.** One-pot four-component synthesis of pyranopyrazoles under microwave irradiation: A green procedure. **D. Bandyopadhyay**, M. Pena-Agudelo
- ORGN 591.** Rh(III)-catalyzed cyclopropanation initiated by C-H activation: Using ligand design to direct diastereoselectivity. **H. Rubin**, T. Plou, T. Rovis
- ORGN 592.** One pot tandem Diels-Alder/Nazarov cyclization. **R.A. Carmichael**, W. Chalfoux
- ORGN 593.** Neat boron trifluoride etherates as reagents for efficient esterification of carboxylic acids and derivatives. **C.J. Cueto**, R.R. Hark
- ORGN 594.** Mn-mediated radical-polar crossover annulation employing a leaving group in the N-acylhydrazone radical acceptor. **K.A. Slater**, G.K. Friestad
- ORGN 595.** Exploration of imine-based Ugi-Smiles reaction. **R. Poornotamed**

ORGN **596**. Rapid, protecting-group free route to acyl pyrrolidines using imines as substrates in the aza-Cope rearrangement—Mannich cyclization. **H.A. Lindsay**, A. Oudeif, J.M. Reder, B. Yambrosic

ORGN **597**. Synthesis of 2-indolinones through microwave-assisted intramolecular transamidation derived from a multicomponent coupling cascade process. **A. Maddirala**, P.R. Andrea

ORGN **598**. Ring opening chemistry of epoxides with new carbon nucleophiles for the synthesis of novel γ -lactones and γ -lactams. **A. Kumar**

ORGN **599**. Toward the miniaturization of chemical library synthesis to the sub-micromole scale using functionalized high loading magnetic nanoparticles. **P.C. Kearney**, P.K. Maity, S. Faisal, P.R. Hanson

ORGN **600**. Ligand-controlled, tunable silver-catalyzed C-H amination. **J.M. Alderson**, A.M. Phelps, R. Scamp, N.S. Dolan, J.M. Schomaker

ORGN **601**. Asymmetric β hydroxylation and amidation of enals via N heterocyclic carbene catalysis. **C. Hoesier**, N.A. White, T. Rovis

ORGN **602**. Solid phase catalysts for the synthesis of α -aryl carboxylic acids. **W.E. Brenzovich**, A. Denton, R. Kohinke, B.R. Craig, D. Moore

ORGN **603**. Synthesis of N-heterocycles via transition metal-catalyzed C-H activation. **K.E. Ruhl**, T. Hyster, T. Rovis

ORGN **604**. New catalytic methods for N-heterocycle synthesis by late transition metal-mediated C-H bond activation. **P. Kilaru**, P. Zhao

ORGN **605**. Substituted 5,6,11,12-tetrahydrodibenzo[a,e] cyclooctenes: Syntheses, properties, and DFT studies of substituted Sondheimer diynes. **F. Xu**, A. Orita, J. Otera

8:45 **PHYS 2**. Contribution of human related sources to indoor volatile organic compounds. **S. Liu**, R. Li, R. Wild, J. Krechmer, S. Thompson, C. Warneke, J.A. de Gouw, S.S. Brown, S. Miller, J.L. Jimenez, P. Ziemann

9:05 **PHYS 3**. Global climate impact of sulphur-plume chemistry and particle formation. **J. Pierce**, R. Stevens

9:30 Intermission.

9:45 **PHYS 4**. Mechanisms of formation and growth of particles in air. **B.J. Finlayson Pitts**

10:50 **PHYS 5**. Detection of low-volatility gas-phase organic compounds from the OH-initiated oxidation of isoprene hydroxyhydroperoxide and their relevance to organic aerosol production. **J. Krechmer**, M. Coggan, J.B. Nowak, J. Kimmel, H. Stark, P. Massoli, J.T. Jayne, J.D. Crouse, T.B. Nguyen, P. Wennberg, J.H. Seinfeld, D.R. Worsnop, J.L. Jimenez, M. Canagaratna

10:25 **PHYS 6**. Nanoparticle growth by carbonaceous matter. **M.V. Johnston**

11:10 **PHYS 7**. Interplay between secondary organic aerosol chemistry, phase state, and growth dynamics. **R.A. Zaveri**, J. Shilling, A. Zelenyuk-Imre, J. Liu, J. Wilson, A. Laskin, B. Wang, J. Fast, R. Easter, J. Wang, C. Kuang, J.A. Thornton, A. Selyan, Q. Zhang, T.B. Onasch, D.R. Worsnop

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Carbon Star Outflows
L. J. Allamandola, T. J. Lee, *Organizers*
J. Oomens, *Presiding*

8:00 **PHYS 8**. Lifecycle of cosmic carbon. **A. Tielens**

8:35 **PHYS 9**. Molecular content of carbon-rich evolved stars and the carbon balance from observations at all wavelengths. **P. Chemicharo**

9:10 **PHYS 10**. Formation of complex organics and carbonaceous grains in the outflow of carbon stars: A laboratory study. **F. Salama**

9:45 Intermission.

10:15 **PHYS 11**. Synthesis of pure and N-substituted cyclic hydrocarbons (e.g. pyrimidine) via gas-phase ion-molecule reactions. **P.P. Bera**, R. Peverati, M.P. Head-Gordon, T.J. Lee

10:50 **PHYS 12**. Computational vibrational spectroscopy and applications to astrochemistry. **R.C. Fortenberry**, X. Huang, W. Morgan, R.A. Theis, T. Crawford, T.J. Lee

11:15 **PHYS 13**. Multiple excited states of PANH anions using informed orbital descriptions. **M.L. Theis**, A. Candian, A. Tielens, T.J. Lee, R.C. Fortenberry

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Accurate Energies for Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
M. S. Gordon, *Presiding*

8:00 **PHYS 14**. Potential energy surfaces for dynamics calculations. **D.G. Truhlar**

8:30 **PHYS 15**. Strategies towards dynamic and non-dynamic electron correlation. **A.K. Wilson**

9:00 **PHYS 16**. Dissecting the effect of morphology on the rates of singlet fission: Insights from theory. **A. Krylov**

9:20 **PHYS 17**. Aerobic oxidation of methanol to formic acid on Au_7^+ : Benchmark analysis based on completely renormalized coupled-cluster and density functional theory calculations. **P. Piecuch**, J.A. Hansen, M. Ehara

9:40 Intermission.

10:00 **PHYS 18**. Complications in potential energy surfaces for molecules involving second row elements. **T.H. Dunning**

10:30 **PHYS 19**. Dynamics of curved carbon π systems. **K.K. Baldrige**

11:00 **PHYS 20**. Mag-walking Monte Carlo and density functional theory calculations of interaction energies in ammonium halide clusters. **R.Q. Topper**, J.J. Biswakarma, V. Cicoci

11:20 **PHYS 21**. Analysis of changes in bonding patterns along reaction paths in terms of molecule-intrinsic quasi-atomic orbitals. **K. Ruedenberg**, A.C. West, M.W. Schmidt, M.S. Gordon

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid β : Structures and Molecular Interactions

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
J. E. Shea, *Presiding*

8:00 Introductory Remarks.

8:05 **PHYS 22**. High resolution insights on the membrane mediated amyloid aggregation. **A. Ramamoorthy**

8:45 **PHYS 23**. Modulation of molecular interactions of Alzheimer's A β peptide fibrils and oligomers with lipid membranes. **F. Tofoleanu**, B. Brooks, **N. Buchete**

9:25 **PHYS 24**. Interaction of A- β with model lipid membranes. **P.S. Cremer**

9:45 Intermission.

10:05 **PHYS 25**. Determining the structural ensemble of intrinsically disordered disease peptides: Applications to Alzheimer's disease biology in solution and membrane. **T.L. Head-Gordon**

10:45 **PHYS 26**. Revealing the interplay between amyloid- β and membranes through molecular simulations. **B. Strodel**

11:25 **PHYS 27**. Structural studies of the membrane disruption pathways induced by β -amyloid peptides in Alzheimer's disease. **W. Qiang**, R.D. Akinlolu, M. Nam, N. Shu, D. Delgado

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Advances in Simulation Methodology

Cosponsored by COMP

A. E. Garcia, *Organizer*
G. Hummer, *Organizer, Presiding*

8:00 **PHYS 28**. Sense and nonsense when performing and interpreting molecular dynamics simulations of biomolecular systems. **W. van Gunsteren**

8:35 **PHYS 29**. Potential function as a variable: Advances in using simulations of multiple states to solve hard biomolecular problems. **M.R. Shirts**

9:10 **PHYS 30**. TRAM: Optimal estimation of trajectory data from multiple thermodynamic states. **F. Noe**

9:45 **PHYS 31**. Exact milestoning. **R. Elber**

10:20 **PHYS 32**. Fluorescent proteins as pH sensors: Insights from constant pH molecular dynamics. **E.N. Laricheva**, C.L. Brooks

10:55 **PHYS 33**. Molecular multipole models for complex biomolecules. **T. Ichihye**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
H. Jaeger, *Presiding*

8:00 **PHYS 34**. Photoinduced proton-coupled electron transfer in solution: Quantum mechanical/molecular mechanical nonadiabatic dynamics. **S. Hammes-Schiffer**

8:40 **PHYS 35**. Energy transfer in closely packed Si quantum dots: The role of surface defects. **S.V. Kilina**

9:20 **PHYS 36**. Cheap models for electronic transitions and their application to lead-halide perovskites. **J. Parkhill**

9:40 Intermission.

10:00 **PHYS 37**. Modeling artificial and natural light harvesting systems with DFT. **E. Jakubikova**

10:40 **PHYS 38**. Photodissociation dynamics of phenol. **X. Xu**, J. Zheng, K. Yang, D.G. Truhlar

11:20 **PHYS 39**. Computational photochemistry of thioanisole. **S.L. Li**, D.G. Truhlar

11:40 **PHYS 40**. Time-dependent density functional theory study of the excited state energy landscape of gold phosphine thioalate complexes. **E.B. Guidez**, C.M. Aikens

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, *Organizer*

S. Link, K. A. Willets, *Organizers, Presiding*

8:00 **PHYS 41**. Ultrafast photoelectron imaging microscopy of plasmonic nanoparticles. **D.J. Nesbitt**

8:35 **PHYS 42**. Tuning the acoustic frequency of a gold nanodisk through its adhesion layer. **W. Chang**, F. Wen, D. Chakraborty, M. Su, Y. Zhang, B. Shuang, P.J. Nordlander, J. Sader, N.J. Halas, S. Link

8:55 **PHYS 43**. Coherent plasmonics for ultrasensitive and single molecule sensing. **N.J. Halas**

9:30 **PHYS 44**. Probing ground-state single-electron self-exchange across a molecule-metal interface and molecule-substrate electronic coupling by simultaneous spectroscopic and topographic Near-field SERS Imaging. **Y. Wang**, P. Sevinc, Y. He, H. Lu

9:50 **PHYS 45**. Using STEM/EELS to probe energy transfer in plasmon-enhanced solar devices. **J.P. Camden**

10:25 **PHYS 46**. Use of electron microscopy to probe quantum plasmonics, hot electrons and energy transport in hybrid nanoparticle/semiconductor systems. **C. Cherqui**

10:45 **PHYS 47**. Cathodoluminescence-activated nano-imaging by resonant energy transfer. **N.S. Ginsberg**, C.G. Bischak, C. Hetherington, Z. Wang, J. Precht, D. Kaz, C. Stachelrodt, D. Schlom

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Recent Advances in Computational Methods

L. Gagliardi, B. Smit, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **PHYS 48**. Self-interaction correction to density-functional approximations with unitary invariance. **M.R. Pederson**

8:35 **PHYS 49**. Toward rational design of small molecule adsorption in open-site metal-organic frameworks with density functional theory. **J. Neaton**

9:05 **PHYS 50**. New density functionals obtained by a genome-scale search approach to functional design. **N. Mardirossian**, M.P. Head-Gordon

9:35 **PHYS 51**. Mechanism of C-H bond activation of C_2H_4 by iron(IV)-oxo sites in magnesium-diluted $Fe_2(dobdc)$. **P. Verma**, K.D. Vogiatzis, N. Planas, J. Borycz, D. Xiao, J.R. Long, L. Gagliardi, D.G. Truhlar

PHYS

Division of Physical Chemistry

E.L. Sibert, Program Chair

OTHER SYMPOSIA OF INTEREST:

ACS Award for Computers in Chemical and Pharmaceutical Research honoring David Case (see *COMP, Mon, Tue*)

Electronic Structure Methods for Highly Polarizable Systems (see *COMP, Sun, Mon*)

Computational Design, Discovery and Optimization of Organic Semiconductor Materials (see *COMP, Sun, Mon*)

Quantum Chemistry (see *COMP, Sun, Mon, Tue, Wed*)

Molecular Mechanics: Force Field Development (see *COMP, Mon*)

Computational Chemistry In The Undergraduate Curriculum: What Is Working And How Do We Assess It? (see *CHED, Wed*)

SUNDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

New Particle Formation and Growth

M. Freedman, *Organizer*

D. Cziczó, *Organizer, Presiding*
J. Pierce, *Presiding*

8:00 Introductory Remarks.

8:05 **PHYS 1**. Aerosol nucleation and growth in the CLOUD experiment at CERN. **J. Curtius**

9:55 Intermission.

10:15 **PHYS 52.** Enantioselective adsorption in zeolites and metal-organic frameworks. R. Bueno-Perez, A. Martín-Calvo, P. Gómez-Alvarez, J. Gutiérrez-Sevillano, P. Merkling, T. Vlucht, van Erp, D. Dubbeldam, S. Calero

10:45 **PHYS 53.** New computational tools for modeling metal-organic frameworks. F. Paesani

11:15 **PHYS 54.** Computational materials design of co-polymers for organic electronics. R.E. Larsen, T.W. Kemper, S. Sides, P. Graf, D.C. Olson

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Dynamics

Sponsored by COMP, Cosponsored by PHYS

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Ice Nucleation

M. Freedman, *Organizer*
D. Cziczó, *Organizer, Presiding*
J. Lu, *Presiding*

1:30 **PHYS 59.** Nucleation of ice: A molecular perspective. V. Molinero

2:10 **PHYS 60.** Homogeneous freezing of single submicron to micron-sized water and hydrocarbon aerosol droplets levitated in a Bessel beam trap. J.W. Lu, M. Isenor, R. Signorell

2:30 **PHYS 61.** Ice formation in ultracold cirrus. E. Moyer, K. Lamb, B. Clouser, L. Sarkozy, M. Bolot, O. Moehler, H. Saathoff, V. Ebert

2:55 **PHYS 62.** Ice nucleation in clouds: Sensitivities to physicochemical IN properties and cloud microphysics. B. Evens, G. Feingold

3:20 Intermission.

3:35 **PHYS 63.** Atmospheric ice nucleating particles from the sea surface microlayer. B. Murray, T.W. Wilson, L. Ladino, P. Alpert, M. Breckels, I. Brooks, J.A. Huffman, C. Judd, W.P. Killthau, R. Mason, G. McFiggans, L. Miller, J. Najera, E. Polishchuk, S. Rae, S. Corinne, M. Si, T. Whale, J. Wong, O. Wurl, J. Yakobi, J.P. Abbatt, J.Y. Aller, A.K. Bertram, D.A. Knopf

4:15 **PHYS 64.** Contact-induced efflorescence of amorphous inorganic microparticles. R.D. Davis, S. Lance, J.A. Gordon, S.B. Ushijima, M. Tolbert

4:35 **PHYS 65.** Studies of the abundance and compositions of organic ice nucleating particles in the atmosphere. P.J. DeMott, T.C. Hill, C.S. McCluskey, E.J. Levin, K.J. Suski, O. Laskina, Y. Tobo, D.B. Collins, C. Sultana, C. Lee, G. Cornwell, H. Al-Mashat, M. Santander, C.M. Beall, F. Malfatti, R. Mason, D. Pham, N.G. Swoboda-Colberg, V.H. Grassian, R. Moffet, A.K. Bertram, K.A. Prather, S. Kreidenweis

5:00 **PHYS 66.** Atmospheric ice nucleation: Microspectroscopic imaging and characterization of individually identified ice nucleating particles. D.A. Knopf, P. Alpert, B. Wang, W.P. Killthau, D. Bothe, R.E. O'Brien, S.T. Kelly, A. Laskin, M.K. Gilles, J.Y. Aller

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Carbon Star Outflows
L. J. Allamandola, T. J. Lee, *Organizers*
F. Salama, *Presiding*

1:30 **PHYS 67.** Observations of organic molecules in carbon-rich proto-planetary nebulae and planetary nebulae. E. Peeters

2:05 **PHYS 68.** Dust formation in carbon stars. I. Cherchneff

2:40 **PHYS 69.** Ion chemistry of cyclic aromatics and interactions with polar molecules leading to the formation of complex organics in the gas phase and on ice grains. M. El-Shall

3:15 Intermission.

3:45 **PHYS 70.** Laboratory infrared spectroscopy of 'hard-to-get' ionized polyaromatics. J. Oomens

4:20 **PHYS 71.** Carbonaceous dust and fullerenes in evolved stars. J. Cami

4:45 **PHYS 72.** Quantum chemical studies of interstellar organic molecules: Formation mechanisms, spectroscopic signatures, and properties. T.J. Lee

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Gas-Phase Kinetics and Dynamics
Cosponsored by COMP
J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
G. C. Schatz, *Presiding*

1:30 **PHYS 73.** Mode-, bond- and stereo-selective bimolecular reactions. K. Liu

2:00 **PHYS 74.** Sudden vector projection model: Mode specificity and bond selectivity made easy. H. Guo

2:30 **PHYS 75.** Mixed quantum/classical theory for rotationally and vibrationally inelastic scattering. D. Babikov

2:50 **PHYS 76.** Sum over histories representation for chemical kinetics. R.T. Skodje

3:10 Intermission.

3:30 **PHYS 77.** Resonances in chemical reactions. X. Yang

4:00 **PHYS 78.** Reaction dynamics on ab initio potential energy surfaces. J.M. Bowman, Y. Wang, Z. Homayoon, R. Conte, P. Houston

4:30 **PHYS 79.** Improved semiclassical tunneling. A.F. Wagner

4:50 **PHYS 80.** Alkyl CH stretch vibrations as a probe local environment. E.L. Sibert, D.P. Tabor, N. Kidwell, J.C. Dean, T.S. Zwier

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid Precursor Protein, Origin of Amyloid β
Cosponsored by COLL and COMP
J. C. Lee, J. E. Straub, *Organizers*
M. T. Zanni, *Presiding*

1:30 **PHYS 81.** Structure, dimerization, and cholesterol binding of the amyloid precursor protein transmembrane C99 domain and amyloidogenesis. C.R. Sanders

2:10 **PHYS 82.** Impact of membrane composition on the structure, stability, and processing of the transmembrane domain of the amyloid precursor p. L. Dominguez, L. Foster, J.E. Straub, D. Thirumalai

2:50 **PHYS 83.** Conformational changes induced by the A21G Flemish mutation in the amyloid precursor protein lead to increased A β secretion in Alzheimer's disease. T. Tang, Y. Hu, P. Kienlen-Campard, L. El Haylani, M. Decock, J. Van Hees, Z. Fu, J. Ocatve, S. Constantinescu, S.O. Smith

3:10 Intermission.

3:30 **PHYS 84.** Titration of charged residues in the context of membrane bilayers; A constant pH molecular dynamics study. A. Panahi, C.L. Brooks

3:50 **PHYS 85.** Dimerization of a transmembrane peptide from amyloid precursor protein. S. Meredith

4:30 **PHYS 86.** Multiscale molecular dynamics simulations of transmembrane structures of amyloid precursor protein in biological membrane. Y. Sugita

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Classical and Quantum Descriptions of Protein Function
Cosponsored by COMP
G. Hummer, *Organizer*
A. E. Garcia, *Organizer, Presiding*

1:30 **PHYS 87.** Proton-coupled electron transfer in soybean lipoxygenase: Hydrogen tunneling and conformational motions. S. Hammes-Schiffer

2:05 **PHYS 88.** Activation mechanisms in RAF kinase dimers. E. Rosta

2:40 **PHYS 89.** Ab initio QM/MM simulations point to an alternative mechanism for the AlkB catalyzed repair of 1-methyl adenine. D. Fang, G.A. Cisneros

3:15 **PHYS 90.** Exploring water penetration in soluble proteins and ion pumps. Q. Cui

3:50 **PHYS 91.** Withdrawn.

4:25 **PHYS 92.** Theoretical analysis and modeling of rhodopsin's unusual kinetics of thermal reactions and its role in dim-light vision. Y. Guo, S. Sekharan, J. Liu, V.S. Batista, J.C. Tully, E.C. Yan

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Complex Materials and Molecules
Cosponsored by COMP
B. G. Levine, S. A. Varganov, *Organizers*
S. W. Kilina, *Presiding*

1:30 **PHYS 93.** Quantum simulation of coherent exciton dynamics in conjugated systems. P.J. Rossky

2:10 **PHYS 94.** Electronic excitation of metal-organic frameworks. H. Jaeger

2:50 **PHYS 95.** Auger relaxation of hot electrons in CdSe quantum dots using GFSH. D. Trivedi, L. Wang, O. Prezhdo

3:10 **PHYS 96.** Nonlinear optical structural properties of room-temperature ionic liquids, calculated with the combined fragment molecular orbital and linear-response time-dependent density functional theory method (FMO/LR-TDDFT). A.D. Findlater, F. Zahariev, M.S. Gordon

3:30 Intermission.

3:50 **PHYS 97.** Evolution of photoexcited states in extended molecular chromophores. S. Tretiak

4:30 **PHYS 98.** Excited state dynamics at metal to semiconductor interfaces. D. Kilin

5:10 **PHYS 99.** Excited states in large molecular systems by the combined quantum Monte Carlo/effective fragment molecular orbital method. F. Zahariev, A.D. Findlater, M.S. Gordon

5:30 **PHYS 100.** Electronic structure study of CIGS solar cells by X-ray absorption spectroscopy: Experiment and theory. C.P. Schwartz, D. Nordlund, T. weng, K. Ramanathan, D. Sokaras, D. Prendergast, S. Christensen

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, D. J. Masiello, *Organizers*
K. A. Willets, *Organizer, Presiding*
J. P. Camden, *Presiding*

1:30 **PHYS 101.** Quantum and molecular plasmonics. P.J. Nordlander

2:05 **PHYS 102.** Single photon interactions with localized surface plasmons: Exploiting fano resonances to generate quantum beats. N. Thakkar, C. Cherqui, D.J. Masiello

2:25 **PHYS 103.** Understanding heterogeneity in plasmonic metal oxide nanocrystals. D.J. Milliron, R. Johns, A. Agrawal, S.D. Lounis, D. Nordlund, H. Bechtel

3:00 **PHYS 104.** Mid-infrared surface phonon polaritons in dolar Dielectrics: An alternative approach. A.J. Giles, J. Caldwell

3:20 **PHYS 105.** Life and times of plasmonically-generated energetic electrons. M. Moskovits

3:55 **PHYS 106.** Characterizing the generation of hot electrons by metal nanoparticles through their interaction with molecular-type electron acceptors. A. Hoggard, B. Foerster, D. Huang, W. Chang, S. Link

4:15 **PHYS 107.** Towards nonphotonic and time-resolved spectroscopy of plasmonic systems. I. Thomann

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Gas Separation & Gas Storage: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

1:30 **PHYS 55.** Accurate first-principles force fields for high-throughput screening of gas uptake in metal-organic frameworks. J.G. McDaniel, S. Li, E. Tyllanakis, R. Snurr, J.R. Schmidt

2:00 **PHYS 56.** First principles simulations in the study of metal-organic frameworks: From stability to activity. N. Lopez

2:30 **PHYS 57.** Metal organic framework based catalyst for release of chemically stored nitric oxide. R. Kumar

3:00 **PHYS 58.** Top-down generation and screening of metal-organic frameworks for gas storage and separation applications. D. Gomez-Gualdrón, Y.J. Colon, Y. Chung, R. Snurr

3:30 Intermission.

3:50 **PHYS 108.** Ab initio simulation of adsorption isotherms for gases and gas mixtures in porous media. J. Sauer

4:20 **PHYS 109.** 2D crystalline zeolites, non-aluminosilicate molecular sieves, and metal organic frameworks. M. Tsapatsis

4:50 **PHYS 110.** Developing a predictive, descriptor based approach for CO and NO adsorption to Fe, Co, Ni and Cu sites in zeolites. F. Goeltl, P. Mueller, I. Hermans, P. Sautet

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems**Embedding: QM/QM and QM/MM**

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry**Methodology**

Sponsored by COMP, Cosponsored by PHYS

MONDAY MORNING**Section A**Colorado Convention Center
Room 501**Atmospheric Chemistry: Transformations of Matter in the Troposphere****Water & Organic Aerosol**D. Cziczo, M. Freedman, *Organizers*
R. Washenfelder, Q. Zhang, *Presiding*

8:00 PHYS **111**. Hydration state of methylglyoxal at the air-water interface. G.L. Richmond, S. Wren, B.P. Gordon, N. Valley, L. McWilliams

8:40 PHYS **112**. Direct and quantitative measurement of the surface tension of airborne microdroplets. B.R. Bzdek, R.M. Power, J.P. Reid

9:00 PHYS **113**. Calculated equilibrium constants for formation of peroxy radical/water complexes to elucidate radical initiated particle formation. R.B. Shirts, S. Kumbhani, E. Burrell, J.C. Hansen

9:20 Intermission.

9:35 PHYS **114**. Liquid/vapor interface of aqueous solutions relevant to tropospheric chemistry. J.C. Hemminger

10:15 PHYS **115**. Single scattering albedo studies of brown carbon formation in evaporating droplets. M. Zauscher, M.A. Symons, D.O. Dehaan

10:35 PHYS **116**. Air-water interface: As influenced by ions, lipids, and electric fields. H.C. Allen

11:00 PHYS **117**. Redistribution of black carbon in aerosol particles undergoing liquid-liquid phase separation. S. Brunamonti, U. Krieger, C. Marcolli, T. Peter

Section BColorado Convention Center
Room 502**Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution****Organic Molecules in the Diffuse Interstellar Medium**L. J. Allamandola, T. J. Lee, *Organizers*
J. Cami, *Presiding*

8:00 PHYS **118**. Carbon bearing molecules in interstellar clouds. J. Krelowski

8:35 PHYS **119**. Molecular laboratory astrophysics: About molecular transients and molecule formation under interstellar conditions. H. Linnartz

9:10 PHYS **120**. Carbon in the galaxy. E. Roueff

9:45 Intermission.

10:15 PHYS **121**. Low temperature formation of polycyclic aromatic hydrocarbons in the interstellar medium via bimolecular neutral-neutral reactions. R. Kaiser

10:50 PHYS **122**. Angle-resolved PEPICO imaging of the dissociative ionization of methyl azide and methylenimine using a tabletop high harmonic generation light source. W.K. Peters, D.E. Couch, C.W. Hogle, D. Beltran, P. Towstik, D.M. Jonas, H. Kapteyn, M.M. Murnane

11:15 PHYS **123**. Electronic excited states of interstellar species: Quantum chemical prediction of spectroscopic signatures using quartic force fields. W.J. Morgan, R.C. Fortenberry

Section CColorado Convention Center
Room 503**Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar****Enzyme Kinetics and Dynamics**

Cospponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
S. Hammes-Schiffer, *Presiding*

8:00 PHYS **124**. Tunneling and the role of barrier width in enzymatic C-H activation. J.P. Klinman

8:30 PHYS **125**. Theoretical studies of enzymatic reactions. W. Thiel

9:00 PHYS **126**. Role of dynamics in enzyme catalysis: Challenges in comparing calculations to measurements. A. Kohen

9:20 PHYS **127**. Quantum mechanical/molecular mechanical simulations of the hydride transfer reactions in quinone reductase 2. C.R. Reinhardt, S. Bhattacharyya

9:40 Intermission.

10:00 PHYS **128**. QM/MM excited state dynamics of complex systems. U. Roethlisberger

10:30 PHYS **129**. Understanding metalloenzyme catalysis with QM/MM free energy simulations. Q. Cui

11:00 PHYS **130**. Adaptive-partitioning QM/MM dynamics simulations of proton transfer. S. Pezeshki, H. Lin

11:20 PHYS **131**. Functional mode electron transfer theory. H. Chen

Section DColorado Convention Center
Room 504**Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease** **α -Synuclein, the Parkinson's Protein**

Cospponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*G. L. Millhauser, *Presiding*

8:00 PHYS **132**. Structure of the toxic core of α -synuclein, the amyloid associated with Parkinson's disease. D. Eisenberg, J.A. Rodriguez, M. Ivanova, M. Sawaya, D. Cascio, F. Reyes, D. Shi, E. Guenther, L. Johnson, J. Hattne, S. Sangwan, B. Nanega, A. Brewster, M. Messerschmidt, S. Boutet, N. Sauter, T. Gonon

8:40 PHYS **133**. NMR approaches to uncovering the molecular basis of inhibition of alpha-synuclein aggregation by beta synuclein. J. Baum, M. Janowska, G. Moriarty, M. Olson, N. Sikka

9:20 PHYS **134**. Examining the folding landscape of α -synuclein using time-resolved FRET. S.K. Hess, J.C. Lee

9:40 Intermission.

10:00 PHYS **135**. Misfolding and membrane interaction of amyloidogenic proteins. R. Langen

10:40 PHYS **136**. Aggregation mechanism of amyloidogenic proteins involved in neurodegenerative disorders. C. Stultz

11:20 PHYS **137**. Amyloidogenic proteins A-beta, alpha-synuclein and Tau interact with and disrupt membranes via different mechanisms and exhibit cell-type dependent toxicity. H. Lashuel

Section EColorado Convention Center
Room 507**Modeling Complex Biomolecules: From Structure to Dynamics & Function****Membrane Proteins**

Cospponsored by COMP

A. E. Garcia, G. Hummer, *Organizers*
E. Tajkhorshid, *Presiding*

8:00 PHYS **138**. Large-scale computer simulations of lipids: Coarse-grained simulations of complex mixed bilayers. D.P. Tieleman

8:35 PHYS **139**. Membrane proteins: From structure refinement and remodeling to functional mechanisms. H. Zhou

9:10 PHYS **140**. Specific protein-lipid interactions stabilize an active state of the beta 2 adrenergic receptor. C. Neale, H.D. Hecce, R. Pomès, A.E. Garcia

9:45 PHYS **141**. Dynamics of dopamine transporter: Molecular simulations and comparison with LeuT dynamics. M.H. Cheng, I. Bahar

10:20 PHYS **142**. Channel rhodopsin: Structure vs. function relationships from molecular dynamics simulations. S.W. Rick, M. VanGordon, S.L. Rempe

10:55 PHYS **143**. Assembly and mechanistic details of drug translocation in MexAB-OprM efflux pump. C.A. Lopez, J. Phillips, B. Alexandrov, G. Gnanakaran

Section FColorado Convention Center
Room 505**Modeling Excited States of Complex Systems****Excited States in Biology**

Cospponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
L. V. Slipchenko, *Presiding*

8:00 PHYS **144**. Excitonic states in natural light-harvesting systems. B. Mennucci

8:40 PHYS **145**. Electronic progression during the photoisomerization of microbial and vertebrate light-sensing rhodopsins. H. Luk, S. Gozem, F. Melaccio, S. Rinaldi, M. Olivucci

9:20 PHYS **146**. Theoretical study of the electron transfer in DNA repair process of the cyclobutane pyrimidine dimer lesion. L. Joubert-Doriot, T. Domratcheva, M. Olivucci, A.F. Izmaylov

9:40 Intermission.

10:00 PHYS **147**. Insights into the role of excimers/excimeres in the photophysics and photochemistry of DNA. S. Matsika

10:40 PHYS **148**. Excited-state electron transfer in fluorescent proteins. A. Krylov

11:20 PHYS **149**. Charge-transfer dynamics of light-harvesting systems in complex solvated environments. B.M. Wong, M. Oviedo

11:40 PHYS **150**. Spectroscopic properties of a cholesteric liquid glass platinum acetylacetyl. T.M. Cooper, A.R. Burke, D.M. Krein, R.F. Ziolo, J.E. Haley, D.J. Stewart, S.L. Long, A.E. Bell

Section GColorado Convention Center
Room 506**Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level**S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer*, *Presiding*
I. Thomann, *Presiding*

8:00 PHYS **151**. Shape and surface control of plasmonic particles. C.J. Murphy

8:35 PHYS **152**. Plasmonic properties of coupled gold nanostructures. C. Liow, A. Li, S. Li

8:55 PHYS **153**. Mechanisms of on-colloid nanoparticle growth. J. Millstone, P. Strane, L. Marbella

9:30 PHYS **154**. Probing G_{33} and G_{41} contents of HIV-1 and ebola virus-like particles through plasmon coupling microscopy. A. Feizpour, C. Silva, H. Akiyama, C.M. Miller, S. Gummuluru, B.M. Reinhard

9:50 PHYS **155**. Surface plasmon polaritons in chemically synthesized nanostructures. G.V. Hartland, P. Johns, M. Devadas, K. Yu

10:25 PHYS **156**. Understanding the STEM/EELS magneto-optical responses of aromatic plasmon-supporting metal oligomers. N. Bigelow, C. Cherqui, A. Vaschillo, H. Goldwyn, D.J. Masiello

10:45 PHYS **157**. Plasmon/exciton and plasmon/photonic mode interaction. G.C. Schatz

Section HColorado Convention Center
Room 607**Design of Materials and Chemical Processes: The Genomic Approach****The Materials Genome and DataMining**L. Gagliardi, B. Smit, *Organizers*, *Presiding*

8:00 PHYS **158**. Materials project for accelerated materials design. K. Persson

8:30 PHYS **159**. Predictive materials discovery: Finding optimal zeolites for challenging separations and chemical conversions. J.I. Siepmann, P. Bai, M. Jeon, L. Ren, C. Knight, M.W. Deem, M. Tsapatsis

9:00 PHYS **160**. Recent applications of databases of crystal structures and experimental data for metal-organic framework materials. D. Sholl, X. Nie, T. Duerinck, K. Walton, D. Nazarian, J. Camp

9:30 PHYS **161**. Computational screening of MOFs with open metal sites for adsorption and catalysis applications. K.D. Vogiatzis, E. Haldoupis, J.I. Siepmann, L. Gagliardi

9:50 Intermission.

10:10 PHYS **162**. Material informatics in discovery of nanoporous materials for energy applications. M. Haranczyk

10:40 PHYS **163**. Prediction of high deliverable capacity metal-organic frameworks with an evolutionary algorithm. Y. Bao, R. Martin, C. Simon, M. Haranczyk, B. Smit, M.W. Deem

11:10 PHYS **164**. Materials genome in action: Finding a nanoporous material for methane storage. C. Simon, J. Kim, D. Gomez-Gualdron, J. Camp, Y. Chung, R. Martin, R. Mercado, M.W. Deem, D. Gunter, M. Haranczyk, D. Sholl, R. Snurr, B. Smit

11:30 PHYS **165**. Cheminformatics-inspired approaches for big materials data. O. Isayev, D. Fourches, E. Muratov, A. Tropsha

MONDAY AFTERNOON**Section A**Colorado Convention Center
Room 501**Atmospheric Chemistry: Transformations of Matter in the Troposphere****Aqueous Chemistry**

D. Cziczo, M. Freedman, *Organizers*
D. O. Dehaan, M. D. Zauscher, *Presiding*

1:30 PHYS **166**. Aqueous-phase and organic-phase photochemistry of atmospheric organic compounds. S.A. Nizkorodov

2:10 PHYS **167**. Laboratory and field studies of brown carbon aerosol in the near-ultraviolet spectral region. R. Washenfelder, J. Flores, G. Adler, C. Brock, J. Lee, J. Laskin, A. Laskin, S.A. Nizkorodov, L. Segev, S.S. Brown, Y. Rudich

- 2:30** **PHYS 168.** Formation and photochemical evolution of phenolic SOA in aqueous phase. **Q. Zhang,** L. Yu, J.D. Smith, C. Anastasio, A. Laskin, J. Laskin
- 2:55** **PHYS 169.** Cloud and fog processing of atmospheric organic matter. **J.L. Collett,** A. Boris, M. Schurman, Y. Desyaterik
- 3:20** Intermission.
- 3:35** **PHYS 170.** Aerosol organics: Formation and processing in the aqueous phase. **V. McNeill**
- 4:15** **PHYS 171.** Multiphase atmospheric chemistry of pyruvic acid. **V. Vaida,** A. Monod, J. Doussin, A.E. Reed Harris, E. Griffith, J.A. Kroll, R.J. Rapf
- 4:40** **PHYS 172.** Aqueous-phase aldehyde photooxidation in the presence of ammonium salts, amines, and SO₂: brown carbon formation. **D.O. Dehaan,** N.G. Jimenez, P.D. Wickremasinghe, K.D. Sharp

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Interstellar Clouds

L. J. Allamandola, T. J. Lee, *Organizers*
H. Linnartz, *Presiding*

- 1:30** **PHYS 173.** Review of the molecular complexity of organic material in the gas-phase ISM. **S.N. Milam**
- 2:05** **PHYS 174.** Global optimization and broadband analysis software for interstellar chemistry. **S.L. Widicus Weaver,** L. Zou, M. Rad, J. Sanders
- 2:40** **PHYS 175.** Molecular line lists of carbon-containing molecules for exoplanets and other hot bodies. **J. Tennyson**
- 3:15** Intermission.
- 3:45** **PHYS 176.** Observations of carbon in interstellar and circumstellar ices. **A. Boogert**
- 4:20** **PHYS 177.** Reliable abundances of extraterrestrial hydrocarbon ices: Interminable quest or end in sight? **R.L. Hudson,** P.A. Gerakines
- 4:45** **PHYS 178.** Optical properties of titan haze analogs using photoacoustic and cavity ring-down spectroscopy. **M.S. Ugelow,** K.J. Zarzana, M.A. Tolbert

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Catalysis

Cosponsored by COMP

- J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
C. T. Campbell, *Presiding*
- 1:30** **PHYS 179.** Silica thin films: From crystals to glass in 2D. **H. Freund**
- 2:00** **PHYS 180.** Doped metal clusters on oxides: Rationalization and design through the prism of chemical bonding. **A. Alexandrova**
- 2:30** **PHYS 181.** Some recent developments in saddle point finding methods: Gradient squared minimization, solid state transitions, and temperature accelerated adaptive Kinetic Monte Carlo. **G.A. Henkelman**
- 3:00** **PHYS 182.** Catalysis with metal clusters anchored at the Zr⁶-based metal-organic framework NU-1000. **L. Gagliardi,** D.G. Truhlar, C.J. Cramer, J. Borycz, L. Fernandez, S. Tussupbayev
- 3:20** Intermission.
- 3:40** **PHYS 183.** New approaches to simulating biological and molecular catalysis. **T.F. Miller**

- 4:10** **PHYS 184.** Organometallic and organocatalytic reactions explored using the automated reaction route mapping method. **K. Morokuma**
- 4:40** **PHYS 185.** Hydrazine decomposition in the gas phase and on an Iridium catalyst. **M.W. Schmidt,** M.S. Gordon
- 5:00** **PHYS 186.** Density functional theory study of lithium ion battery anode materials: Ruthenium (IV) oxide, tin (IV) oxide, and tin (IV) sulfide. **B.R. Ramachandran,** A.S. Hassan, K. Moyer, T. Dixon, C.D. Wick

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Islet Amyloid Polypeptide (IAPP) at the Water/Lipid Interface

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
T. L. Head-Gordon, *Presiding*

- 1:30** **PHYS 187.** Islet amyloid polypeptide: Membrane interactions and cytotoxicity. **D.P. Raleigh**
- 2:10** **PHYS 188.** Aggregation and Orientation of amyloid proteins at lipid/water interfaces probed by chiral sum frequency generation spectroscopy. **L. Fu, Z. Wang, D. Xiao, V.S. Batista, E.C. Yan**
- 2:50** **PHYS 189.** β -Sheet intermediate dictates the fiber formation kinetics of amylin from type 2 diabetes. **M.T. Zanni**
- 3:30** Intermission.
- 3:50** **PHYS 190.** Islet amyloid and the shared molecular origins of membrane poration and cytotoxicity. **A. Miranker**
- 4:30** **PHYS 191.** Exploring the free energy and conformational landscape of amyloidogenic peptides upon aggregation and amyloid formation. **R. Winter**
- 5:10** **PHYS 192.** Protein folding and assembly on membrane-mimics in constant volume replica-exchange simulations. **Z.A. Levine,** R.G. Mullen, J.E. Shea
- 5:30** **PHYS 193.** Structure of insulin at the air/water interface: monomers or dimers? **S. Mauri, T. Weidner, H. Arnolds**

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Molecular Machines

Cosponsored by COMP

A. E. Garcia, *Organizer*
G. Hummer, *Organizer, Presiding*

- 1:30** **PHYS 194.** Modeling the function of molecular motors and other challenging biological systems. **A. Warshel**
- 2:05** **PHYS 195.** Energy barriers and driving forces in tRNA translocation through the ribosome. **K. Grubmueller,** L.V. Bock, G.F. Schroder, I.I. Davydov, M.V. Rodnina, H. Stark, A.C. Vaiana, N. Fischer, C. Blau
- 2:40** **PHYS 196.** Simulating conformational changes of the ribosome. **K. Sanbonmatsu**
- 3:15** **PHYS 197.** Unraveling the mystery of ATP hydrolysis in actin filaments. **G.A. Voth**
- 3:50** **PHYS 198.** Specificity, mechanism, and membrane organization of ATP synthases. **J. Feraldo-Gomez**
- 4:25** **PHYS 199.** Visualizing complex functional motions of membrane transporters using advanced simulation and free energy techniques. **E. Tajkhorshid**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Multiple Chromophores

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
A. F. Izmaylov, *Presiding*

- 1:30** **PHYS 200.** Ab initio exciton model for nonadiabatic dynamics of multichromophoric systems on GPUs. **A. Sisto,** D.R. Glowacki, **T.J. Martinez**
- 2:10** **PHYS 201.** New electronic structure methods for describing excited states in multichromophore and other large systems. **J.M. Herbert,** X. Zhang, A.F. Morrison
- 2:50** **PHYS 202.** Charge transfer-like excitations in solution: A critical assessment of TDDFT/continuum models. **C.A. Guido,** D. Jacquemin, C. Adamo, B. Mennucci
- 3:10** **PHYS 203.** Modeling protein - chromophore electrostatic interactions with multiple electronic states: Diabatic population matrix approach. **J.W. Park, Y.M. Rhee**
- 3:30** Intermission.
- 3:50** **PHYS 204.** Vibronic interactions in bi- and multi-chromophores. **L.V. Slipchenko**
- 4:30** **PHYS 205.** Accurate simulation of exciton dynamics for hundreds to tens of thousands of chromophores: Theoretical methods and acceleration by general-purpose graphics processing units (GPGPU). **A. Aspuru-Guzik**
- 5:10** **PHYS 206.** Photoexcited energy transfer in a weakly coupled dimer. **L. Alfonso Hernandez, T. Nelson, S. Tretiak, S. Fernandez-Alberti**
- 5:30** **PHYS 207.** Theoretical investigation of singlet fission in quinoindol bithiophenes. **A. Chien, A. Molina, T.G. Goodson, P.M. Zimmerman**

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer, Presiding*
P. K. Jain, *Presiding*

- 1:30** **PHYS 208.** Mechanistic study of serum albumin interaction with therapeutic nanoparticles. **C.F. Landes, S. Dominguez-Medina, L. Kisley, S. Link**
- 2:05** **PHYS 209.** Biological targeting of plasmonic nanoparticles improves cellular imaging via the enhanced scattering in the aggregates formed. **M. Aioub, B. Kang, M. Mackey, M.A. El-Sayed**
- 2:25** **PHYS 210.** Probing single metal-semiconductor heterostructures for visible light photocatalysis. **N. Fang, B. Dong, F. Zhao**
- 3:00** **PHYS 211.** Triplet-state mediated super-resolution imaging of fluorescently-labeled gold nanorods. **K. Blythe, K.A. Willets**
- 3:20** **PHYS 212.** Plasmon-enhanced fluorescent protein emission: A new paradigm for improved single-molecule bio-imaging. **J.S. Biteen**
- 3:55** **PHYS 213.** Superstudies of plasmonically mediated emission: Beyond the Gaussian point-spread function. **E.J. Titus, K.A. Willets**
- 4:15** **PHYS 214.** Energy conversion within a single nanocavity structure. **T.W. Odom**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Gas Separation & Gas Storage: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

- 1:30** **PHYS 215.** Experimental and theoretical approach to the study of CO₂ adsorption in an extensive family of metal-organic frameworks. **W.L. Queen,** E.D. Bloch, J.S. Lee, J.D. Howe, J.A. Mason, M.I. Gonzalez, M.R. Hudson, K. Lee, S.J. Teat, J. Neaton, B. Smit, J.R. Long, C.M. Brown
- 2:00** **PHYS 216.** Engineering metal organic framework materials for optimum methane storage. **T. Yildirim**
- 2:30** **PHYS 217.** Computational screening of MOFs for gas separations. **S. Keskin**
- 3:00** **PHYS 218.** Parasitic energy: A potential building block for the prediction of CCS materials. **J. Huck, L. Joos, R. Mercado, L. Lin, A. Berger, A. Bhowan, K.U. Reuter, B. Smit**
- 3:20** Intermission.
- 3:40** **PHYS 221.** Small molecule adsorption in metal organic frameworks with open meal sites. **B. Vlaisavljevich, R. Mercado, L. Lin, K. Lee, J. Huck, B. Smit**
- 4:00** **PHYS 220.** Robust metal-organic frameworks: rational design and gas storage. **D. Feng, H. Zhou**
- 4:30** **PHYS 219.** Gas separations in metal-organic frameworks. **T.M. McDonald, E.D. Bloch, Z.R. Herm, J.A. Mason, B.M. Wiers, M.T. Kapelewski, M.I. Gonzalez, J. Oktawiec, G. Barin, D. Gygi, W. Queen, J.R. Long**

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Excitons

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry

Methodology

Sponsored by COMP, Cosponsored by PHYS

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E.L. Sibert, Organizer

8:00 - 10:00

32, 43, 88, 113, 175, 196, 205, 212. See previous listings.

PHYS222. Discovery and Innovation of inorganic graphene analogs by computations. **Z. Chen**

286, 316, 324, 376, 405, 409, 463, 483, 519, 532, 557, 580. See subsequent listings.

TUESDAY MORNING

Section B

Colorado Convention Center
Room 607

PHYS Award Symposium

E. L. Sibert, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 **PHYS 223.** Award Address (Peter Debye Award in Physical Chemistry sponsored by E. I. du Pont de Nemours & Co.). Single molecule biophysical chemistry: Life at the single molecule level. **S. Xie**

8:35 PHYS 224. Award Address (Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids sponsored by ExxonMobil Research and Engineering). Dynamics of polar solvation. M. Maroncelli

9:05 PHYS 225. Award Address (Francis P. Garvan–John M. Olin Medal sponsored by the Francis P. Garvan–John M. Olin Medal Endowment). Theoretical development and modeling across the periodic table: Toward accurate and inaccurate energetic prediction. A.K. Wilson

9:35 PHYS 226. Award Address (ACS Award in Theoretical Chemistry sponsored by the ACS). Fragmentation: A route to accurate calculations on large molecular systems. M.S. Gordon

10:05 PHYS 227. Address Award (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation). Bringing bioelectricity to light. A.E. Cohen

10:35 Intermission.

10:55 PHYS 228. Award Address (Ahmed Zewail Award in Ultrafast Science and Technology sponsored by the Ahmed Zewail Endowment Fund established by Newport). Multidimensional electronic and vibrational spectroscopy of molecules using attosecond X-ray pulses and quantum light. S. Mukamel

11:25 PHYS 229. Award Address (E. Bright Wilson Award in Spectroscopy sponsored by the ACS Division of Physical Chemistry). Mapping atomic motions with ultrabright electrons: The chemists' gedanken experiment enters the lab frame. R. Miller

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Organic Aerosol

D. Cziczo, M. Freedman, *Organizers*
N. Riemer, J. Surratt, *Presiding*

1:30 PHYS 230. Sources, properties, aging, and anthropogenic influences on OA and SOA over the Southeast US and the Amazon during SOAS, DC3, SEAC4RS, and GoAmazon. J.L. Jimenez

2:10 PHYS 231. Isoprene-derived SOA formation across multiple sites in the southeastern U.S.: Implications for air quality and human health. J.D. Surratt, S. Budisulistiorini, W. Rattanavaraha, Y. Lin, X. Li, M. Arashiro, A. Gold, Z. Zhang, S. Shaw, P. Croteau, M. Canagaratna, E. Knipping, S. Bairai, R.L. Tanner, M. Riva, T.P. Riedel, K. Chu

2:35 PHYS 232. Gas-phase vs. aqueous-phase aging of secondary organic aerosol. J.H. Kroll, J. Hunter, K. Daumit, A.J. Carrasquillo

3:00 PHYS 233. Influence of particle phase and viscosity on the heterogeneous OH-initiated oxidation of organic aerosol. J.F. Davies, K.R. Wilson

3:20 Intermission.

3:35 PHYS 234. On the surface chemistry of secondary organic aerosol particles. F. Geiger

4:00 PHYS 235. Lifetime of photosensitizer triplet states in model tropospheric aerosol. E. Woods, M. Barthold, J. Wan, M. Tigue

4:20 PHYS 236. Organic aerosol composition and aging in the atmosphere: How to fit laboratory experiments, field data, and modeling together. C.L. Heald, C. Chen

4:45 PHYS 237. On the connection of organic aerosol ageing to viscosity. F.A. Houle, W. Hinsberg, K.R. Wilson

5:05 PHYS 238. Oxidation flow reactors for the study of atmospheric chemistry systematically examined by modeling. Z. Peng, D.A. Day, A.M. Ortega, W. Hu, B.B. Palm, R. Li, K. Tsigaridis, J.A. de Gouw, W.H. Brune, J.L. Jimenez

Section B

Colorado Convention Center
Room 607

Ahmed Zewail Prize in Molecular Sciences

R. van Daalen, *Organizer*
D. C. Clary, *Presiding*

2:00 Introductory Remarks.

2:10 PHYS 239. Chemical adventures using the unified principles of homogeneous and heterogeneous catalysis. J.M. Thomas

3:00 PHYS 240. 4D electron microscopy: Developments and applications. A.H. Zewail

3:50 Intermission.

4:10 PHYS 241. Catalytic chemistry: a subtle blend of voids and single sites. M. Che

4:45 PHYS 242. Solution metallic catalysis on the nanoscale. M.A. El-Sayed

5:20 PHYS 243. From single sites to nanostructured assemblies: Designing tools for high-precision chemical transformations. T. Maschmeyer

5:55 Concluding Remarks.

Section C

Colorado Convention Center
Room 503

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of O₂

A. Co, D. A. Scherson, *Organizers*
J. M. Feliu, U. S. Ozkan, *Presiding*

1:30 Introductory Remarks.

1:35 PHYS 244. Bi adatoms at the surface of Pt single crystals. J.M. Feliu

2:15 PHYS 245. Impurity effects on the oxygen reduction reaction (ORR). A. Jacob Jebaraj, N. Georgescu, D. Scherson

2:35 PHYS 246. Effect of nitrogen functionalization on stability and performance of carbon-supported PtRu electrocatalysts in acid and alkaline media. S. Pilypenko, P. Joghoe, K. Wood, A.R. Corpuz, J. Christ, G. Bender, R. O'Hayre

2:55 PHYS 247. Galvanic displacement of Pt on nanoporous copper: An alternative synthetic route for obtaining robust and reliable oxygen reduction and alcohol oxidation catalysts. E. Coleman, H. Choi, K. Walz, A. Co

3:15 Intermission.

3:35 PHYS 248. Tuning of perovskite oxides electrocatalytic activity for water oxidation and oxygen reduction. K.J. Stevenson, T. Mefford, W. Hardin, K.P. Johnston

4:15 PHYS 249. Development of oxide-based materials for oxygen reduction and oxygen evolution reactions. P.B. Atanrossov, A. Serov, I. Matanovic, A. Roy, N. Andersen

4:55 PHYS 250. Theoretical investigation of water oxidation processes on small pure and Ca-doped MnO₂ complexes. K. Weerawardena, C.M. Aikens

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease Prions and Beyond

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
D. P. Raleigh, *Presiding*

1:30 PHYS 251. Surprising new structure for the cellular prion protein, and how this structure may influence membrane processes and prion disease. G.L. Millhauser

2:10 PHYS 252. Influence of induced polarization on amyloid peptide misfolding in different solution environment. J.A. Lemkul

2:50 PHYS 253. Role of cofactor molecules in encoding mammalian prion infectivity. S. Supattapone

3:30 Intermission.

3:50 PHYS 254. Curli: Functional bacterial amyloid fibers. C. Reichhardt, D.M. Rice, J. Uang, L. Ceglanski

4:10 PHYS 255. Membrane microdomain composition may temporally modulate or determine protein function. H. Jang, A.L. Gillman, J. Lee, S. Ramachandran, F. Teran Arce, B. Kagan, R. Lal, R. Nussinov

4:50 PHYS 256. What can theory and computations teach us about protein aggregation? D. Thirumalai

5:30 Closing Remarks.

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Electronic Structure

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
K. A. Lopata, *Presiding*

1:30 PHYS 257. Excited electronic states: Solvent effects and dynamics. M.S. Gordon, F. Zahariev, K. Keipert, Y. Harabuchi

2:10 PHYS 258. Relativistic variational density functional theory of electronic excited states. F.A. Evangelista, W.D. Dericotte, P. Verma

2:50 PHYS 259. Photoelectron spectra and photoelectron angular distributions from ab initio electronic structure methods. S. Gozem, A. Krylov

3:10 Intermission.

3:30 PHYS 260. Potential energy surfaces for excited electronic states. R. Dawes

4:10 PHYS 261. New developments in complete active space spin-flip methods for ground and excited states of large molecules with strong electron correlations. N. Mayhall, M.P. Head-Gordon

4:50 PHYS 262. Time-resolved spectroscopy: A challenge for time-dependent density functional theory. K. Luo, J.I. Fuks, E. Sandoval, N. Maitra

5:10 PHYS 263. Capturing geometric phase effects by mixed quantum-classical methods. R. Gherib, I.G. Ryabinkin, A.F. Izmaylov

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry

Applications

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Heterogeneous Chemistry, Sea Spray, Mineral Dust, and Black Carbon

D. Cziczo, M. Freedman, *Organizers*
J. G. Navea, E. Woods, *Presiding*

8:00 PHYS 264. Water uptake and heterogeneous chemistry of model and authentic sea spray aerosol particles. V.H. Grassian

8:40 PHYS 265. Transformations of nitrogen oxides at the troposphere–soil interface. J.D. Raff

9:05 PHYS 266. Optical properties of mineral dust components and mixtures. D. Veghte, J. Moore, L. Jensen, M. Freedman

9:25 Intermission.

9:40 PHYS 267. Determination of near UV absorption crosssections of surface-adsorbed H₂O and heterogeneous nucleation of H₂O on fused silica surfaces. L. Zhu

10:00 PHYS 268. From the particle scale to the global scale: Quantifying black carbon climate impacts using a stochastic particle-resolved model. N. Riemer

10:25 PHYS 269. Comparative photochemistry of nitric acid chemisorbed on different components of tropospheric particulate matter. J.G. Navea

10:45 PHYS 270. Probing the impacts of aerosol sources on cloud microphysics and precipitation through in situ measurements of aerosol chemical mixing state. K.A. Prather

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Interstellar Clouds

L. J. Allamandola, T. J. Lee, *Organizers*
S. N. Milam, *Presiding*

8:00 PHYS 271. Organic molecules in ices and their release into the gas phase. E. Fayolle, K. Oberg, R.T. Garrod, E.F. van Dishoeck, M. Rajappan, M. Berlin, C. Romanzin, J. Fillon

8:35 PHYS 272. Ice chemistry in interstellar dense molecular clouds, protostellar disks, and comet. S.A. Sandford

9:10 PHYS 273. Like a fly and the fire — polycyclic aromatic hydrocarbons (PAHs) in icy environments: A historical perspective. M.S. Gudipati

9:45 Intermission.

10:15 PHYS 274. Theoretical studies of interstellar ice chemistry involving polycyclic aromatic hydrocarbons and other compounds. D.E. Woon

10:50 PHYS 275. Formation of aromatic heterocycles from the UV-photoirradiation of aromatic hydrocarbons in ices. C.K. Matereze, M. Nuevo, S.A. Sandford

11:15 PHYS 276. Infrared spectroscopic properties of polycyclic aromatic nitrogen heterocycles (PANHs): The acridine series. A.L. Mattioda, J. Bregman, C. Bauschlicher, A. Ricca, D. Hudgins, L.J. Allamandola

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Properties and Processes in Solvated Systems

Cosponsored by COMP

J. Gao, B. C. Garrett, *Organizers*
B. Mennucci, *Organizer, Presiding*

8:00 PHYS 277. 25 years of SMx models: Quantum and classical continuum solvation. C.J. Cramer, D.G. Truhlar

8:30 PHYS 278. Protein aggregation, collapse, and disorder: Model systems. B.M. Pettitt, D. Karandur

9:00 PHYS 279. BioEFP: Effective fragment potential method for biological systems. L.V. Slipchenko

9:20 PHYS 280. Role of solvent structure on the rate of ion-pairing. M.D. Baer, C.J. Mundy, G.K. Schenter

9:40 Intermission.

10:00 PHYS 281. Quantum-classical path integral: A rigorous methodology. N. Makri

10:30 PHYS 282. Structure, properties, excited states and reactivity of complex systems in solution: Putting together the pieces. G. Scalmani, M.J. Frisch

11:00 **PHYS 283**. How reliable are calculations of absorption spectra of solvated molecules with CC theory and PCM? M. Caricato

11:20 **PHYS 284**. Continuum solvation calculations of solvatochromic shifts: Recent advances and perspectives. A.V. Marelich, C.J. Cramer, D.G. Truhlar, G. Scalmani, M.J. Frisch

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrochemical Formation of Semiconductors

D. A. Scherson, *Organizer*
A. Co, *Organizer, Presiding*
S. Maldonado, *Presiding*

8:00 **PHYS 285**. Investigations into the electrochemical formation of germanene. J.L. Stickney, M. Ledina, J. Jung

8:40 **PHYS 286**. Electrocatalytic crystallization of covalent inorganic semiconductors. S. Maldonado

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of H₂O and H₂

A. Co, *Organizer*
D. A. Scherson, *Organizer, Presiding*
S. Maldonado, *Presiding*

10:00 **PHYS 287**. Withdrawn.

10:40 **PHYS 288**. Graphene oxide-promoted hydrogen and oxygen evolution. N. Wu

11:00 **PHYS 289**. Electrocatalytic hydrogen production performed by model protein scaffolds. H.S. Shafaat, J.W. Slater, A.C. Manesis, S.L. Cirino, H.A. Monaco

11:20 **PHYS 290**. Electrocatalytic water oxidation by iridium ions. K. Glusac

11:40 **PHYS 291**. Electrocatalytic water oxidation on model cobalt oxide dimer and cubane complexes. A. Fernando, C.M. Aikens

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Modeling of Macromolecular Structure and Function

Cosponsored by COMP

A. E. Garcia, G. Hummer, *Organizers*
M. Chu-Moyer, *Presiding*

8:00 **PHYS 292**. Integrative structural biology. A. Sali

8:35 **PHYS 293**. Unveiling the function of macromolecular assemblies using integrative dynamic modeling. M. Dal Peraro

9:10 **PHYS 294**. Introducing molecular flexibility in Monte Carlo simulations of many-protein systems. V. Prytkova, M. Heyden, J.A. Freitas, D.J. Tobias

9:45 **PHYS 295**. Building toy models of proteins using co-evolutionary information. R.R. Cheng, M. Raghunathan, J.N. Onuchic

10:20 **PHYS 296**. Atomistic and coarse-grained simulations of histones, Nucleosomes and DNA. G. Papoian, D. Winoogradoff, H. Zhao, I. Echeverria, Y. Dalal

10:55 **PHYS 297**. Relative resolution: A hybrid strategy for molecular modeling. A. Chaimovich, K. Kremer, C. Peter

11:30 **PHYS 298**. Beyond Hofmeister: Interactions between ions and proteins in water. P. Jungwirth

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Electronic Structure

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
F. A. Evangelista, *Presiding*

8:00 **PHYS 299**. Understanding photochemistry and photoelectron spectra with highly correlated electronic structure methods based on coupled-cluster theory. P. Piecuch, J.A. Hansen, N.P. Bauman

8:40 **PHYS 300**. Electronic structure methods for high-energy excited states. X. Li, P. LeStrange, D.B. Williams-Young, J.J. Goings

9:20 **PHYS 301**. Linear response time-dependent complex generalized Hartree-Fock for frustrated spin systems. J.J. Goings, D.B. Williams-Young, F. Ding, M.J. Frisch, X. Li

9:40 **PHYS 302**. Graphical processing unit acceleration of "two-step" complete active space configuration interaction (CASCI) methods. B. Fales, B. Levine

10:00 Intermission.

10:20 **PHYS 303**. Above-ionization excited states with non-Hermitian time-dependent density functional theory. K.A. Lopata

11:00 **PHYS 304**. Caution when using real-time TDDFT: Two-electron Rabi oscillations and peak-shifting. C. Isborn, M. Provorise, B. Habenicht

11:40 **PHYS 305**. Charge transfer and other non-linear electron dynamics: the problem of detuning in TDDFT. J.I. Fuks, K. Luo, E. Sandoval, N. Maltra

12:00 **PHYS 306**. Experimental perspective on the electronic structure and dynamics of higher-lying electronic states. C.G. Elles, C.L. Ward, A.L. Houk, T.J. Quiny

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer, Presiding*
J. S. Biteen, *Presiding*

8:30 **PHYS 307**. Probing the mechanistic of charge transfer from optically excited plasmonic metal nanoparticles to adsorbates leading to chemical transformations. S. Linc

9:05 **PHYS 308**. Electrochemistry on plasmonic nanoparticle electrodes. A. Wilson, K.A. Willets

9:25 **PHYS 309**. Collective behavior in the solid-state elucidated by plasmonic spectroscopy. P.K. Jain

10:00 **PHYS 310**. Single-particle absorption spectroscopy of plasmonic nanostructures. M. Yorulmaz, S. Nizzero, W. Chang, L. Wang, S. Link

10:20 **PHYS 311**. Atomistic simulations of surface-enhanced spectroscopies. L. Jensen

10:55 **PHYS 312**. Design and optimization of plasmonic crystals for surface enhanced Raman spectroscopy using the finite-difference time-domain method. R. Petit, J.M. Montgomery

11:15 **PHYS 313**. Electron microscopy and spectroscopy of plasmonic alloys. E. Ringe, S.M. Collins, C.J. DeSantis, S.E. Skrabalak, P.A. Midgley

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Catalysis and Materials for Catalysis: Experiments & Calculations

L. Gliardini, B. Smit, *Organizers, Presiding*

8:00 **PHYS 314**. Global energy and emissions reduction potential of new materials development. C. Tway, E.G. Rightor, J. Liu, C. Han, M. McAdon, J. Goss, K. Andrews

8:30 **PHYS 315**. Thermodynamics and kinetics of elementary reaction steps on late transition metal catalysts, and using them to search for better catalysts. C.T. Campbell

9:00 **PHYS 316**. Tailored mesoscale gold alloy materials for energy- and resource-efficient catalysis. M.L. Personick, B. Zugic, C.M. Friend

9:20 Intermission.

9:40 **PHYS 317**. Impact of location and concentration of acid sites in zeolites for acid catalyzed reactions in condensed phase. J.A. Lercher

10:10 **PHYS 318**. Harnessing polymorphism for the rational design of new nanoporous materials: assessing mechanical, thermal stability, and experimental feasibility. F. Trouselet, L. Bouessel du Bourg, F. Coudert

10:30 **PHYS 319**. Material descriptor of oxygen vacancy formation energies in wide band gap oxides. A. Deml, A. Holder, R. O'Hayre, C. Musgrave, V. Stevanovic

Quantum Chemistry

Quantum Dynamics & Monte Carlo Simulations

Sponsored by COMP, Cosponsored by PHYS

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Sponsored by CHED, Cosponsored by PHYS

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Gas Phase Atmospheric Chemistry

D. Cziczco, M. Freedman, *Organizers*
K. T. Kuwata, C. Womack, *Presiding*

1:30 **PHYS 320**. Photochemical and multiphase sources of isoprene derived secondary organic aerosol. J.A. Thornton, B. Lee, C. Gaston, E. D'Ambro, F. Lopez-Hilfiker, J. Liu, J. Shilling, C. Mohr, T.P. Riedel, Z. Zhang, A. Gold, J. Surratt, W. Hu, D. Day, P. Campuzano-Jost, B. Palm, J.L. Jimenez, N. Ng, L. Xu

2:10 **PHYS 321**. Atmospheric chemistry in the southeast U.S. J. de Gouw, C. Warneke, M. Trainer

2:35 **PHYS 322**. Uncertainties in global atmospheric composition due to uncertainties in inorganic and organic rate constants. M.J. Evans, B. Newsome

3:00 Intermission.

3:15 **PHYS 323**. Relative abundances of gas phase amines and ammonia in the ambient atmosphere. J. Murphy, T.C. Vandenboer, G. Wentworth, M. Markovic, P. Gregoire

3:40 **PHYS 324**. Probing the composition of atmospheric interfaces through measurement of trace gas reactive uptake and product yields. T.H. Bertram, O.S. Ryder, N. Campbell

4:05 **PHYS 325**. Heterogeneous chemistry of nitrogen oxides: Results from recent field studies. S.S. Brown

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Clouds and Star and Planet Forming Regions

L. J. Allamandola, T. J. Lee, *Organizers*
E. Peeters, *Presiding*

1:30 **PHYS 326**. Complex organic molecules in star-forming regions: Sweet results from ALMA. E.F. van Dishoeck

2:05 **PHYS 327**. Polycyclic aromatic hydrocarbons as catalysts for interstellar molecular hydrogen formation. L. Hornekaer

2:40 **PHYS 328**. Modeling grain surface chemistry in dense molecular clouds. H. Cuppen, L. Karssemeijer

3:15 Intermission.

3:45 **PHYS 329**. Formation of complex organic molecules in protoplanetary disks. T. Millar

4:20 **PHYS 330**. Time-domain terahertz spectroscopy of polycyclic aromatic hydrocarbons. M.A. Alldif, P. Carroll, S. Ioppolo, B.A. McGuire, G.A. Blake

4:45 **PHYS 331**. Tackling the theoretical anharmonic infrared spectra of polycyclic aromatic hydrocarbons. C. Mackie, A. Candian, X. Huang, T.J. Lee, A. Tielens

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Nonadiabatic Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
X. Li, *Presiding*

1:30 **PHYS 332**. Beyond the Born-Oppenheimer approximation: Construction of accurate multicomponent wave function using explicitly-correlated and projection-based methods. A. Chakraborty

2:00 **PHYS 333**. Directly correlating electronic and vibrational motions with multidimensional coherent spectroscopies. M.H. Khallil

2:30 **PHYS 334**. Approximate time-dependent diabatic states computed using a measure driven tessellation technique for use in on-the-fly quantum dynamics methods. S.S. Iyengar

3:00 **PHYS 335**. Avoiding the Born-Oppenheimer separation between electrons and protons in wavefunction and density functional theory calculations. S. Hammes-Schiffer

3:20 Intermission.

3:40 **PHYS 336**. Surface hopping and spectroscopy. J.E. Subotnik, A.S. Petit

4:10 **PHYS 337**. Novel approaches to nonadiabatic molecular dynamics. O.V. Prezhdo

4:40 **PHYS 338**. Time-dependent electronic and nuclear potentials that exactly capture electron-ion coupling. N. Maitra

5:00 **PHYS 339**. Time-derivative coupling scheme for accurate electronic state transition probabilities in nonadiabatic molecular dynamics. G. Meek, B. Levine

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

In Situ Characterization

A. Co, D. A. Scherson, *Organizers*
C. L. Korzeniewski, D. Scherson, *Presiding*

1:30 **PHYS 340**. Vibrational spectroscopy and 2D correlation analysis applied to probe structure in ionomer membrane materials. C.L. Korzeniewski, T. Zhang

- 2:10** **PHYS 341.** Operando X-ray studies of electrocatalysis for energy conversion. **D. Friebel**
- 2:50** Intermission.
- 3:10** **PHYS 342.** Irrelevance of CO poisoning in methanol oxidation on PtRu electrocatalysts: A re-visit of the bifunctional mechanism. **Y. Tong**
- 3:50** **PHYS 343.** In operando optical studies of solid oxide fuel cells operating with biogas: heterogeneous surface chemistry vs. electrochemical oxidation. **R.A. Walker, J. Kirtley, J. Owrutsky, D.A. Steinhurst**

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function**Folding and Aggregation**

Cosponsored by COMP

A. E. Garcia, G. Hummer, Organizers
R. Nussinov, Presiding

- 1:30** **PHYS 344.** Accurate atomistic simulations of intrinsically disordered proteins. **R.B. Best, W. Zheng, J. Mittal**
- 2:05** **PHYS 345.** Regulation and aggregation of intrinsically disordered peptides. **J.E. Shea**
- 2:40** **PHYS 346.** Multiscale and multiresolution simulations of aggregation in polyglutamine containing block copolymers. **R.V. Pappu**
- 3:15** **PHYS 347.** Spontaneous formation of oligomers and fibrils in large scale molecular dynamics simulations of peptides. **C.K. Hall, M. Cheon, D.C. Latshaw, I. Chang**
- 3:50** **PHYS 348.** Alzheimer's disease: Aggregation of WT and protective A β peptides, free or in the presence of inhibitors and under shear flow by all-atom and coarse-grained simulations. **J. Nasica-Labouze, P. Nguyen, B. Tarus, F. Sterpone, M. Chiriccio, O. Berthoumieu, P. Fallar, A. Doig, S. Melchionna, P. Derreumaux**
- 4:25** **PHYS 349.** Protein folding and recognition in the cell — an in silico approach. **M.S. Cheung**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems**Electronic Structure**

Cosponsored by COMP

B. G. Levine, S. A. Varganov, Organizers
J. I. Fuks, Presiding

- 1:30** **PHYS 350.** Modeling excited states with multireference quantum chemical methods. **L. Agliardi, R. Carlson, D.G. Truhlar, K. Vogliatzis**
- 2:10** **PHYS 351.** Single- and multireference quantum chemical methods for nonadiabatic molecular dynamics. **H. Lischka, M. Barbatti**
- 2:50** **PHYS 352.** Low valency in rare earth diatomics. **G. Schoendorff, A.K. Wilson**
- 3:10** Intermission.
- 3:30** **PHYS 353.** Active space decomposition. **T. Shiozaki**
- 4:10** **PHYS 354.** Representation of adiabatic potential energy surfaces coupled by conical intersections and their use in describing nonadiabatic processes. **D.R. Yarkony, X. Zhu, J. Dillon, C. Malbon**
- 4:50** **PHYS 355.** Electronic structure of diatomic rare earth species. **C. South, G. Schoendorff, A.K. Wilson**
- 5:10** **PHYS 356.** Size-inconsistency effects in transition moments for quasi-degenerate variational perturbation theory and averaged coupled-pair functional theory. **K. Dzwile, R.J. Cave**

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, K. A. Willets, Organizers
S. Link, Organizer, Presiding
R. R. Frontiera, Presiding

- 1:30** **PHYS 357.** Raman scattering in time and frequency on a nanantenna and its molecular load. **V.A. Apkarian**
- 2:05** **PHYS 358.** Photoluminescence quantum yield of strongly coupled gold plasmonic molecule. **D. Huang, C. Byers, L. Wang, A. Hoggard, B. Hoener, W. Chang, C.F. Landes, S. Link**
- 2:25** **PHYS 359.** Plasmons and intraband transitions. **P. Guyot-Sionnest**
- 3:00** **PHYS 360.** Electron dynamics in gold nanoparticles under strong laser fields. **J. Powell, A. Rudenko, C.M. Sorensen**
- 3:20** **PHYS 361.** Controlling and probing spatially dependent plasmonic field effect and charge transfer dynamics using single quantum dot modified AFM tips. **T. Lian**
- 3:55** **PHYS 362.** Strong coupling between individual plasmonic metal nanostructures and quantum dots. **M. Pelton**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach**Catalysis and Materials for Catalysis: Experiments & Calculations**

L. Agliardi, B. Smit, Organizers, Presiding

- 1:30** **PHYS 363.** Computational design of highly selective transition metal catalysts encapsulated by metal-organic frameworks for butane oxidation to 1-butanol. **S. Dix, R. Getman**
- 2:00** **PHYS 364.** Metal-organic frameworks as highly functional catalytic arrays. **O.K. Farha**
- 2:30** **PHYS 365.** Metal-organic framework materials for solar energy applications. **W. Lin**
- 3:00** **PHYS 366.** Performance descriptors for the design of solar energy materials. **A. Walsh**
- 3:20** Intermission.
- 3:40** **PHYS 367.** Withdrawn.
- 4:10** **PHYS 368.** In silico prediction of emergent catalysts. **D.G. Vlachos**
- 4:40** **PHYS 369.** Impact of MOF topology upon solvent organization, dynamics, and solution phase stability. **A.E. Clark, W. Queen, X. Yang**

Quantum Chemistry**Applications**

Sponsored by COMP, Cosponsored by PHYS

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Sponsored by CHED, Cosponsored by PHYS

WEDNESDAY EVENING**Section G**

Colorado Convention Center
Hall C

Physical Chemistry Poster Session

E. L. Sibert, Organizer

6:30 - 9:30

- PHYS 370.** Quantum numerical control for particles at matter surface. **Q. Wang**
- PHYS 371.** Scaled quantum mechanical scale factors for vibrational calculations using alternate polarized and augmented basis sets with the B3LYP density functional calculation model. **W.B. Collier, C.R. Legler, N.R. Brown, R.A. Dunbar, M.D. Harness, K. Nguyen, O.O. Oyewole**

- PHYS 372.** Calculating the infrared spectra of the eigenion using anharmonic vibrational theory. **B. Thomsen, K. Yagi, Y. Sugita**
- PHYS 373.** Theory and efficient computation of vibrational difference spectra. **T. Joutsuka, A. Morita**
- PHYS 374.** Diabatic states of a delta function model. **T. Middlemas, R.J. Cave**
- PHYS 375.** Lifetimes of vibrational states of XY ions (X=Li, Na; Y=Be, Mg) calculated using the CCSDT potential energy and dipole moment curves. **D.K. Barnes, D. Fedorov, S.A. Varganov**
- PHYS 376.** Probing vibrational-electronic interactions of a sensitizing dye at the TiO₂ surface using heterodyne detected doubly resonant sum-frequency generation spectroscopy. **C.C. Rich, M. Mattson, A.T. Krummel**
- PHYS 377.** Time-resolved infrared spectroscopy of [FeFe]-hydrogenase model compounds. **R. Meyer, A. Zhandosova, E.J. Heilweil, C.J. Stromberg**
- PHYS 378.** Statistically weight averaged vibrational spectrum over molecular fragments for studying the amide I vibration of sphingomyelin bilayer. **K. Yagi, P. Li, K. Shirota, T. Kobayashi, Y. Sugita**
- PHYS 379.** Structural and energetic properties of lanthanide trivalents via DFT and ab initio approaches. **R.J. Weber, G. Schoendorff, A.K. Wilson**
- PHYS 380.** Ferrocene - ozone reactions: A matrix-isolation and DFT study. **R.W. Kugel, L. Pinelo, B.S. Ault**
- PHYS 381.** Mechanistic investigations of siderophore complexation via density functional theory. **M.F. Skaro, M.S. Hughey, J.L. Sonnenberg**
- PHYS 382.** Theoretical phase diagram for Fe₂O₃ (111) surfaces using a DFT + U(Fe) approach. **X. Huang, S. Ramadugu, S.E. Mason**
- PHYS 383.** DFT and ab initio composite method investigations of oxygen fluorides and related hydrides. **Z.H. Alsunaidi, A.K. Wilson**
- PHYS 384.** Effect of choline chloride on secondary structure conformation for two small peptides: A circular dichroism study. **M. Giordano, M. Vermeuel, P. Gupta, D. Léon, M.R. Bunagan**
- PHYS 385.** Deconstructing solvent organization in confined nanoporous materials: Implications for separation. **C. Wang, A.E. Clark**
- PHYS 386.** Crystallographic characterization of three furan-substituted benzimidazolones and calculation of C-H/ π and π/π interaction energies. **D.K. Geiger, C. Geiger**
- PHYS 387.** Quantum electronic kinetics from an atom-centered bath model. **T. Nguyen, S. Blau, T. Markovitch, J. Parkhill**
- PHYS 388.** Impact of resonance stabilization on H-atom shift isomerization and ring closure reactions. **K. Wang, S. Villano, A.M. Dean**
- PHYS 389.** Sodium dodecyl sulfate monomers induce XAO peptide polyproline II to β -helix transition. **Z. Hong, D. Krishnan Achary, S.A. Asher**
- PHYS 390.** Multishells vs. gradient-alloyed shells on core quantum dots: Ensemble and single particle optical properties. **P. Bajwa, F. Gao, B.O. Omogo, C.D. Heyes**
- PHYS 391.** Physicochemical investigation of ionic liquid mixtures. **M.T. Clough, J. Gråsvik, P. Hunt, H. Niedermeyer, T. Welton**
- PHYS 392.** Antibunching in small clusters of quantum dots. **J.Q. Geisenhoff, K.J. Whitcomb, D. Ryan, M.P. Gelfand, A.K. Van Orden**
- PHYS 393.** Modification method of natural zeolite by ultrasonic and sodium chloride. **W. Qun, Y. Zhichao, G. Mingkun, X. He, C. Bin, C. Shuang**
- PHYS 394.** Understanding nanoconfined hydrogen: first ever quantum free-energy profiles of diffusion of hydrogen and the importance of condensed phase environment in sil clathrate hydrate. **A. Powers, O. Marsalek, L. Ulivi, M.E. Tuckerman, Z. Bacic**
- PHYS 395.** Solution dynamics of group 8 metal pentacarbonyls in fluorinated benzene solvents. **C.P. Baryames, A. Devanny, C. Laperle**

- PHYS 396.** Solution dynamics of osmium pentacarbonyl in alcohol solvents. **C. Laperle, A. Devanny**
- PHYS 397.** Surface thermodynamics and vesicle formation of decanoic acid. **B. Kessenich, R. Rapf, R.J. Perkins, V. Vaida**
- PHYS 398.** Molecular dynamics simulation of ion transports through liquid-liquid interface. **N. Kikkawa, A. Morita, L. Wang**
- PHYS 399.** Raman spectroscopic study of graphene photochlorination dynamics in the gas phase and in solution. **K.Z. Rinaldi, N. Patel, S. Ramrattan, A. Crowther**
- PHYS 400.** Decomposing hydrogen bond dynamics into multiscale components: Understanding the hydrophobic effect. **T. Zhou, A.E. Clark**
- PHYS 401.** Diabatic electronic population matrix and its utilization in simulating electronically excited state dynamics. **J. Park, Y.M. Rhee**
- PHYS 402.** Decoherence in nonadiabatic dynamics from an approximate mixed quantum-classical Poisson bracket mapping equation formalism. **H. Kim, Y.M. Rhee**
- PHYS 403.** Interdomain dynamics of chloroplast signal recognition particle proteins studied by time-resolved single-molecule FRET. **D. Baucom, F. Gao, P. Patel, A. Kight, R. Goforth, R. Henry, C. Heyes**
- PHYS 404.** Molecular dynamics to study energy transduction in the ATP powered translocation of PcrA along DNA. **R.B. Davidson, M. McCullagh**
- PHYS 405.** Two-photon spectroscopy, dynamics, and quantum yields of a photochromic molecular switch. **A.L. Houk, C.G. Elles**
- PHYS 406.** Global potential energy surfaces of O₂ and dynamics of high-energy O₂-O₂ collision-induced energy transfer and dissociation. **Y. Paukku, Z. Varga, W. Lin, R. Meana-Pañeda, J. Bender, G.V. Candler, D.G. Truhlar**
- PHYS 407.** Time-dependent excited-state molecular dynamics of photofragmentation of gas-phase tris(isopropylcyclopentadienyl) lanthanum complexes. **Y. Han, Q. Meng, P.S. May, M.T. Berry, D. Kilin**
- PHYS 408.** Structural characterization of supported noble metal nanocatalyst from atomistic simulations. **S. Xiong, R. Diwan, Y. Li**
- PHYS 409.** Investigating the efficient conversion of unsaturated acids to olefins over acid catalysts. **T.J. Evans, J.M. Clark, C. Mukarakate, M.M. Yung, M.R. Nimios, D.J. Robichaud**
- PHYS 410.** First principles treatment of photoluminescence linewidth in semiconductors. **D.J. Vogel, D. Kilin**
- PHYS 411.** Investigating the best type of gold and platinum bimetallic nanoparticle catalyst for alcohol oxidation reactions. **A. Earle, J.M. Petroski**
- PHYS 412.** Laser-assisted nickel liquid phase deposition on surface of dielectrics and semiconductors. **E. Khairullina, S. Araslanova, S. Safonov**
- PHYS 413.** Reaction kinetics of NO and NO₂ with pyrite. **H.M. Bewsek**
- PHYS 414.** Probing the mechanism of DNA duplex formation in sequences with consecutive versus alternating purines and pyrimidines using stopped flow kinetics experiments. **S.P. Carney, R. Stratil, A. Deckert**
- PHYS 415.** Monitoring internal temperatures and kinetics in nitrogen- and oxygen-containing plasma systems. **E. Sutor, J. Blechle, E.R. Fisher**
- PHYS 416.** Effects of organic matter on polycyclic aromatic hydrocarbon photolysis kinetics in ice and at ice surfaces. **P. Malley, T. Kahan**
- PHYS 417.** Dissociation processes of deprotonated nucleobases: Astrobiological implications. **C.A. Cole, Z. Wang, T.P. Snow, V.M. Bierbaum**
- PHYS 418.** Carbon chains in low-mass young stellar objects. **O.H. Wilkins, D.M. Graninger, K. Oberg**

[†] Cooperative Cosponsorship

- PHYS 419.** Formation mechanism of interstellar PANH cations: Experimental and computational studies. **Z. Wang**, V.M. Bierbaum, C.A. Cole, T.P. Snow
- PHYS 420.** Spectral characteristics and lightfastness of fluorescent dyes absorbed on nanoparticles of aerosil dispersed in polymer matrix. **N. Barashkov**, S. Sheshenia, T. Sakhno, V. Granchak, S. Kuchmii, I. Irgibayeva
- PHYS 421.** Investigation of two alternative methods of introducing fluorescent dyes in the Au nanoparticles-polysiloxane composites. **N. Barashkov**, I. Irgibayeva, A. Aldongarov, A. Mantel, A. Ishchenko, T. Sakhno
- PHYS 422.** Electron and nuclear dynamics in gold and silver nanoparticles. **R.D. Senanayake**, C.M. Aikens
- PHYS 423.** Electrochemical fabrication of CdSe/TiO₂ nanotubes for photoelectrocatalytic water splitting application. **F. de Souza Lucas**, M. Sant'anna, R.G. Freitas, L.H. Mascaro, E.C. Pereira
- PHYS 424.** Pseudo-direct bandgap transitions in silicon nanocrystals: Effect on optoelectronics and thermoelectrics. **V. Singh**, Y. Yu, **Q. Sun**, B. Korgel, P. Nagpal
- PHYS 425.** Work function modification of various electrodes by deposition of carbon nanotubes via aerosol jet printing. **C.A. Jordan**, R.S. Aga, E. Kreit, C.M. Bartsch, E.M. Heckman, R.S. Aga
- PHYS 426.** Temperature dependent solubility of gold nanoparticle suspensions. **J. Powell**, K. Bayliff, E. Herman, C.M. Sorensen
- PHYS 427.** Doping of wide-bandgap titanium-dioxide nanotubes: Optical, electronic and magnetic properties. **Y. Ding**, Y. Alivov, V. Singh, P. Nagpal
- PHYS 428.** Computational studies of pathways toward the growth of small boron and boron-carbon nanomaterials. **D.C. Woods**, A.L. Dibble, J.R. Rocha
- PHYS 429.** Withdrawn.
- PHYS 430.** Quantitative SERS-based detection using Ag-Fe₃O₄ nanocomposites with an internal reference. **P.B. Joshi**, Y. Zhou, T. Ozkaya, P. Zhang
- PHYS 431.** Singlet oxygen generation under NIR and light visible light excitation of Chlorin e6 on the surface of fluorescent polymer coated NaYF₄ upconversion nanoparticles. **P.B. Joshi**, P. Zhang
- PHYS 432.** Novel approach to modeling the absorption spectra and colloidal stability of few- and single-chirality single walled carbon nanotubes. **K.C. Tvrđy**, K. Prescott, K. Rosenthal
- PHYS 433.** Withdrawn.
- PHYS 434.** Preparation of metal oxide substrates for surface-enhanced Raman scattering. **B. Li**, C. Weng, C. Yang, C. Lin, S. Lee
- PHYS 435.** Spin-forbidden transitions between electronic states of the active site of rubredoxin. **G. dePolo**, D. Kalliak, S.A. Varganov
- PHYS 436.** Charge transfer complexes and photochemistry of ozone with n-butylferrocene and ferrocene: A UV-Vis matrix isolation study. **L. Pinelo**, R. Kugel, B.S. Ault
- PHYS 437.** Engineering long range ferromagnetism in 2D transition metal dichalcogenide WSe₂. **C. Gil**, A. Pham, S. Li
- PHYS 438.** Structure and bonding of metal complexes containing possible hepatitis C inhibitors. **R.M. Drazenovic**, D.N. Ward, P.J. Smith, J.L. Sonnenberg
- PHYS 439.** Interaction of niobium-containing chloride melts with niobium metal. **M.V. Chernyshov**, I.B. Polovov, V.A. Volkovich, O.I. Rebrin
- PHYS 440.** Organic nanowire waveguide excitation-polariton nanolaser and its photonic application. **Q. Liao**
- PHYS 441.** Triplet states of pyrazine. **R. Bendiak**, R.J. Cave
- PHYS 442.** Effect of reaction environment on atmospheric photochemistry of pyruvic acid. **A.E. Reed Harris**, B. Ervens, R.K. Shoemaker, J.A. Kroll, R.J. Rapf, E.C. Griffith, A. Monod, J. Doussin, V. Vaida
- PHYS 443.** Kirkwood-Buff derived force field for esters. **G. Pallewela**, P.E. Smith
- PHYS 444.** Stabilization of a Cl—Cl— anion pair in the gas phase: Ab initio microsolution study. **A.S. Ivanov**, G. Frenking, A.I. Boldyrev
- PHYS 445.** Detecting organic nitrates using thermal dissociation cavity ringdown spectroscopy. **N. Keehan**, B. Ayres, J.L. Fry
- PHYS 446.** Rotational and hyperfine analysis of the E2T_{1/2} state of TaO. **T.D. Varberg**, C.R. Christopher, S.Y. Lee, F.B. Gwandu, A.J. Matsumoto, B.J. Knurr, T.K. Mahle, Z.W. Morrow
- PHYS 447.** Metal-mediated proton transfer in maleic acid and implications for enzyme catalysis. **M.T. Ruggiero**, T.M. Korter
- PHYS 448.** Combined photoelectron spectroscopy and ab initio studies of pure, carbon-doped, and transition-metal-doped boron clusters. **I.A. Popov**, W. Li, Z.A. Piazza, R. Pal, V.F. Popov, K.V. Bozhenko, I. Černušák, X.C. Zeng, A.I. Boldyrev, L. Wang
- PHYS 449.** Raman spectra of EDAB and its analogs in various solvents. **S. Farmer**, M.L. Fetterolf, G. Rowe
- PHYS 450.** QM/MM simulations reveal the involvement of excimers in the photophysics of adenine based oligonucleotides. **V.A. Spata**, S. Matsika
- PHYS 451.** TiO₂ mediated photooxidation of squalene: A kinetic and mechanistic study. **M.L. Kaak**, J.A. Ganske
- PHYS 452.** Is ketene an intermediate in the addition of imines to azlactone to a scanlon β-lactam? **C. Kordes**, P. Willoughby, J. Scanlon
- PHYS 453.** Aerosol formation initiated by nucleation of radical-water complexes. **E. Burrell**, S. Kumbhani, R.B. Shirts, J.C. Hansen, L. Hansen
- PHYS 454.** Drinking water disinfection by a low-voltage pulsed electric field device. **P. Hung**, Y. Li, O. Lee, K. Lam, S. Kwan, J. Kwan, K.L. Yeung
- PHYS 455.** Experimental and computational investigation of the dissociation pathways of first generation protonated nitrile-terminated PPI dendrimer. **W.D. Price**
- PHYS 456.** Photophysical properties and electronic structure of strongly coupled hydroporphyrin dyads with extended near-infrared absorption. **H. Kang**, N.N. Esemoto, J.R. Diers, D.M. Niedzwiedzki, J.A. Greco, J. Akgigbe, Z. Yu, C. Panchoi, G.V. Bhagavathy, J.K. Nguyen, R.R. Birge, C.R. Kirmaier, D.F. Bocian, M. Ptasek, D. Holtzen
- PHYS 457.** Investigation of the hygroscopicity of glycine and lysine aerosols and their mixtures with Na₂SO₄. **J.P. Darr**, P. Morales, S. Gottuso, A. Johnson
- PHYS 458.** Docking studies of binding of *Plasmodium falciparum* plasmeprin II to normal and sickle hemoglobin. **S.C. Marguet**, V.F. Waingeh
- PHYS 459.** Correlation consistent composite approach (ccCA): Application to organics and beyond. **A. Morris**, A. Wilson
- PHYS 460.** Charge-transfer in fullerene: Molecular cluster co-crystals. **N. Patel**, K.Z. Rinaldi, E. O'Brien, X. Roy, A. Crowther
- PHYS 461.** Raman spectroscopic study of solvent-mediated electron-transfer chemical doping of graphene. **J. Karten**, B. Janicek, A. Crowther
- PHYS 462.** Rapid scan electron paramagnetic resonance improves sensitivity relative to conventional methods. **G.R. Eaton**, S. Eaton, M. Tseytlin, R. Quine, G. Rinard, D. Mitchell, J. Biller, Z. Yu, Y. Shi
- PHYS 463.** Photon and water mediated sulfur oxide and acid chemistry in planetary atmospheres. **J.A. Kroll**, V. Vaida
- PHYS 464.** Theoretical analysis on the methods to derive surface molecular orientation by sum frequency generation spectroscopy. **A. Morita**, T. Ishihara, K. Saito, T. Ishiyama, L. Wang
- PHYS 465.** Thermodynamics of uranium in gallium-aluminum based liquid alloys. **V.A. Volkovich**, D.S. Maltsev, L.F. Yamshchikov, I.B. Polovov, A.G. Osipenko
- PHYS 466.** Thermodynamic modeling and experimental verification of f-elements separation employing Ga-Sn eutectic alloys. **S.Y. Melchakov**, D.S. Maltsev, **V.A. Volkovich**, L.F. Yamshchikov, D.G. Lisienko, M.A. Rusakov
- PHYS 467.** Thermodynamic properties of lanthanum in alloys based on gallium-aluminum eutectic mixture. **A.V. Shchetinskiy**, A.S. Dedyukhin, **V.A. Volkovich**, L.F. Yamshchikov, A.G. Osipenko
- PHYS 468.** Characterization of aqueous metal-pyrazole complexes. **A.K. Huff**, G. Turcios, S. Miller
- PHYS 469.** Photodissociation of cis- and trans-CH₃ONO: Is conformation destiny? **J. Lantis**, M. Birkdorf, J.A. Bartz
- PHYS 470.** Photodissociation of t-butyl nitrite: Steric influences on vector correlations. **M. Birkdorf**, J. Lantis, J.A. Bartz
- PHYS 471.** Effects of large water box on anatase thin film surface: A computational analysis on changing electronic properties. **S.J. Jensen**, D. Kilin
- PHYS 472.** Influence of various solvents on the physical properties of materials for organic electronic devices. **A. Foote**, R. Aga, E. Niwemukiza
- PHYS 473.** BOMD study of M+(tryptamine)(H₂O)_n cluster ions. **P.E. Hoerner**, J. Beck, M.P. Gaigeot
- PHYS 474.** Spectroscopic study of the effects of local environment and deuteration on the structure of trimethylamine N-oxide (TMAO). **L. McNamara**, D.N. Reinemann, H.U. Valle, J.C. Prather, P.L. Reves, D.H. Magers, T.K. Hollis, G.S. Tschumper, N. Hammer
- PHYS 475.** Thermal decomposition of iron dithiocarbamates. **J.C. Becca**, **J.F. Fuller**
- PHYS 476.** Enzymatic activation of nitric oxide. **J.C. Pearson**, A.K. Wilson
- PHYS 477.** Characterizing novel solid-state reaction intermediates using advanced in situ X-ray diffraction techniques. **C. Benson**, J. Cox, I. Walton, J.B. Benedict
- PHYS 478.** Withdrawn.
- PHYS 479.** Withdrawn.
- PHYS 480.** Spectroscopic characterization of free-base bis(arylethynyl)porphyrins bearing p-hydroxyphenyl substituents. **K.K. Evens**, K.E. Splan
- PHYS 481.** Fingerprinting molecular structure via photoionization out of Rydberg states and microwave Rayleigh scattering. **R.D. Oster**, S. Purohit, S. Atkins, F. Rudakov
- PHYS 482.** Impact of basis set completeness on computed dissociation energies of transition metal complexes. **J. Plascencia**, A.K. Wilson
- PHYS 483.** On the B800-850 LH2 antenna complex of the purple sulfur bacterium *Allochrochromatium vinosum*. **A. Kell**, M. Jassas, K. Hacking, R.J. Cogdell, R. Jankowiak
- PHYS 484.** Comments on the optical lineshape function: Application to transient hole burned spectra of bacterial reaction centers. **A. Kell**, M. Reppert, T.O. Pruitt, D. Sanchez, R. Jankowiak
- PHYS 485.** Critical assessment of the low-temperature optical spectra of the CP47 antenna protein complex of Photosystem II: Revised structural assignments. **J. Chen**, A. Kell, T. Reinot, M. Jassas, R. Jankowiak
- PHYS 486.** Heat capacity of oxygen atoms at high temperatures. **L. Biolsi**
- PHYS 487.** Membrane catalyzed aggregation of amylin using 2D IR spectroscopy. **K. Rich**, M.T. Zanni
- PHYS 488.** Ab initio approaches for accurate predictions of lanthanide thermochemistry. **C.C. Peterson**, A.K. Wilson
- PHYS 489.** Evaluation of charge density analysis methods. **C.C. Jeffrey**, **M.J. Carlson**, A.K. Wilson
- PHYS 490.** Electron transfer rate modulation in a compact Re(II) donor-acceptor complex. **Y. Yue**, T. Grusenmeyer, M. Zheng, P. Zhang, R.H. Schmehl, D.N. Beratan, I.V. Rubtsov
- PHYS 491.** Study of low temperature oxidation reactions of 2-methylfuran using synchrotron photoionization mass spectrometry. **A.R. Smith**, G. Meloni
- PHYS 492.** Gas-phase acidities of nitrated azole species from the extended kinetic method. **C.M. Nichols**, W. Old, W.C. Lineberger, V.M. Bierbaum
- PHYS 493.** Modeling stopped-flow data for nucleic acid duplex formation reactions. **A. Deckert**, J. Sikora, B. Rauzan
- PHYS 494.** DSC and rheological study of supercooled ethylene glycol-water mixture. **S. Kim**, R. Fore, E. Kook, B.H. Milosavljevic
- PHYS 495.** Using kinetic models to understand H atom reactions in solid parahydrogen. **F.M. Mutunga**, D.T. Anderson
- PHYS 496.** Evaluation of a novel nontraditional processing aid for the pulp and paper industry. **C. Kirwan**, R. Hamm, B. Wilson, L. Bava
- PHYS 497.** Template and model sets of protein structures. **I. Anishchanka**, P. Kundrotas, A. Tuzikov, I. Vakser
- PHYS 498.** Overcoming costly sampling simulations using non-Boltzmann Bennet's acceptance ratio method to generate potentials of mean force. **P.S. Hudson**, **F.L. Kearns**, S. Boresch, H.L. Woodcock
- PHYS 499.** Development of bacteriorhodopsin a potential energy surface by quantum chemical calculations. **C. Kim**, Y.M. Rhee
- PHYS 500.** Environmental effect on excited energy transfer in photosynthetic light harvesting complex: Comparing Poisson bracket mapping equation and reduced hierarchical equation of motion. **W. Lee**
- PHYS 501.** Evaluation of defoamer chemistries for brown stock washing. **R. Hamm**, C. Kirwan, B. Wilson, L. Bava
- PHYS 502.** DsDNA-assisted dissolution of tungsten (IV) disulfide in aqueous solution. **M. Simmons**, X. Xu, W. Zhao
- PHYS 503.** Computational study of the reduction by 2-propanol of acetophenone in supercritical 2-propanol. **D.B. Lawson**
- PHYS 504.** Electron transmission in molecular electronics: A computational study. **B. Topham**
- PHYS 505.** Effect of substitution on the rate of benzyloxyl radical generation through a 1,2-Hydrogen atom shift: A computational study. **D.J. Van Hooymissen**, S. Vyas
- PHYS 506.** Computational studies of inhibitor binding to human immunodeficiency virus, Type 2 (HIV-2) protease. **R. Summay**, V.F. Waingeh
- PHYS 507.** Solid phase microextraction with polystyrene- poly(dimethylsiloxane) block copolymers. **A. Schlaus**
- PHYS 508.** Mixed polarization vibrational sum frequency generation spectra of organic semiconducting thin films. **P.M. Kearns**, A.M. Massari
- PHYS 509.** Stochastic approach to reaction diffusion modeling of the fragmentation processes during heterogeneous oxidation of organic aerosol. **A.A. Wiegell**, K.R. Wilson, W. Hinsberg, F.A. Houle
- PHYS 510.** Characterization of a real-time tfor isoprene epoxydiols-derived secondary organic aerosol (IEPOX-SOA) from aerosol mass spectrometer measurements. **W. Hu**, P. Campuzano-Jost, B. Palm, D. Day, A. Ortega, P. Hayes, Q. Chen, M. Kuwata, Y. Liu, S. Simoes de Sa, S.T. Martin, M. Hu, S. Budisulistiorini, J. Surratt, K. Docherty, G. Isaacman, A. Goldstein, J. Clair, J.D. Crouse, P. Wennberg, J. Jimenez
- PHYS 511.** Water vapor enhancement of peroxy radical reactions. **S. Kumbhani**, T. Cline, M. Killian, J. Clark, L. Hansen, R.B. Shirts, D. Robichaud, J.C. Hansen
- PHYS 512.** Kinetics of acid-catalyzed dehydration of aerosol cyclic hemiacetals formed from the OH radical-initiated reaction of n-pentadecane. **A.P. Ranney**, P. Ziemann
- PHYS 513.** Heterogeneous oxidation of liquid and solid alkanes by OH in the presence and absence of NO or SO₂. **N.K. Richards-Henderson**, M.D. Ward, A. Goldstein, K.R. Wilson

PHYS 514. Investigating index of refraction trends in ammonium sulfate and glyoxal reactions. **M. Symons**, M.D. Zauscher, M.M. Galloway, D.O. Dehaan

PHYS 515. Determination of N-containing conjugated brown carbon products in glycolaldehyde, methylamine, and glycine reaction mixtures. **T. Kress**

PHYS 516. Measurements of in-situ SOA formation and chemistry using an oxidation flow reactor. **B.B. Palm**, P. Campuzano-Jost, D. Day, W. Hu, A.M. Ortega, S.S. de Sá, R. Seco, J. Park, A. Guenther, S. Kim, J. Brito, F. Wurm, P. Artaxo, R. Thalman, J. Wang, L. Kaser, W. Judd, T. Karl, A. Hansel, J. Fry, S.S. Brown, D. Draper, K.J. Zarzana, W.P. Dubé, N. Wagner, L. Hacker, A. Kiendler-Scharr, L. Yee, G. Isaacman, A. Goldstein, R. Souza, A. Manzi, O. Vega, J. Tota, M. Newburn, M. Alexander, S.T. Martin, W. Brune, J.L. Jimenez

PHYS 517. SOA derived from isoprene epoxydiols: Insights into formation, aging and distribution over the continental US from the DC3 and SEAC4RS campaigns. **P. Campuzano Jost**, B.B. Palm, D. Day, W. Hu, A.M. Ortega, J. Jimenez, J. Liao, K.D. Froyd, I. Pollack, J. Peischl, T.B. Ryerson, J. Clair, J.D. Crouse, P. Wennberg, T. Mikoviny, A. Wisthaler, L. Ziemba, B.E. Anderson

PHYS 518. Depositional ice nucleation on NX illite and mixtures of NX illite with organic acids. **K.M. Primm**, M. Tolbert, G. Schill

PHYS 519. Does the reaction of HO₂ with NO produce HONO, and HOONO? **L.A. Mertens**, H.M. Allen, M. Okumura, S.P. Sander

PHYS 520. Gas/particle partitioning of organic acids during the southern oxidant and aerosol study (SOAS): Measurements and modeling. **S. Thompson**, L. Yatawelli, H. Stark, J. Kimmel, W. Hu, B.B. Palm, P. Campuzano-Jost, D. Day, G. Isaacman, A. Goldstein, R. Holzinger, A. Khan, F. Lopez-Hilfiker, C. Mohr, J.A. Thornton, J.T. Jayne, D.R. Worsnop, J.L. Jimenez

PHYS 521. Reactions of resonantly-stabilized free radicals that impact molecular weight growth kinetics. **K. Wang**, S. Villano, A.M. Dean

PHYS 522. Hydration of Krypton in dilute and concentrated solutions. **M. Chaudhari**, S.L. Rempel, D. Sabo, L.R. Pratt

PHYS 523. Theoretical and experimental studies on the radical-radical reaction: NO₂ + N₂H₂. **G.L. Vaghjani**, H. Sun, S.D. Chambreaux, A. Schenck, K.K. Law

PHYS 524. Estimation of quantum effects in atomic solids using quantum trajectory dynamics with dissipation. **B. Gu**, V. Rassolov, S. Garashchuk

PHYS 525. Characterizing the effects of noncovalent interactions on hydrated azabenzene clusters: Charge localization and charge transfer. **J.T. Kelly**, K.H. Bowen, G.S. Tschumper, N. Hammer

PHYS 526. Intrinsic bonding patterns via localized orbitals. **J. Duchimaza**, A. West, M.W. Schmidt, M.S. Gordon, K. Ruedenberg

PHYS 527. Origins of long timescales in solvation dynamics of nanoconfined liquids. **J. Harvey**, W. Thompson

PHYS 528. Magnetic stability and relaxation in single-molecule magnets: Insights from new stochastic theories. **D. Packwood**, K. Reaves, F. Federici Canova, I. Hamada, H. Katzgraber, W. Teizer

PHYS 529. Multireference diagnostic criteria for 4d transition-metal-containing molecules. **J. Wang**, S. Manivassagam, A.K. Wilson

PHYS 530. In search of an intrinsic chemical bond. **A. Morgenstern**, T. Wilson, T. Jones, J. Miorelli, M. Eberhart

PHYS 531. Density functional theory study of the reduction of substituted quinones by lumiflavine. **E. Song**, C.R. Reinhardt, S. Bhattacharyay

PHYS 532. First-principles interpretation of ultrafast time-resolved core-level spectroscopies investigating photo-induced charge transfer. **S. Pamaraju**, S. Neppi, K. Siefertmann, D. Prendergast, O. Gessner

PHYS 533. Hydrocarbon structure impacts on the fumarate addition mechanism: Perspectives on the biodegradation susceptibility of fuels from electronic structure calculations. **V.S. Bharadwaj**, S. Vyas, S. Villano, C.M. Maupin, A.M. Dean

PHYS 534. Intramolecular oxygen bond re-arrangement reactions studied with density functional theory: Thermodynamics vs. kinetics. **F.X. Vazquez**

PHYS 535. Creating transferrable multiscale models from all-atom data. **M. McCullagh**

PHYS 536. Molecular polarizability as a descriptor of molecular conductance. **S. K. S. Mazinani**, R. Vatan, T. Pilarisetty, J.L. Palma, V. Mujica

PHYS 537. Modeling electron transfer through hydrogen bonding. **M. Wimmer**, R. Vatan, T. Pilarisetty, V. Mujica, J.L. Palma

PHYS 538. Raft environments assist the aggregation of the transmembrane region of Amyloid Precursor Protein. **N. Miyashita**, F. Ogushi, Y. Sugita

PHYS 539. Influence of sequence and lipid type on membrane perturbation by human and rat amyloid β-peptide (1-42). **A. Brown**, D.R. Bevan

PHYS 540. Lipid chain internalizes into human cardiomyocytes in a Dynamin-independent way. Amyloid fibrils recruit soluble protein in media and accelerate its internalization. **M. Marin-Argany**, M. Ramirez-Alvarado

PHYS 541. Revisiting Thioflavin T as fibrilization sensor: What is actually probed? **J. Brefkke**, M. Maroncelli

PHYS 542. Contributions of collision-induced dissociation to collision crossSections measured using the crossSectional areas by Fourier transform ion cyclotron resonance (CRAFT) approach. **C. Harper**, D.V. Dearden

PHYS 543. Theoretical study of the two-photon circular dichroism of molecular structures simulating aromatic amino acids residues in proteins with secondary structures. **Y.K. Vesga Prada**, M. Higgs, C. Diaz, F. Hernandez

PHYS 544. Analyzing small DNA constructs via chromophore model within the point dipole approximation. **P.G. Romano**

PHYS 545. Octa-coordination and the hydrated Ba²⁺(aq) ion. **M. Chaudhari**, S.L. Rempel, M. Soniat

PHYS 546. Inferring latent states and force estimates via hierarchical Dirichlet process modeling in single particle tracking experiments. **C.P. Calderon**

PHYS 547. Structure-activity and conformational-activity relationships of inhibitor of κB kinase-β. **M. Jones**, A.K. Wilson

PHYS 548. New insight into the FMO antenna protein: Hole burning and modeling study. **A. Kell**, K. Acharya, M. Jassas, T. Reintot, J. Tang, R. Jankowiak

PHYS 549. Computational study of folding thermodynamics and mechanism of fold-cage mutants with RSFF2. **C. Zhou**, F. Jiang, Y. Wu

PHYS 550. Engineering Aspects of Titania Nanotube Synthesis. **S.A. Ferdousi**, K.L. Yeung

PHYS 551. Natural boundary condition for hydrodynamic transport is the slip boundary condition for all molecule sizes and all solvents. **S.R. Aragon**

PHYS 552. Docking of protein models. **P. Kundrotas**, I. Anishchenko, A. Tuzikov, I. Vakser

PHYS 553. Solvent effects on azobenzene photodynamics with spin-flip time-dependent density functional theory and effective fragment potential methods. **K. Keipert**, Y. Harabuchi, M.S. Gordon

PHYS 554. Controlling the reactivity of large molecules by remote protonation of a side-group. **J. Ditkovich**, D. Pines, **E. Pines**

PHYS 555. Bond energy orbitals: The concept and some applications. **E.A. Boudreaux**

THURSDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Gas Phase Atmospheric Chemistry

D. Cziczo, M. Freedman, *Organizers*

T. H. Bertram, *J. Murphy, Presiding*

8:00 **PHYS 556.** Reactions of atmospheric peroxy radicals studied by synchrotron VUV multiplexed photoionization mass spectrometry. **L.G. Dodson**, L. Shen, J. Savee, D.L. Osborn, N.C. Eddingsaas, S.P. Sander, C.A. Taatjes, F.J. Grieman, **M. Okumura**

8:40 **PHYS 557.** Observation of the simplest cregee intermediate, CH₂OO, in the gas-phase ozonolysis of ethylene. **C. Womack**, M. Martin-Drumel, R. Field, M. McCarthy

9:00 **PHYS 558.** Comprehensive theoretical mechanism for the Cregee intermediate-sulfur dioxide reaction. **K.T. Kuwata**, E.J. Guinn, M.R. Hermes, J.A. Fernandez

9:20 Intermission.

9:35 **PHYS 559.** Ozone responses to climate change and NO_x reductions. **R.C. Cohen**

10:15 **PHYS 560.** New 'bond and photons' paradigm for the tropospheric ozone budget. **P.M. Edwards**, M.J. Evans

10:35 **PHYS 561.** How does nighttime oxidation of biogenic VOCs impact daytime ozone? **J. Mao**, J. Li, L. Horowitz, V. Naik, F. Paulot, M. Lin, I. Pollack, T.B. Ryerson, P.M. Edwards, K. Min, S.S. Brown, M. Graus, C. Warneke, J. Gilman, B. Lerner, A. Neuman, J.B. Nowak, P. Veres, J. Roberts, F. Lopez-Hilfiker, B. Lee, J.A. Thornton, J. Kaiser, F. Keutsch, G.M. Wolfe, T.F. Hanisco, K. Wells, D. Millet, B. Henderson, K. Aikin, J. de Gouw

11:00 **PHYS 562.** Novel method to estimate and evaluate OH rate constants for atmospherically relevant VOCs. **R.T. Rdister**, J.F. Hamilton, A.C. Lewis, M.J. Evans, A.R. Rickard, D.E. Heard, L.K. Whalley, D.R. Cryer, J.C. Young

11:20 Concluding Remarks.

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

PAH-Related Processes

L. J. Allamandola, T. J. Lee, *Organizers*
H. Cuppen, *Presiding*

8:00 **PHYS 563.** Organic molecules in protoplanetary disks: Probes of planet formation and chemical evolution. **J. Najita**

8:35 **PHYS 564.** Gas phase ion chemistry of complex organic species. **V.M. Bierbaum**, C.A. Cole, Z. Wang, T.P. Snow

9:10 **PHYS 565.** Tying interstellar PAH emission spectra and (photo)chemistry to local physical conditions in the emission zones. **C. Boersma**

9:45 Intermission.

10:15 **PHYS 566.** Dehydrogenation of PAHs: First steps towards fullerenes in the ISM. **P. Castellanos Nash**, J. Zhen, A. Candian, H. Linnartz, A. Tielens

10:50 **PHYS 567.** Photochemical model of the top down formation of fullerenes in the interstellar medium. **O. Berne**, J. Montillaud, C. Joblin

11:25 **PHYS 568.** Anharmonic bands in the 3-μm region of acenes: A combined experimental and theoretical study. **A. Petrigiani**, E. Maltseva, A. Candian, A. Tielens, J. Oomens, W. Buma

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Macromolecular Dynamics

Cosponsored by COMP

J. Gao, B. Mennucci, *Organizers*

B. C. Garrett, *Organizer, Presiding*

8:00 **PHYS 569.** Computationally guided design and optimization of inhibitors of macrophage migration inhibitory factor. **W.L. Jorgensen**, D.J. Cole, M.J. Robertson

8:30 **PHYS 570.** Multiscale characterization of macromolecular dynamics. **C. Clementi**

9:00 **PHYS 571.** Dynamic effects in dihydrofolate reductase catalysis. **R.K. Allemann**, L. Luk, J. Loveridge

9:30 **PHYS 572.** Advancing ab initio molecular dynamics via multiple-timestep methods. **R. Steele**

9:50 Intermission.

10:10 **PHYS 573.** Toward a molecular theory of early and late events in monomer to amyloid fibril formation. **J.E. Straub**

10:40 **PHYS 574.** Large spatiotemporal-scale quantum molecular dynamics simulations: A divide-conquer-recombine approach. **A. Nakano**, R.K. Kalia, K. Nomura, K. Shimamura, F. Shimajo, P. Vashishta

11:10 **PHYS 575.** Sorbate dynamics in hierarchical porous materials. **J.I. Siepmann**, P. Bai, E. Haldoupis, M. Tsapatsis

11:30 **PHYS 576.** Molecular dynamics simulations of ion transport in carbon nanotubes. **K.L. Shuford**, O. Samoylova, E. Calixte

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of CO₂

D. A. Scherson, *Organizer*

A. Co, *Organizer, Presiding*

A. R. Asthagiri, *Presiding*

8:30 **PHYS 577.** Understanding CO₂ electroreduction on Cu electrodes through first-principles modeling. **A.R. Asthagiri**

9:10 **PHYS 578.** Extended π-attraction α-repulsion model for carbon monoxide adsorbed on platinum-ruthenium-osmium-iridium quaternary alloys. **N. Dimakis**, N.E. Navarro, E.S. Smotkin

9:30 **PHYS 579.** Charge-state dependent electrocatalytic activity of discretely charged, atomically-precise Au_n(SR)_n⁺ nanoclusters (q = -1, 0, +1). **D. Kauffman**, D. Alfonso, C. Matranga, X. Deng, P. Ohodnicki, R. Silva, R. Jin

9:50 **PHYS 580.** Investing the electroreduction pathway of carbon dioxide using surface enhanced Raman spectroscopy. **J. Billy**, E. Coleman, K. Muhlenkamp, **A. Co**

10:10 **PHYS 581.** Pyridine-catalyzed CO₂ reduction on p-GaP photoelectrodes: First-principles investigation of possible reaction mechanisms. **M. Lessio**, C. Riplinger, A.B. Muñoz-García, E.A. Carter

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Dynamics in Function and Inhibitor Design

Cosponsored by COMP

G. Hummer, *Organizer*

A. E. Garcia, *Organizer, Presiding*

8:00 **PHYS 582.** Predicting drug-target binding kinetics through enhanced sampling simulations. **F. Gervasio**

POLY

Division of Polymer Chemistry

M. Jeffries-El, D. Boday and T. White, Program Chairs

SOCIAL EVENTS:

POLY Luncheon, 12:30 PM: Sun
POLY Luncheon, 12:30 PM: Mon
POLY Reception, 5:30 PM: Tue
POLY Breakfast, 7:30 AM: Tue
POLY Reception, 5:30 PM: Wed

BUSINESS MEETINGS:

POLY Programming Committee Meeting (Lunch), 12:00 PM: Tue

SUNDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Cosponsored by PMSE†

Y. C. Simon, *Organizer*
E. B. Berda, J. Foster, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY 1. Poly(phthalaldehydes) as stimuli-responsive, depolymerizable materials that are capable of providing amplified responses. A.M. DiLauro, S.T. Phillips

9:05 POLY 2. Making "smarter" heparin-mimicking polymers. N. Ayres, Y. Huang, Q. Chi

9:35 POLY 3. Nucleobase hydrogen bonding in polymers as a source of intelligence. T.E. Long, K. Zhang, M. Aiba, S. Cheng, W.D. Chiang

10:05 Intermission.

10:15 POLY 4. Poly(phosphoester)s: From adhesives to stealth polymers. F. Wurm

10:45 POLY 5. Light-degradable polymers: amplification strategies, response to new wavelengths, and application to a clinical challenge. J. Olejniczak, C. Carling, V. Nguyen Huu, A. Garcia, J. Luo, K. Zhang, A. Almutairi

11:15 POLY 6. Folding single polymer chains. C. Barner-Kowollik, J. Willenbacher, O. Altintas

11:45 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Putting Renewable Polymers to Work

D. Boday, E. C. Hagberg, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 POLY 7. Poly(β -methyl δ -valerolactone) as a scalable and renewable soft segment for aliphatic polyester block polymers. M.A. Hillmyer

8:35 POLY 8. Commercialization of triglyceride-based thermoplastic elastomers for polymer modified asphalt pavements: Where the (bio)rubber meets the road. E.W. Cochran, R. Williams, N. Hernandez, M. Yan, A. Hohmann, M.J. Forrester

9:05 POLY 9. Conversion of agricultural residues into value-added products. H. Cheng, A. Biswas

9:35 Intermission.

9:50 POLY 10. Synthesis and functional properties of renewable polymers. R.M. Waymouth, X. Zhang, B. Timothy, A.J. Ingram, K. Chung, W. Ho, J. Hedrick

10:20 POLY 11. Design and synthesis of eumelanin-inspired polymers derived from vanillin. T.L. Nelson, R.P. Hopson, S. Selvaraju, N. Sachinthan

10:40 POLY 12. Thiol-ene films derived from phenolic acids. G. Yang, H. Tesefay, M.L. Robertson

11:10 POLY 13. Glass transition dynamics of bioabsorbable poly(ethylene 2,5-furandicarboxylate). A. Codou, N. Guigo, M. Moncel, L. Martino, J. Van Berkel, E. De Jong, N. Sbirrazzuoli

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Celebrating the Fifth Year Anniversary of Polymer Chemistry (RSC)

Financially supported by Royal Society of Chemistry

D. M. Haddleton, B. S. Sumerlin, W. You, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 POLY 14. Nature's functionality on synthetic polymers — zwitterions and inverse zwitterions. T. Emrick

9:10 POLY 15. Mimicry of photosynthesis: for the synthesis of well-defined polymers. S. Sharmugam, J. Xu, C. Boyer

9:40 POLY 16. New methodology for controlled supramolecular polymerization. X. Zhang

10:10 Intermission.

10:30 POLY 17. Sequential one-pot organocatalytic polymerization of epoxides and cyclic esters/carbonates. J. Zhao, D. Pahovnik, Y. Gnanou, N. Hadjichristidis

11:00 POLY 18. Building smart materials from poly(2-vinyl-4,4-dimethylazlactone) scaffolds. A.B. Lowe

11:30 POLY 19. Self-immolative polymersomes for high-efficiency triggered release and programmed enzymatic reactions. G. Liu, X. Wang, S. Liu

Section D

Sheraton Denver Downtown Hotel
Governor's Square 9

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
A. Carlmark, F. Horkay, *Presiding*

8:00 POLY 20. Cartilage: architecture and function. F. Horkay, P.J. Bassar

8:20 POLY 21. Drug-functionalized cell-penetrating peptides for enhanced delivery and binding in myotonic dystrophy type 1 treatment. Y. Bai, L. Nguyen, Z. Song, J. Cheng, S.C. Zimmerman

8:40 POLY 22. Novel biodegradable, biocompatible and bifunctional block copolymer scaffolds for tissue engineering applications. P.P. Smith, A.L. Rightler, B.K. McConnell, F. Zhang, S.O. Streubel, S. Lu, D. Price, S.G. Boyes

9:00 POLY 23. Protein:polymer conjugates via graft-from ring-opening metathesis polymerization. S.A. Isarov, J.K. Pokorski

9:20 POLY 24. Polylactic acid composite with natural fibers in food packaging. S. Sedaghat

9:40 POLY 25. N-heterocyclic carbenes in the organopolymerization of N-substituted N-carboxy-anhydrides to polypeptoid. I. Falivene, M. Alghamdi, L. Cavallo

10:00 POLY 26. Surface-initiated ring opening polymerization of carbonates and siloxanes from cellulose surfaces. S. Pendergraph, G. Klein, M.K. Johansson, A. Carlmark

10:20 POLY 27. Optimizing photo-CuAAC polymerization kinetic for dental restorative materials. H. Song, A.D. Baranek, M. McBride, T. Gong, A. Flores, J.W. Stansbury, C.J. Kloxin, C. Bowman

10:40 POLY 28. Chemical modification reactions of polysaccharides studied in real time by light scattering and viscometry-based methods. V.C. Spier, A.M. Alb

11:00 POLY 29. Radiolabeled polymers to probe the enhanced permeability and retention effect. M.C. Parrott

11:20 POLY 30. Investigating polymerization reactions with thermography: Differentiating between bulk effects, thermal diffusion and oxygen inhibition. C. Wappel, R. Geier, H. Freiszmuht, C. Slugovc, G. Gescheidt

11:40 POLY 31. High performance hydrogels based on melt-assembled networks of sphere-forming block copolymers. J. Lewis, T.S. Bailey

12:00 POLY 32. Smart polymers for on-demand drug delivery. Y. Zhang, K. Cai, J. Cheng

Section E

Sheraton Denver Downtown Hotel
Directors Row I

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY 33. Size exclusion chromatography/gel permeation chromatography – a blessing and curse of science and technology of synthetic polymers. D. Berek

9:15 POLY 34. Industrial polymer analysis using a solvent elimination IR detector. R. Allen, S. Moyses, N. Jestel

9:45 POLY 35. Is SEC-Raman a feasible way of measuring copolymer chemical heterogeneity? A.M. Striegel, L. Pitkanen, A.A. Urbas

10:15 Intermission.

10:30 POLY 36. Probing serum phase oligomer in acrylic emulsion polymerization process by GPC-RI/MS. T. Zhang, W. Gao, R. Even, D. Kline

11:00 POLY 37. Characterization of novel high temperature thermoplastic elastomers polybenzofulvene-block-polyisoprene-block-polybenzofulvene. J.W. Mays, W. Wang, T. White, N. Kang, K. Hong, R. Schlegel, M. Beiner, K. Williams, S.P. Gido

11:30 POLY 38. Ultrahigh performance size exclusion chromatography of synthetic polymers. M. Janco, J.N. Alexander, E.S. Bouvier, D. Morrison

12:00 POLY 39. Advanced polymer chromatography: Method development tools for SEC polymer analysis. D. Morrison, M. O'Leary

SUNDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Cosponsored by PMSE†

E. B. Berda, Y. C. Simon, *Organizers*
J. Foster, *Organizer, Presiding*

N. Zacharia, *Presiding*

1:30 Introductory Remarks.

1:35 POLY 40. Progress towards the efficient synthesis of polymers with precisely defined mass, sequence, and stereochemistry. J. Barnes, D. Ehrlich, F. Leibfarth, T.F. Jamison, J.A. Johnson

2:05 POLY 41. Programmed block copolymers: At the end it is always good to be smart. E.B. Coughlin

2:35 POLY 42. Tunable solid state fluorescent materials for supramolecular encryption. X. Hou, C. Ke, J.F. Stoddart

3:05 Intermission.

3:25 POLY 43. Dynamic-covalent nanoparticles and self-healing hydrogels. S. Mukherjee, C.C. Deng, W. Brooks, M. Hill, B.S. Sumerlin

3:55 POLY 44. Chirality-selected phase behavior in ionic polypeptide complexes. M.V. Tirrell

8:35 PHYS 583. Activation and drug design of a muscarinic G-protein coupled receptor. Y. Miao, J.A. McCammon

9:10 PHYS 584. Prediction of mechanically hot spots in protein-protein interactions using perturbation response scanning method. H. Abdizadeh, A. Atlgan, C. Atlgan

9:45 PHYS 585. Nucleotide-dependent interaction of K-Ras4B hypervariable region with Ras active site. T.S. Chavan, H. Jang, L. Khavrutskii, V. Gaponenko, N.I. Tarasova, R. Nussinov

10:20 PHYS 586. Elucidating protein function and dynamics through molecular simulations and Markov state modeling: Allostery through conformational selection. R.E. Amaro, R. Malmstrom, S.S. Taylor, A. Kornev

10:55 PHYS 587. Folding kinetics and local dynamics of the 60 nucleotide rRNA GTPase center RNA. M.J. Rau, K.B. Hall

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Nonadiabatic Effects

B. G. Levine, *Organizer*
S. A. Varganov, *Organizer, Presiding*

8:00 PHYS 588. Excited state dynamics at complex interfaces: time-domain ab initio studies. O.V. Prezhdo

8:40 PHYS 589. Geometric phase effects in non-adiabatic dynamics near two-state conical intersections. A.F. Izmaylov

9:20 PHYS 590. PYXAID program: a tool for modeling excited state dynamics in complex systems. A.V. Akimov, O.V. Prezhdo

9:40 PHYS 591. Self-trapping of excitons, violation of condon approximation, and efficient fluorescence in conjugated cycloparaphenylenes. L. Adamska, J. Liu, S. Fernandez-Alberti, R. Jasti, S.K. Doorn, S. Tretiak

10:00 Intermission.

10:20 PHYS 592. Current view of surface hopping. J.E. Subotnik, B.R. Landry

11:00 PHYS 593. Multidimensional effects in nonadiabatic statistical theories of spin-forbidden kinetics. A. Jasper

11:40 PHYS 594. Semiclassical Monte-Carlo: A first principles approach to nonadiabatic molecular dynamics. A. White, V. Gorshkov, R. Wang, S. Tretiak, D. Mozyrsky

12:00 PHYS 595. Modeling nonadiabatic photo-dynamics in aqueous environments with the ab initio multiple spawning and effective fragment potential methods. K. Keipert, S.R. Pruitt, M.S. Gordon

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, *Organizer*
S. Link, K. A. Willets, *Organizers, Presiding*

8:30 PHYS 596. Single molecule chemistry probed by SERS and TERS at the nanometer length scale and picosecond time scale. R.P. Van Duyne

9:05 PHYS 597. Optical characterization of pinholes in passivation layers on electrode surfaces. K. Marchuk, C. Renault, A.J. Bard, K.A. Willets

9:25 PHYS 598. Plasmonic application in imaging at the single cancer cell level. M.A. El-Sayed

10:00 PHYS 599.

Withdrawn.

10:20 PHYS 600. Probing magneto-plasmonic phenomena at the single nanostructure level. K.L. Knappenberger

10:55 PHYS 601. Following plasmonically-enhanced chemical reactions with ultrafast Raman spectroscopies. R.R. Frontiera

4:25 POLY 45. Responsive polypeptide-based star and triblock copolymers: Smart function through morphology transitions. G.A. Strange, A.J. Johnson, I. Smith, J.G. Ray, D.A. Savin

4:55 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Putting Renewable Polymers to Work

D. Boday, E. C. Hagberg, *Organizers, Presiding*

1:00 POLY 46. Diisocyanates and tackifiers from isosorbide. M.D. Zerner, J.S. Chen

1:20 POLY 47. Benzyl chloride functionalized polycarbonates: A versatile platform for the synthesis of functional biodegradable polycarbonates. R. Ono, S. Liu, S. Venkataraman, W. Chin, Y. Yang, J. Hedrick

1:50 POLY 48. Synthesis, characterization, and bimodal blend studies of renewable biobased epoxy resins from vanillyl alcohol. E.D. Hernandez, J.M. Sadler, J.J. La Scala, J.F. Stanzione

2:10 POLY 49. Selective organic catalysis in the synthesis of materials from sustainable resources by ring-opening polymerization. A.P. Dove

2:40 Intermission.

2:55 POLY 50. Renewable polymers in hydraulic fracturing applications. J.R. Dorgan

3:25 POLY 51. Soy-based polymer surfactants for personal care applications. A. Popadyuk, H. Kalita, B.J. Chisholm, A.S. Voronov

3:45 POLY 52. From biorefinery to performance technology: Transforming methathesized renewables oils into high value products. K.O. Havelka

4:15 POLY 53. Renewable feedstocks for the polymer industry. E.C. Hagberg, P.D. Bloom

4:45 POLY 54. Polysaccharide circuit boards for epidermal electronics. M.A. Daniele, J.S. Erickson, A.J. Knight, S.A. Roberts, K. Radom, S. Walper, J. Yuen

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Celebrating the Fifth Year Anniversary of Polymer Chemistry (RSC)

Financially supported by Royal Society of Chemistry

D. M. Haddleton, B. S. Sumerlin, W. You, *Organizers, Presiding*

1:30 POLY 55. Hierarchical polymeric nanostructures from precision polymer chemistry. S. Perrier

2:00 POLY 56. Sequence-controlled polymerizations: The Holy Grail is near. J. Lutz

2:30 POLY 57. Protein-polymer conjugates by grafting to and grafting from methods. H.D. Maynard, C. Decker, J. Ko, J. Lee, T.H. Nguyen, E. Pelegrí-O'Day, N. Matsumoto

3:00 Intermission.

3:20 POLY 58. Synthesis of protein-polymer conjugates with controllable activity through site-specific conjugation. X. Li, L. Wang, Y. Cai, L. Yuan, H. Wang, G. Chen, H. Chen

3:50 POLY 59. Entropy driven chain effects on ligation. C. Barner-Kowollik, A. Lederer, M. Coote, G. Gryn'ova, K. Pahnke, F.G. Schmidt, J. Brandt, N. Guimard

4:20 POLY 60. Mimicking complex biological membranes and their programmable glycan ligands. V. Percec

Section D

Sheraton Denver Downtown Hotel
Governor's Square 9

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
N. S. Sampson, W. Xi, *Presiding*

1:00 POLY 61. Solution processable polydiacetylenes (PDAs) through acyclic enediyne metathesis polymerization (AEDMET). Y. Qiu

1:20 POLY 62. Very long, linear polymers from tandem isomerization/alternating ring-opening metathesis polymerization (*t*-AROMP). L. Tan, K.A. Parker, N.S. Sampson

1:40 POLY 63. Ring-opening metathesis emulsion polymerization: A comparison of commercial and homemade surfactants and catalysts. S.R. Almahdali, K. Bukhriakov, V. Rodionov

2:00 POLY 64. Withdrawn.

2:20 POLY 65. Incorporation and use of imidazoles as a dually dopable moiety in conjugated polymers. J.D. Harris, K.R. Carter

2:40 POLY 66. Pushing the limit of the RAFT process: One-pot preparation of multiblock copolymers. G. Gody, S. Perrier

3:00 POLY 67. RAFT polymerization of tertiary amine-based methacrylate pH-responsive monomers for smart MRI contrast agents. L. Zhu, S. Powell, S.G. Boyes

3:20 POLY 68. Stille catalyst-transfer polycondensation using palladium catalysts for the synthesis of well-defined conjugated materials. Y. Qiu, T. Kowalewski, K.J. Noonan

3:40 POLY 69. "Click" by "click" strategy in sequence controlled polymers synthesis. W. Xi, S. Pattanayak, C.J. Kloxin, C. Bowman

4:00 POLY 70. New polymer synthesis strategy based on multicomponent reactions. R. Kakuchi, P. Theato

4:20 POLY 71. Design and synthesis of segmented conjugated polymers via acyclic diene metathesis (ADMET). G. Singh, R.M. Peetz

4:40 POLY 72. Synthesis and polymerization of new 2-substituted vinylimidazolium salts. D. Smith, T. Muzio, T.W. Smith

5:00 POLY 73. Aza-Diels-Alder route to polyquinolines. D.J. Dibble, M. Umerani, A. Mazaheripour, Y. Park, A.A. Gorodetsky

Section E

Sheraton Denver Downtown Hotel
Directors Row J

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY 74. Size and composition-based nanoparticles separations and analyses using field-flow fractionation. K.R. Williams

2:15 POLY 75. Self-organization phenomena in biomacromolecules investigated by field flow fractionation. A. Lederer

2:45 POLY 76. Asymmetrical flow field-flow fractionation for the comprehensive characterization of polymer assemblies. F.M. Winnik

3:15 Intermission.

3:30 POLY 77. Measurement of size and certain structural features of sub-nanokilometer particles in suspension. P.J. Wyatt

4:00 POLY 78. Asymmetric flow field-flow fractionation: A versatile tool for nanoparticle separation. C. Rosu, R. Cueto, E. Reichmanis, P.S. Russo

4:30 POLY 79. Semipreparative asymmetric flow field-flow fractionation for nanoparticle characterization. C. Bria, A. Ashames, P. Skelly, S.R. Williams

5:00 POLY 80. Synthesis and characterization of functional polymer nanoparticles via sonogashira coupling. A. Prasher, D. Chao, E.B. Berda

Nanotechnology: Delivering on the Promise Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Materials with Special Optical, Electronic and Mechanical Behavior

Cosponsored by PMSE†

E. B. Berda, J. Foster, *Organizers*
Y. C. Simon, *Organizer, Presiding*
C. K. Lyon, *Presiding*

8:30 Introductory Remarks.

8:35 POLY 81. Mechanochromism of block copolymer photonic gels. E. Chan, E.L. Thomas

9:05 POLY 82. Development of mechanochemical and thermal triggers for release of small organic molecules. A.J. Boydston

9:35 POLY 83. Responsive photonic multilayers from photo-crosslinkable polymers and nanocomposites. R.C. Hayward

10:05 POLY 84. Voxellated liquid crystal elastomers. T.J. White, T.H. Ware, J. Wile

10:35 Intermission.

10:45 POLY 85. Stretchable electronic materials and devices. Z. Bao

11:15 POLY 86. Applying reconfigurable networks of charge-transporting polycyclic aromatic hydrocarbons to problems in energy storage. B.A. Helms, P.D. Frischmann, L.C. Gerber, S.E. Doris, C. Li

11:45 POLY 87. Creating new architectures for π -conjugated semiconducting polymers. C.K. Luscombe

12:15 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Putting Renewable Polymers to Work

Cellulose

D. Boday, E. C. Hagberg, *Organizers, Presiding*

8:00 POLY 88. High performance cement via cellulose nanocrystal addition. J.P. Youngblood, R. Moon, J. Weiss, P. Zavattieri, Y. Cao

8:30 POLY 89. Effect of the electrical double layer on surface-initiated controlled radical polymerization from cellulose nanocrystals in aqueous media. J.O. Zoppe, X. Xu, H.A. Klok

8:50 POLY 90. Can hemicelluloses be used for durable wood adhesives? E.E. Malmström, E. Norström, L. Fogelström, P. Nordqvist, F. Khabbaz

9:10 POLY 91. Multifunctional fluorescent sensors for imaging the interphase in polymer nanocomposites. J. Gilman, D. Fox, J. Woodcock, J. Liddle, S. Stranick, R. Beams, G. Myers, C. Davis, N. Chen, L. Sacui

9:40 Intermission.

9:55 POLY 92. Structured and functionalized nanocellulose for controlled release and implantation. J. Foster

10:25 POLY 93. Renewable thermoplastic materials from cellulose. J.H. Wang, Y. Bai, B. Zhou, Z. Yu, Q. Jia, W. Wang, H. Tan

10:55 POLY 94. Renewable thermoplastics from lignin. A.K. Naskar, C.D. Tran, A.S. Bova

11:15 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by IAB (ACS Polymer Division Industrial Advisory Board)

C. J. Ellison, T. E. Long, *Organizers*
H. N. Cheng, C. J. Landry-Coltrain, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY 95. Post-electrospinning derivatization of polymer nanofibers with bioactive species using translationally-relevant chemical methods. J. Zheng, D.H. Reneker, M. Becker

8:55 POLY 96. Sequential inverse vulcanization and electropolymerization for conductive plastic sulfur. P.T. Dirlam, J. Pyun

9:15 POLY 97. Manipulating conjugation in electronic polymers: Chemical sensors and precursor routes. J.G. Weis, T.M. Swager

9:35 POLY 98. Poly(ionic liquid)s and their block copolymers: Synthesis, characterization, self-assembly, and applications. H. He, H. Nulwala, K. Matyjaszewski

9:55 Intermission.

10:10 POLY 99. Facile post-polymerization modification of blocked isocyanate and hydrazide containing polymers. E.A. Hoff, B. Abel, C.A. Tretbar, C.L. McCormick, D.L. Patton

10:30 POLY 100. Sequencing in step-growth polymerization: Influence of segment length on thermomechanical properties of poly-sulfone-containing segmented polyesters. J.M. Dennis, G.B. Fahs, R.B. Moore, S.R. Turner, T.E. Long

10:50 POLY 101. Olefin cross-metathesis, a mild, modular and efficient approach towards functionalized cellulose esters. X. Meng, J.B. Matson, K.J. Edgar

11:10 POLY 102. Scalable production of mechanically tunable block polymers from sugar. D.K. Schneiderman, M. Xiong, F.S. Bates, K. Zhang, M.A. Hillmyer

11:30 Remarks by ACS President, Dr. Diane G. Schmidt, and Photo Session

Section D

Sheraton Denver Downtown Hotel
Governor's Square 15

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys

Barrier and Separation Behavior

Cosponsored by PRES

Financially supported by Avery Dennison, 3M, Bayer MaterialScience, Kuraray

J. C. Grunlan, M. Priolo, L. Wagberg, *Organizers*
P. Larsson, D. F. Schmidt, *Presiding*

8:30 Introductory Remarks.

8:35 POLY 103. Electrospun composite membranes of cellulose acetate (CAC) and poly(vinyl alcohol) (PVA). L. Baghernejad, R. Ozer, R. Mohan, O. Shohan, S. Oduyungbo, E.V. Iski

8:55 POLY 104. Assessing gas permeability in polymer nanolaminates. E. Dunckerley, D.F. Schmidt

9:25 POLY 105. Thermally reduced graphene oxide-PEI multilayer thin films as electrically conductive gas barrier layer. B. Stevens, J.C. Grunlan

9:45 POLY 106. Stretchable gas barrier achieved with partially hydrogen-bonded multilayer nanocoating. K.M. Holder, F. Xiang, B.R. Spears, M. Huff, M. Priolo, E. Harth, J.C. Grunlan

10:05 Intermission.

10:25 POLY 107. Multilayered nanocomposites containing high aspect ratio particulates. S. Nazarenko

10:55 POLY 108. Polymer membranes for gas and liquid separations. B.D. Freeman

11:25 POLY 109. Polymer composites for gas separation membranes and sorbents. W. Koros

11:55 POLY 110. Biomaterial-based barrier materials and composites: A review on how to prevent unwanted water interactions and water-induced property deterioration. P. Larsson, L. Wagberg

† Cooperative Cosponsorship

Section E

Sheraton Denver Downtown Hotel
Directors Row I

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY 111. Polysaccharide characterization using asymmetrical flow field-flow fractionation and multiangle light scattering (AF4-MALS): Successes and challenges. L. Nilsson

9:20 POLY 112. Asymmetrical flow FFF coupled with light scattering for the separation and the structural characterization of gluco-polymers with various branching patterns. A. Roland-Sabate, F. Grimaud, R. Irague, S. Guilois, D. Lourdin, J. Putaux, G. Potocki-Véronèse, A. Buléon

9:55 POLY 113. Characterization of hyaluronic acid and polymer JR using size exclusion chromatography with advanced detection techniques. X.M. Liu, E. Maziarz

10:30 Intermission.

10:45 POLY 114. Challenges associated with size exclusion chromatography of amphiphilic cellulose ether materials. D.M. Meunier, Y. Li, E.M. Partain, M. Brackhagen, P. Oliver

11:20 POLY 115. New approach to overcome hydrophobic interaction in cellulose ethers for reliable molecular weight characterization. Y. Li, D.M. Meunier, D. Redwine, M. Brackhagen, R. Adden

Nanotechnology: Delivering on the Promise Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Integrating Chemistry and Polymer Science Research into the Classroom

Sponsored by CHED, Cosponsored by PMSE and POLY

MONDAY AFTERNOON**Section A**

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials Composite Materials and Smart Processes

Cosponsored by PMSE†

Y. C. Simon, *Organizer*
E. B. Berda, J. Foster, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY 116. Ionic polymer carbon composites as a new design for electroactive actuators and sensors. R.B. Moore

2:05 POLY 117. Thermal properties of polymer-inorganic composites. M. White

2:35 POLY 118. Covalently linked polymer-clay nanocomposites: Polymer brushes grafted from lamellar organosilicates. S.L. Burkett, K.A. Winchell, E.W. Vaimberg

2:55 Intermission.

3:15 POLY 119. Synthesis and characterization of ionically crosslinked polymer networks. K.A. Cavicchi

3:45 POLY 120. Vinylic vitrimers. M. Röttger, R. Nicolay, L. Leibler

4:15 POLY 121. Combined hydrophobicity and mechanical durability through surface nano-engineering. P.R. Elliott, S.P. Stagon, H. Huang

4:45 Concluding Remarks.**Section B**

Sheraton Denver Downtown Hotel
Governor's Square 12

Innovations in Macromolecular Network Chemistry

*Industrial Innovations in Polymer Chemistry
Cosponsored by BMGT*

M. Hunt, C. Lipscomb, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY 122. Sustainable carbon sources for the chemical industry: CO₂ is becoming a direct and indirect component in polyurethane plastics. C. Guertler, K. Malsch, M. Wohak, A. Wolf, A. Bardow, N. von der Assen, W. Leitner, T.E. Mueller

2:05 POLY 123. Building a portfolio of renewable diols for unsaturated polyester resins. E.C. Hagberg, P.D. Bloom

2:35 POLY 124. From literature research to industrial production and back again: A polymer's tale. L.M. Stratton, B. Gordon III, T.W. Smith, K.M. Kayne

3:05 POLY 125. Living polymerization routes to siloxane macromers. J.D. Goff, B. Arkles

3:35 POLY 126. Enhanced material properties from new isomer configurations of polyetherimides. P.M. Johnson

4:05 Intermission.

4:20 POLY 127. Pushing the boundaries for hydrocarbon extraction in the oil & gas industry through block copolymer technology. E.B. Murphy

4:50 POLY 128. Advances in polyethylene. M. Demirors

5:20 POLY 129. Abundant, low cost U.S. shale gas supply stimulates polyolefins renaissance. P. Brant

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Excellence in Graduate Polymer Research

*Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by IAB (ACS Polymer Division Industrial Advisory Board)*

H. N. Cheng, C. J. Landry-Coltrain, *Organizers*
C. J. Ellison, T. E. Long, *Organizers, Presiding*

1:30 Introductory Remarks.**1:35 Recognition of Poster Presenters.**

1:45 POLY 130. Unexpected anomalous diffusion in associating protein hydrogels. S. Tang, M. Wang, B.D. Olsen

2:05 POLY 131. Reducing-environment sensitive synthetic hydrogels for controlled delivery of therapeutics. P.M. Kharkar, A.M. Kloxin, K.L. Krick

2:25 POLY 132. Photodegradable hydrogels for studying axon guidance and the user-directed formation of neural circuits. T. Brown, D. McKinnon, K.S. Anseth

2:45 POLY 133. Molecular N-dopants and N-dopable conjugated polymers. B. Naab, S. Zhang, X. Gu, E. Evans, T. Kurosawa, K. Vandewal, A. Salleo, G.L. Millhauser, S. Barlow, S.R. Marder, Z. Bao

3:05 Intermission.

3:20 POLY 134. High-throughput screening of electrochromic polymers toward neutral colors. M.T. Otley, G.A. Sotzing

3:40 POLY 135. Chiral transmission to self-assembling nanostructures from circularly polarized light. J. Yeom, B. Yeom, H. Chan, K. Smith, S. Dominguez-Medina, J. Bang, G. Zhao, W. Chang, S. Chang, A. Chuvilín, D. Melnikau, A. Rogach, P. Zhang, S. Link, P. Kral, N. Kotov

4:00 POLY 136. Polymer-particle rheological analysis of adsorbed cement additives for improved processing. L.R. Murray, E.G. Soltys, K.A. Erk

4:20 POLY 137. Efficient simulation of the molecular scale behavior of polymer melts: Understanding polymer dynamics and rheology. N.A. Rorrer, J.R. Dorgan

Section D

Sheraton Denver Downtown Hotel
Governor's Square 15

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys

*Energy, Electrical & Thermal
Cosponsored by PRES*

Financially supported by Avery Dennison, 3M, Bayer MaterialScience, Kuraray

J. C. Grunlan, M. Priolo, L. Wagberg, *Organizers*
S. T. Iacono, J. P. Youngblood, *Presiding*

1:30 Introductory Remarks.

1:35 POLY 138. Electrical and thermal conductivity of PAN/CNT composite fibers for heating behavior. A. Chien, S. Kumar

1:55 POLY 139. Aqueous MWCNT dispersions and their highly thermally conducting coatings. J. Texter, X. Ma, R. Crombez

2:25 POLY 140. Thermal and other properties in cellulose nanocrystal composite materials. J.P. Youngblood, J.A. Diaz, A. Martini, R. Moon

2:55 POLY 141. Thermal and electrical transport in nanoconfined poly(3-hexylthiophene)-multi-walled carbon nanotube composite fibers. M.K. Smith, V. Singh, K. Kalaitzidou, B.A. Cola

3:15 Intermission.

3:25 POLY 142. Metallized perfluoropolyether nanocomposites: New materials for structural energetics. S.C. Kettwich, J. McCollum, K.S. Kappagantula, N. Clayton, E. Avjian, H.A. Miller, D.W. Ball, M. Pantoya, S.T. Iacono

3:55 POLY 143. Soft, compressible and fully interdigitated 3D energy storage devices built by layer-by-layer assembly inside aerogels. M.M. Hamedi, L. Wagberg, G. Nyström, A. Marais, E. Karabulut, Y. Cui

4:25 POLY 144. Hybrids of conducting polymers and carbon nanotubes for harvesting electrical energy and thermoelectric cooling. C. Yu

Section E

Sheraton Denver Downtown Hotel
Directors Row J

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY 145. Temperature gradient interaction chromatography: Principle and applications. T. Chang

2:15 POLY 146. Gradient elution at critical point of adsorption: Separation by chemical composition and microstructure. Y. Brun, C.J. Rasmussen

2:45 POLY 147. Use of 2-D chromatographic techniques to elucidate macromolecular structures. J.A. McConville, P. Kilz, M. Adler, W. Radke, D. Lohmann

3:15 Intermission.

3:30 POLY 148. Online 2D aTREF-hSEC technique for polyolefins characterization. Y. Yu, M. Hildebrand, M.A. Stepp, P.J. DesLauriers, C.C. Tso

4:00 POLY 149. High temperature liquid chromatography of Polyolefin. R. Cong, W. deGroot

4:30 POLY 150. Dual flow refractive index detection for polymer analysis by high temperature gel permeation chromatography. A.K. Brewer

5:00 POLY 151. Exploring a chiral cross-linker by molecular imprinting using chromatographic and batch rebinding techniques. B. Hebert, D. Meador, D. Spivak

Nanotechnology: Delivering on the Promise**Bridging the Gap to a Thriving US Marketplace**

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Undergraduate Research Posters**Polymer Chemistry**

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING**Section A**

Colorado Convention Center
Halls C/D

Sci-Mix

M. Jeffries-EI, D. Boday and T. White, *Organizers*

8:00 - 10:00

POLY 152. Polyalkylmethacrylate-functionalized inorganic nanoparticles as solid-solid phase change materials: Effect of spacer length, molecular weight and graft density on heat storage capacity. K.A. Stockmal, S. Granados Focil

233-234, 243-245, 249-250, 256, 267, 270, 274, 278-279, 282, 284, 286, 288-289, 292-293, 296, 298, 306, 310-313, 315, 319-320, 323, 330, 343, 347, 369-371. See subsequent listings.

STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum**Polymer Science Education and the NGSS**

Sponsored by CHED, Cosponsored by PMSE, POLY†, RUBB and SCC†

TUESDAY MORNING**Section A**

Sheraton Denver Downtown Hotel
Governor's Square 14

Carl S. Marvel Creative Polymer Chemistry Award in Honor of Todd Emrick

M. Jeffries-EI, T. P. Russell, *Organizers*
R. C. Hayward, J. Pyun, *Presiding*

8:30 Introductory Remarks.

8:35 POLY 153. From molecules to functional materials: Controlling structure and properties through synthesis. R.B. Grubbs

9:05 POLY 154. Metal oxide nanoparticle hybrids: New photoresists with extraordinary sensitivity. J. Jiang, B. Zhang, L. Li, E.P. Giannelis, C.K. Ober

9:35 POLY 155. Harnessing biomimetic catch bonds to create mechanically robust nanoparticle networks. B. Iyer, V.V. Yashin, A.C. Balazs

10:05 POLY 156. Exploiting reversible-covalent chemistry to investigate materials and mechanisms. H. Sun, C.P. Kabb, S. Mukherjee, B.S. Sumerlin

10:35 POLY 157. Importance of the intricate linkage of the needs of particular biomedical applications to the design characteristics of functionally-sophisticated nanoscopic macromolecules to achieve efficacy. K.L. Wooley

11:05 POLY 158. Bioconjugate and hybrid systems prepared by atom transfer radical polymerization. K. Matyjaszewski

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

Cosponsored by PMSE

S. T. Iacono, *Organizer*
S. Clarson, A. Sellinger, *Organizers, Presiding*

8:30 Introductory Remarks.

- 8:40 POLY 159.** Stability of substituted benzyltrimethyl ammonium cations in caustic environments. **M.R. Sturgeon**, H. Long, C. Macomber, D.M. Knauss, Y. Yang, B.S. Pivovar
- 9:10 POLY 160.** Interplay between relaxations and structure in anion-exchange membranes (AEMs). **V. Di Noto**, G. Nawn, K. Vezzù, F. Bertasi, E. Negro, S. Lavina, A. Maes, A.M. Herring, S. Ertem, E. Coughlin
- 9:30 POLY 161.** Hydroxide conductive benzyltrimethylammonium functionalized polysulfone-polyformal multiblock copolymers for alkaline fuel cells. **D.J. Strasser**, D.M. Knauss
- 9:50 POLY 162.** Understanding ionomer thin films. **A.Z. Weber**, A. Kusoglu, S. Shi, M. Testfay
- 10:20** Intermission.
- 10:35 POLY 163.** Diffusion NMR as a tool for understanding ion and solvent transport in anion exchange membranes. **H. Sarode**, Y. Yang, A.M. Herring
- 10:55 POLY 164.** Hydroxide degradation mechanism for cations in anion exchange membranes: A computational study. **H. Long**, B.S. Pivovar
- 11:15 POLY 165.** Polymer materials for energy applications: Structure-function studies of porous polymers. **S. Sivaram**
- 11:35 POLY 166.** Carbon/zirconia/fluoroionomer nanocomposites as polyelectrolyte-membrane fuel cell electrocatalyst support. **S.E. Creager**, J.A. Shetzline

Section C

Sheraton Denver Downtown Hotel
Plaza Court 8

Undergraduate Research in Polymer Science

Financially supported by Sabc Innovative Plastics, IAB (ACS Polymer Division Industrial Advisory Board)

- S. E. Morgan, S. I. Nazarenko, *Organizers, Presiding*
- 8:00 POLY 167.** Hydrolytically stable bio-adaptable thiol-ene network. **D.A. Zomorano**, R. Reit, D. Simon, B.R. Lund, T. Ware, W. Voit
- 8:15 POLY 168.** Synthesis of p(NIPAM)-p(DMA) copolymers for protein conjugation. **D. Park**, M.N. Zhou, J.W. Lowe, K. Chiu, S.L. Goh
- 8:30 POLY 169.** Protein adsorption characteristics of amphiphilic starch-containing hybrid polymer films. **A.R. Linehan**, A. Sengupta, P.M. Iovine
- 8:45 POLY 170.** Expanding the one step acid hydrolysis/Fischer esterification of cellulose nanocrystals. **S. Spinella**, V. Hepworth, A. Maiorana, Q. Qian, R.A. Gross
- 9:00 POLY 171.** Design and synthesis of pH-responsive polymers to aid in cancerous tumor detection. **K. Farquhar**, L. Zhu, S.G. Boyes
- 9:15** Intermission.
- 9:30 POLY 172.** Antioxidant copolymers in biological applications. **D.M. Barber**, T.A. Brenner, L. Qiao, S.L. Goh
- 9:45 POLY 173.** Fabrication of conducting polymer/silk composite films with topographically nanopatterned surfaces. **N. Ostrovsky-Snyder**, S. Severt, J. Larson, A. Murphy
- 10:00 POLY 174.** Synthesis of hollow polydimethylsiloxane microspheres. **S.J. Fuchs**, J.M. Rankin, K.S. Suslick
- 10:15 POLY 175.** Synthesis of resorcinarene-core polylactide/polyethylene glycol star block copolymers using click chemistry: Optimizing polymer coupling reactions using No-D NMR spectroscopy. **W.H. Horn**, A.E. Tipton, P.S. Corbin
- 10:30 POLY 176.** Shrinkage stress in two-stage reactive polymer systems. **B. Earle**, S. Chatani, M. Podgorski, C. Bowman
- 10:45 POLY 177.** Investigation of trans-1,4-polyisoprene as an organogelator for organic solvents. **P.G. Thomas**, K.A. Cavicchi

Section D

Sheraton Denver Downtown Hotel
Governor's Square 9

General Topics: New Synthesis & Characterization of Polymers

- B. Barkakaty, D. Garcia, *Organizers*
K. M. Miller, T. Yokata, *Presiding*
- 8:00 POLY 178.** Michael addition polyester networks from imidazolium and 1,2,4-triazolium polymerizable ionic liquids. **K.M. Miller**
- 8:20 POLY 179.** Novel polyurethane/polyhydroxyurethane hybrid polymers and their applications as elastomers and adhesive bonding agents. **E.K. Leitsch**, W.H. Heath, J.M. Torkelson
- 8:40 POLY 180.** Polyurea glycopolymers from lactose and mannose modified-diamines with different diisocyanate comonomers: Synthesis and anticoagulant properties. **Y. Huang**, M.A. Shaw, E.S. Mullins, N. Ayres
- 9:00 POLY 181.** Novel poly(borosiloxane)s and their properties. **P. Puneet**, R. Vedrajan, N. Matsumi
- 9:20 POLY 182.** Reverse anomeric effect (RAE)-mediated syntheses of sugar poly(orthoesters). **L. Li**, K. Knickelbein, J. Wang, M.J. Obrinske, W. Du
- 9:40 POLY 183.** New monomers and catalysts for nonisocyanate polyurethanes. **R. Lambeth**
- 10:00 POLY 184.** Synthesis of biodegradable conjugated polymers with controlled backbone flexibility. **T. Yokata**, J. Moon
- 10:20 POLY 185.** Baylis-Hillman reaction as a versatile platform for the synthesis of densely functionalized polymers. **A. Joy**, C. Peng
- 10:40 POLY 186.** Redox-switchable copolymerization reactions. **J. Byers**, A.B. Biernesser, K. Delle Chiaie, J. Curley
- 11:00 POLY 187.** Reverse-selective gas separation membranes based on segmented copolymers of PEO and ipitycene-containing polyimides. **R. Guo**, S. Luo, G. Kline
- 11:20 POLY 188.** Donor-acceptor conjugated polymers with modular electronic properties and very narrow band gaps. **J.D. Azoulay**, B. Zhang

Section E

Sheraton Denver Downtown Hotel
Directors Row I

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

8:30

- 8:30** Introductory Remarks.
- 8:35 POLY 189.** Polymer separations utilizing 2D liquid chromatography: Inherent limitations and perspectives. **M.R. Schure**
- 9:15 POLY 190.** Computational/theoretical studies of polymer separations by liquid chromatography at critical condition (LCCC). **Y. Wang**
- 9:45 POLY 191.** Framework for exploring the effect of physical and chemical heterogeneities on polymer-surface interactions. **C.R. Snyder**, C.M. Gutman, E.A. Di Marzio
- 10:15** Intermission.
- 10:30 POLY 192.** Measurement of the surface interaction of solvated chains via model end-tethered polymer layers and self-consistent field theory. **R. Sheridan**, S.V. Orski, R.L. Jones, S. Satija, K. Beers
- 11:00 POLY 193.** Computations related to nanoparticle characterization and nanocomposite property estimation. **F. Vargas-Lara**, A. Hassan, E.J. Garboczi, J. Douglas
- 11:30 POLY 194.** Monovalent counter-ion mediated self-assembly of dendrimers. **S. Eghesadi**

TUESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Governor's Square 14

Carl S. Marvel Creative Polymer Chemistry Award in Honor of Todd Emrick

M. Jeffries-El, T. P. Russell, *Organizers*
R. C. Hayward, J. Pyun, *Presiding*

- 1:30 POLY 195.** Surface modification of porous polymer membranes to reduce fouling by oil/water emulsion. **B.D. Freeman**
- 2:00 POLY 196.** Micelle engineering via crystallization-driven self-assembly. **I. Manners**
- 2:30 POLY 197.** Tuning dispersion of nanoparticles in polymer matrices. **R.C. Hayward**
- 3:00 POLY 198.** Getting dopey with polymers and nanoparticles. **J. Pyun**
- 3:30 POLY 199.** New approaches to designer polymers. **C.J. Hawker**
- 4:00 POLY 200.** Structuring liquids with nanoparticles. **M. Cui**, T. Emrick, C. Huang, T.P. Russell
- 5:00 POLY 201.** Tailoring polymer synthesis for materials and devices. **T. Emrick**
- 5:30** Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

Cosponsored by PMSE

S. T. Iacono, *Organizer*

S. Claron, A. Sellinger, *Organizers, Presiding*

- 1:30 POLY 202.** Method of fabricating perfluorosulfonimide (PFSI) electrolyte materials. **J.S. Thrasher**, T.S. Saylor, A.V. Matsnev, R.E. Fernandez
- 2:00 POLY 203.** Highly conductive alkaline poly(phenylene oxide) poly(vinyl benzyl trimethyl ammonium) diblock membrane for anion exchange membrane fuel cell applications. **T.P. Pandey**, M.W. Liberatore, A.M. Herring
- 2:20 POLY 204.** Diblock copolymers of poly(2,6-dimethyl-1,4-phenylene oxide)-*b*-poly(vinylbenzyltrimethylammonium) prepared by nitroxide mediated polymerization for anion exchange membranes. **Y. Yang**, D.M. Knauss
- 2:40 POLY 205.** Transport and morphology of polymerized ionic liquid block copolymer anion exchange membranes with various cations. **K.M. Meek**, F.L. Beyer, Y.A. Elabd
- 3:10** Intermission.
- 3:25 POLY 206.** High-modulus, high-conductivity nanostructured polymer electrolyte membranes via polymerization-induced phase separation. **M.W. Schulze**, L.D. McIntosh, M.A. Hillmyer, T.P. Lodge
- 3:45 POLY 207.** Morphology and transport in a tris(2,4,6-trimethoxyphenyl) phosphonium functionalized PPO for alkaline fuel cells. **Y. Liu**, B. Zhang, Y. Yang, S. Seifert, Y. Yan, M.W. Liberatore, A.M. Herring
- 4:05** POLY 208. Withdrawn.
- 4:25 POLY 209.** Ion transport in polymer electrolyte membranes for state of the art energy conversion technologies. **A.M. Herring**, G.A. Voht, T. Witten, E.B. Coughlin, D.M. Knauss, Y. Yan, M.W. Liberatore

Section C

Sheraton Denver Downtown Hotel
Plaza Court 8

Undergraduate Research in Polymer Science

Financially supported by Sabc Innovative Plastics, IAB (ACS Polymer Division Industrial Advisory Board)

S. E. Morgan, S. I. Nazarenko, *Organizers, Presiding*

- 1:30 POLY 210.** Rheological and morphological characterization of fractionated rigid-rod sulfone polymers. **J. Tropp**, K.M. Knauer, S.E. Morgan

- 1:45 POLY 211.** Improving flame resistance and softness of cotton fabric with ultrasonication rinsing of multilayered nanocoating. **M. Krecker**, T. Guin, A. Milhorn, J.C. Grunlan
- 2:00 POLY 212.** Development of hybrid magnetic cylindrical nanoparticles for pollutant remediation in aqueous environments. **S.M. Ward**, A. Pavia-Sanders, J.A. Flores, J.D. Russell, K.L. Woolley
- 2:15** Intermission.
- 2:30 POLY 213.** Dynamic topology of thermally-responsive materials via Diels-Alder chemistry. **M. Markmann**, M.R. Martinez, E.D. Crenshaw, T. Klein, P.J. Costanzo
- 2:45** POLY 214. Withdrawn.
- 3:00 POLY 215.** Strategies for recovery of Ru catalyst residues in olefin metathesis reactions. **W. Guzman**, J. Suriboot, J. Andrews, D. Bergbreiter
- 3:15 POLY 216.** Synthesis and characterization of a block copolymer containing and self-immolative block. **A. Engler**, A. Lane, C.G. Willson
- 3:30** Intermission.
- 3:45** Panel Discussion.

Section D

Sheraton Denver Downtown Hotel
Directors Row E

Polymer Composites and High Performance Materials

Functional High Performance Polymers

J. W. Gilman, M. Meador, M. Meador, S. E.

Morgan, D. Savin, *Organizers*

J. Woodcock, *Presiding*

- 1:30 POLY 217.** Interactions between structure and properties that control moisture uptake in high-performance polycyanurates. **A.J. Guenther**, M. Wright, A. Chafin, J.T. Reams, K.R. Lamson, M.D. Ford, S.P. Kirby, J.J. Zavala, V. Vij, J.M. Mabry
- 2:00 POLY 218.** Tuning the glass transition temperature and energy damping capabilities of thiol-ene theroset networks. **O. McNair**, A. Janisse, D.A. Savin
- 2:30 POLY 219.** Alternative high performance polymers for ablative thermal protection systems. **T. Boghozian**
- 2:50 POLY 220.** Versatile conjugated polymer/di-ureasil hybrid materials: From enhanced emission quantum yields to white light emission. **N. Willis-Fox**, A. Marques, M. Kraft, U. Scherf, H. Burrows, R.C. Evans
- 3:10 POLY 221.** Intrachain radical chemistry as a facile route to well-defined polymeric nanostructures. **E.B. Berda**, J. Dickinson, J. Cole
- 3:40 POLY 222.** Oxygen permeation and theroset degradation with temperature. **M.C. Celina**, N. Giron, A. Quintana
- 4:10 POLY 223.** Improving mechanical properties of highly branched perfluorinated polymer membranes. **M.J. Quast**, A.D. Argall, C.J. Hager, A. Mueller
- 4:30 POLY 224.** Development of flexible polyimide-urea aerogels cross-linked with a triisocyanate. **B.N. Nguyen**, M. Meador

Section E

Sheraton Denver Downtown Hotel
Directors Row J

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

1:30

- 1:30** Introductory Remarks.
- 1:35 POLY 225.** Asymmetric flow field flow fractionation: An effective separation technique for polymers for which SEC/GPC fails. **S. Podzimek**

- 2:15 POLY 226. Root causes of molecular weight loss of poly(cyclic butylene terephthalate) in pCBT/clay nanocomposites during processing. J.W. Lyons, J.J. Kiefer
- 2:45 POLY 227. Leveraging polymer separation science to design new materials. S. Moyses, R.W. Allen, N. Jesterl
- 3:15 Intermission.
- 3:30 POLY 228. Monitoring kinetics of polymeric processes. M.F. Drenski, C.A. McFaul, A.M. Alb, F. Twigg, C. Jarand, W.F. Reed
- 4:00 POLY 229. Polymeric antileaching agents that facilitate homogeneous catalysis. M.L. Harrell, C. Torres-Lopez, G. Gonzalez, D.E. Bergbreiter
- 4:30 POLY 230. Combined hydrophobic/oleophobic membrane separation and extraction for fuel treatment. A.J. Guenther, J.T. Reams, K.T. Greeson, K.R. Lamison, A.S. Vam, S.P. Kirby, A. Kota, G. Kwon, A. Tutaja, J.M. Mabry
- 5:00 POLY 231. Surface patterning of ultrafiltration membranes to mitigate particulate and protein fouling. S. Maruf, Y. Ding, A.R. Greenberg, J. Pellegrino

TUESDAY EVENING

Section F

Colorado Convention Center
Hall D

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys

Cosponsored by PRES

Financially supported by Kuraray, Avery Dennison, Bayer MaterialScience, 3M

J. C. Grunlan, M. Priolo, L. Wagberg, Organizers

6:00 - 8:00

- POLY 232. Polyethylene-based composites containing graphene platelets: Enhanced barrier and electrical properties via multilayer coextrusion and interdiffusion. K.P. Meyers, J.J. Decker, D.R. Paul, D.A. Schiraldi, S.I. Nazarenko
- POLY 233. Investigating the reactivity of aluminum-based thermites with PFPE additive. J.M. McCollum, M. Pantoya, S.T. Iacono
- POLY 234. Effect of reinforcement fabrics on free standing thin film thermite mechanical properties and combustion. B. Clark, M. Pantoya, R. Heaps, M. Daniels
- POLY 235. Polyketone nanocomposite with non-covalently functionalized graphene for enhanced moisture barrier property. I. Jeon, T. Lee, J. Cho
- POLY 236. Inter- and Intra- molecular interactions in some oligoethylenes and ethylenedioxythiophenes: X-ray single crystal structural analysis. P.T. Pham, M.M. Bader
- POLY 237. Molecular modeling of electrical and thermal resistance across carbon nanotube and graphene nanoribbon contacts. B.L. Farmer, V. Vasrney, S. Shenogin, J. Lee, A.A. Voevodin, A.K. Roy
- POLY 238. Withdrawn.
- POLY 239. Improved dielectric breakdown strength of nanocomposites containing surface modified fillers. M.H. Bell, M. Mohammadkhani, B.C. Benicewicz, T. Krentz, Y. Huang, L. Schadler, S. Vitanen
- POLY 240. Energy transport in molecules with repeating units occurs ballistically. N. Rubtsova, C.M. Nyby, H. Zhang, J. Jayawickramarajah, I.V. Rubtsov

Section F

Colorado Convention Center
Hall D

Energy and Materials

Cosponsored by ENFL and PMSE

S. Clarson, S. T. Iacono, A. Sellinger, Organizers

6:00 - 8:00

- POLY 241. Synthesis of dendronized polymers and their self-assembly to nanostructured materials. P.E. Guzmán, R.H. Grubbs

- POLY 242. Effects of Confinement on Structure and Proton Conductivity of PFSA. V. Sim, W. Han, S.A. Ferdousi, K.L. Yeung
- POLY 243. Design and synthesis of stable angular polycyclic aromatic hydrocarbons. J.T. Ly, L. Zhang, A.L. Briseno
- POLY 244. Preparation of polypyridylruthenium light harvesting polymers and application in water oxidation catalyst assembly. J. Jiang, G. Leem, Z. Chen, T. Pho, S. Keinan, Z. Fang, E. Puodziukynaite, J.R. Reynolds, K.S. Schanze
- POLY 245. Development and characterization of layer-by-layer assembled ferrocene polymer/enzyme films for usage as biofuel cell anodes. N.P. Godman, J. DeLuca, D. Schmidtke, D.T. Glatzhofer
- POLY 246. Synthesis and characterization of semifluorinated polyarylene copolymers. S.M. Budy, J. Jin, D.A. Loy, S.T. Iacono
- POLY 247. Bandgap tuning of silicon quantum dots using organic surface ligands. R. Anderson, J. Bell, B. Gorman, A. Sellinger, M. Lusk
- POLY 248. Synthesis and characterization of water stable, silicoticungstic acid functionalized perfluorocyclobutyl polymer electrolyte. A. Motz
- POLY 249. Cyclopentadiene-containing π -conjugated polymers. L. Chen, A. Pietrangelo
- POLY 250. Modifying the bandgap of ITO and ZnO by 2eV using novel conjugated aromatic phosphonic and carboxylic acid ligands. B.W. McNichols, U. Koldemir, J.L. Braid, A. Morgenstern, M.E. Eberhart, R.T. Collins, D.C. Olson, A. Sellinger

Section F

Colorado Convention Center
Hall D

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by IAB (ACS Polymer Division Industrial Advisory Board)

H. N. Cheng, Organizer

C. J. Ellison, C. J. Landry-Coltrain, Organizers

6:00 - 8:00

- POLY 251. Fluorescence conjugated microporous polymers with amino receptors as metal cation chemosensor. A. Chen, J.L. Duffy-Matzner, W.E. Bernier, W.E. Jones
- POLY 252. Roles of quinoidal character, regularity, and polydispersity in determining the photovoltaic performance of conjugated copolymers. T. Zheng, L. Yu
- POLY 253. Magnetic core-fluorescent conjugated polymer shell nanoparticles prepared by surface-initiated Kumada polymerization. S. Chatterjee, C. Rosu, P.S. Russo, E.E. Nesterov
- POLY 254. Fast initiating nickel precatalysts for π -conjugated polymer synthesis. A.O. Hall, S. Lee, A.J. McNeil
- POLY 255. Growing green polymers using the sun: Organocatalyzed photoredox mediated polymerization. J.C. Theriot, G. Miyake
- POLY 256. Oximes as eversible links in polymer chemistry: Dynamic macromolecular stars. S. Mukherjee, A. Bapat, M. Hill, B.S. Sumerlin
- POLY 257. Molecule to morphology chirality-transfer in ABC triblock terpolymers. A. Sarkar
- POLY 258. Solid-state self-assembly: For advanced functional materials. Y. Kim, N. Kotov
- POLY 259. How processing affects dispersion and thermomechanical properties of waterborne epoxy and cellulose nanocrystal composites. N. Girouard, J.C. Meredith, M. Shofner, G. Schuenneman
- POLY 260. Functional polymers via post-polymerization modification of poly(methionine). E.G. Gharakhnian
- POLY 261. Withdrawn.

Section F

Colorado Convention Center
Hall D

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, T. Saito, Organizers

6:00 - 8:00

- POLY 262. One-step synthesis of poly(oxazoline)-based amphiphilic block copolymers using a dual initiator for RAFT polymerization and CROP. Y. Yu, J. Youk
- POLY 263. New binuclear α -diimine nickel catalysts for ethylene polymerization. A.A. Alsaygh
- POLY 264. Preparation of helical star polymers using tris-nickel Initiators. D.A. Siriwardane, J.F. Reuther, B.M. Novak
- POLY 265. Novel styrene sulfonate copolymer and its application. S. Ozoe
- POLY 266. Synthesis, morphological behavior, and ODT of poly(cyclohexadiene)-based copolymers. K. Mischronis, J. Chen, K.J. Kakh, A. Imel, M.D. Dadmun, J.G. Kennemur, F.S. Bates, J.W. Mays, K. Hong, A.T. Avgeropoulos
- POLY 267. Synthesis and facile end-group quantitation of functionalized PEG azides. J.E. Semple, B.T. Sullivan, K.N. Sill
- POLY 268. Effect of ethers on BF_3 -initiated cationic ring-opening polymerization of glycidol. C.M. Staton, A.A. Chaudhry, E.A. Shcherbina, L.A. Searcy, A.T. Royappa
- POLY 269. Novel functional copolymers of styrene and alkoxy ring-substituted butyl 2-cyano-3-phenyl-2-propenoates. H. Feng, G.B. Kharas
- POLY 270. Chain-growth condensation rigid rod polymer brushes: Design and synthesis of a new polymer brush technique. F.C. Prehn Jr, S.G. Boyes
- POLY 271. Chemical reactivity of hydroxyl end-groups in bis-MPA based hyperbranched polymers. M. Syed, S. Nazarenko
- POLY 272. Comb-type triblock copolymers synthesized by RAFT polymerization and their capability for heavy crude oil emulsification. J. Huang, J. Xu, K. Chen, T. Wang, C. Cui, R. Zhang, L. Li, X. Guo
- POLY 273. Polymerization of PEEK AB monomers with oxyalkylene linkages via NAS and Friedel-Crafts reactions. S. Hennelly, W.A. Feld
- POLY 274. Synthesis of eumelanin-inspired polyindoles. K. Sachinthan, T.L. Nelson
- POLY 275. Synthesis of fluorescently labelled sodium polystyrenesulfonate via atom transfer radical polymerization. P. Balding, A.M. Blake, P.S. Russo, W. Huberty, R. Cueto
- POLY 276. Cyclic polymers via a solid-supported ruthenium-based metathesis catalyst system. J.P. Edwards, R.H. Grubbs
- POLY 277. Synthesis and characterization of eumelanin-inspired ethynylene-linked polymers. S. Adhikari, S. Selvaraju, T.L. Nelson
- POLY 278. Synthesis and characterization of alkoxy-functionalized polyselenophenes. D. Khambhati, T.L. Nelson
- POLY 279. Withdrawn.
- POLY 280. Broad spectrum antimicrobial effectiveness for synthetic mimic of antimicrobial peptides. A.L. Fogel, S.E. Exley, G. Sahukhal, B. Abel, M.O. Elarsi, C.L. McCormick, S.E. Morgan
- POLY 281. PEGylated Q_7 -riched enzyme conjugatable polymer for long-term high performance electrochemical glucose sensors. Z. Li, S. Vaddiraju, F. Papadimitrakopoulos
- POLY 282. Biodegradable, functional polyesters for fused deposition modeling. K. Dube, M. Guvendiren, V.B. Damodaran, J.B. Kohn
- POLY 283. Regulation of protein properties via site-specific polymer conjugation. L. Wang, X. Li, H. Wang, L. Yuan, H. Chen
- POLY 284. Toward side-selective modification of microdialysis sampling polyethersulfone (PES) membranes. S. Phillips, J. Stenken
- POLY 285. Tuning the physical properties of poly(arylene ether)s prepared from 3,5-difluorobenzenesulfonamides. R. Mitton, E. Fossum

POLY 286. Triplet-triplet annihilation upconversion from rationally designed polymeric emitters with tunable interchromophore distances. X. Yu, X. Cao, X. Chen, N. Ayres, P. Zhang

POLY 287. Investigating the effects of a low refractive index counter-diffusive component in two-chemistry holographic photopolymer. M. Alim, B. Kowalski, C. Bowman, R. McLeod

POLY 288. Polycraft: polymer chemistry in the evolving paradigm of education. S. Parker, B.R. Lund, W. Voit

POLY 289. Chemo- and stereoselective polymerization of polar divinyl monomers by metallocenium catalysts. F. Vidal, E.Y. Chen

POLY 290. Starch-containing hybrid polymers: Studying protein adsorption via quartz crystal microbalance with dissipation (QCM-D). A. Sengupta, A.R. Linehan, P.M. Iovine

POLY 291. Synthesis and characterization of new low band gap polymers containing ethyl and phenyl ester functionalized polythiophene derivatives. D.M. Shircliff, B.M. Boardman

POLY 292. Renewable polymers derived from ferulic acid, biobased diols and fatty acid derivatives via ADMET. I. Barbara, A.L. Flourat, F. Allais

POLY 293. Electrochemical redox-unlocked smart polymeric ring. A. Feng, L. Peng, J. Yuan

POLY 294. Study of polymer dynamics in linear low density polyethylene by solid state NMR. L. Caire da Silva, R. Graf, C. Bowers, K.B. Wagener

POLY 295. Water based PEDOT conducting coating. X. Liu, J. Shen, Y. Feng, C. Ma, Z. Xiao, T. Fan, S. Tong, W. Zeng, Y. Liu, Y. Min

POLY 296. Synthesis of shell-crosslinked nanoparticles from polyhydroxylsaccharides block-poly lactides. J. Wang, L. Li, M. Obrinske, L. Bitterman, W. Du

POLY 297. Development of graphene/polyurea nanocomposites based on admicellar polymerization. T. Karim

POLY 298. Flocculation of emulsified oil using a novel amphiphilic and cationic chitosan-based flocculant. T. Lyu, H. Zhao

POLY 299. Effects of Fullerene Chain Ends on Polymer Reptation. A. Zhou, R. Chen, S. Li, X. Sun, Y. Mi, X. Wang

POLY 300. Large molecule incorporation into polyimide aerogel matrix for enhanced aerospace application. S.L. Vivod, M.B. Meador, C.R. Pugh

Section F

Colorado Convention Center
Hall D

Innovations in Macromolecular Network Chemistry

Cosponsored by PMSE

B. R. Lund, L. M. Stratton, A. J. Guenther Organizers

6:00 - 8:00

- POLY 301. Novel chlorine-containing hypercross-linked polymers as adsorbent for removing organic pollutants from humid streams. W. Wang, C. Wang, K. Wang, J. Chen, Z. Liu, Z. Hao, Z. Liu
- POLY 302. Control of kinetics and stress development in polymer networks with acrylated vs. methacrylated polymer nanoparticles. P.K. Shah, J.W. Stansbury
- POLY 303. Light controlled thiol-Michael addition initiated by photocaged superbases. X. Zhang, W. Xi, S. Chatani, M. Podgorski, C. Bowman
- POLY 304. Synthesis of a biocompatible hydrogel platform for drug delivery using oxime click chemistry. K.A. Gilmore, D.B. Beezer, D.M. Stevens, E.A. Delesky, E.M. Harth
- POLY 305. Thiol-vinyl sulfone and thiol-vinyl sulfone-isocyanate crosslinking reactions to generate glassy and tough network polymers. M. Podgorski, D. Nair, E. Becka, C. Bowman

- POLY 306.** Thiol-alkyne photopolymerization in miniemulsion: A facile route to functional polymer nanoparticles. **D.N. Amato**, D.A. Amato, M. Brei, R.F. Storey, D.L. Patton
- POLY 307.** Visible-light initiator with potential for bottom-up photocuring. **S. Lewis**, M. Barros, K. Sarao, M. Makhlja, J.W. Stansbury
- POLY 308.** Toward "green" thermosets: Characterization of poly(alkylene mercaptosuccinates). **G. Sternhagen**, N. Levenhagen, J.P. Droske
- POLY 309.** Studies on the synthesis and ion conductivities of sp³-hybridized boron-linked macrocycle-based covalent-organic network. **Y. Du**, H. Yang, W. Zhang

Section F

Colorado Convention Center
Hall D

Interacting with the Immune System using Polymeric Systems

B. De Geest, A. P. Esser-Kahn, *Organizers*

6:00 - 8:00

- POLY 310.** Light controlled activation of immune cells via photocaged NOD1 agonist. **A.C. Chon**, A. Esser-Kahn
- POLY 311.** Effect of spatially predetermined agonist presentation on immune response via polymeric systems. **K. Ryu**, K. Slowinska, R. Mancini, A.P. Esser-Kahn
- POLY 312.** Synthesis of a photocaged NOD2 agonist for stimulation of innate immune cells. **A.M. Dark**, A. Esser-Kahn
- POLY 313.** Enhancing CpG immunotherapy in brain cancer through improved delivery. **E. White**, D. Alizadeh, B. Badie, J.M. Berlin

Section F

Colorado Convention Center
Hall D

Macromolecular and Nanoparticle Separation Science

Joint POLY/PMSE Poster Session

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, Green Materials – ICE Science, University of Dallas

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers*

6:00 - 8:00

- POLY 314.** Use of high speed/high resolution size based chromatographic separation of polymeric materials with micro viscometric detection. **M.J. O'Leary**
- POLY 315.** Online coupling of specialty detectors in GPC for chemical and molar mass detection. **J.A. McConville**, D. Lohmann, T. Hofe, M. Cudaj, G. Guthausen, M. Wilhelm
- POLY 316.** Carbohydrate based hyper cross-linked organic polymers with -OH functional group for CO₂ separation. **H. Li**, B. Meng, S.M. Mahurin, S. Chai, D.C. Baker, H. Liu, S. Dai

Section F

Colorado Convention Center
Hall D

Next Generation Smart Materials

Cosponsored by PMSE†

Y. C. Simon, E. B. Berda, J. Foster, *Organizers*

6:00 - 8:00

- POLY 317.** Flexible SiO₂ nanofilms assembled on poly(ethylene terephthalate) substrates through a room temperature fabrication process. **S. Yamamoto**, K. Sonobe, M. Mitsuishi, T. Miyashita
- POLY 318.** Degradable nanoparticles for light-assisted cancer invasion inhibition. **H. Chong**, S. Wang
- POLY 319.** 3D printing of mechanochromic polycaprolactone on entry-level printers. **G.I. Peterson**, M.B. Larsen, M. Ganter, D. Storti, A.J. Boydston

- POLY 320.** Nature-inspired intramolecular cyclization for fast light-triggered nanogel degradation. **C. de Gracia Lux**, J. Lux, G. Collet, S. He, M. Chan, J. Olejniczak, A. Almutairi
- POLY 321.** Supramolecular polymers synthesized by thiol-ene click polymerization from supramonomer. **Q. Song**, F. Li, L. Yang, Z. Wang, X. Zhang
- POLY 322.** ROS responsive tellurium-containing hyperbranched polymer. **R. Fang**, W. Cao, X. Zhang, H. Xu
- POLY 323.** Endothelial cell attachment on shape memory polymer surfaces. **T. Govindarajan**, R. Shandas
- POLY 324.** Interfacial fabrication of functional supramolecular polymeric networks for photocatalysis. **B. Yuan**, H. Yang, Z. Wang, X. Zhang
- POLY 325.** Cooperative effect of cucurbit[8]uril-based π-π interaction. **Z. Huang**, K. Qin, L. Yang, Z. Wang, X. Zhang
- POLY 326.** Withdrawn.
- POLY 327.** Application of bioluminescence resonance energy transfer (BRET) in anticancer and antifungal research. **H. Bai**, S. Wang, X. Zhang
- POLY 328.** Pursuing ordered microphase separation in mixed polymer brushes. **C.K. Simocko**, A.D. Price, D. Huber, A.L. Frischknecht, S. Hur, G.H. Fredrickson
- POLY 329.** Shape memory properties of polymer networks formed using photomediated copper(I)-catalyzed azide alkyne cycloaddition (photo-CuAAC). **M. McBride**, A.D. Baranek, C. Bowman
- POLY 330.** Bioderived polymers prepared from *N*-(acryloyl-2-pyrrolidone)s with ether and thio-ether-based residues. **R. Bhat**, A. Pietrangelo
- POLY 331.** Fabrication and characterization of a radiopaque embolic hydrogel coil. **T. Lee**, H. Song, I. Jeon, J. Cho
- POLY 332.** Novel hydrogelator for the creation of supramolecular structures for biomedical applications. **Y. Gao**, C. Berciu, D. Nicastro, B. Xu, F. Horkay
- POLY 333.** Electrochemical redox responsive micelles based on host-guest interactions and star polymers. **L. Peng**, A. Feng, J. Yuan
- POLY 334.** Production of polymeric composites with self-healing functionality by multi-axis electrospinning. **J. Seyyed Mofared Zanjani**, B. Saner Okan, M. Yildiz, Y.Z. Menciloglu
- POLY 335.** Detecting early metal corrosion via "turn-on" fluorescence in smart epoxy coatings. **D. Ghosh**, W. Ming
- POLY 336.** Withdrawn.
- POLY 337.** Chemistry of MoS₂ solvent-assisted exfoliation: Correlation between moisture and the in-situ formation of reduction species. **R. Vaia**, D. Nepal, L.F. Drummy, K. Park
- POLY 338.** Two-component molecular gels as smart biocompatible soft materials. **J. Miravet**, B. Escuder Gil, C. Berdugo, C. Felip, S. Diaz-Oltra
- POLY 339.** Preparation of neutral color polymeric electrochromic devices using an commercial organic dye. **Y. Zhu**, M.T. Otley, X. Zhang, M. Li, G.A. Sotzing
- POLY 340.** Rationally engineering phototherapy modules of eosin-conjugated responsive polymeric nanocarriers via intracellular endocytic pH gradients. **G. Liu**, S. Liu

Section F

Colorado Convention Center
Hall D

Putting Renewable Polymers to Work

D. Boday, E. C. Hagberg, *Organizers*

6:00 - 8:00

- POLY 350.** Polymeric materials from biomass. **B.M. Upton**, A.M. Kasko
- POLY 351.** Recycle method of waste plastics based on physical degradation theory. **S. Yao**, A. Tominaga, N. Takenaka, N. Oda, H. Sekiguchi, R. Nakano
- POLY 352.** Aluminum(III) isopropoxide initiated polymerization of gluconolactone. **D. Saxon**, J. Scanlon

Section F

Colorado Convention Center
Hall D

Undergraduate Research in Polymer Science

S. E. Morgan, S. I. Nazarenko, *Organizers*

6:00 - 8:00

- POLY 353.** Synthesis, characterization, and optical properties of perfluorocyclic arylamine polymers. **D.B. Barbee**, F. Carty, S.T. Iacono
- POLY 354.** Synthesis, characterization, and utilization of tri(perylene bisimides) as an electron accepting material for polymer solar cells. **M. Roth**, L. Moore, S.E. Morgan
- POLY 355.** Incorporation of Diels-Alder chemistry into polymer matrices via an iminer approach. **E.D. Crenshaw**, M. Markmann, T. Kleine, A.E. London, P.J. Costanzo
- POLY 356.** Development of fluorocyclic silsesquioxanes as model templates for organically modified silica composites. **C. Thrasher**, A.R. Jennings, S.T. Iacono
- POLY 357.** Toward high temperature elastomers based on poly(arylene ether)s derived from 3,5-difluorobenzene sulfonamides. **J. Schmitz**, E. Fossium
- POLY 358.** Tailoring the mechanical properties of conducting polymer films via crosslinking. **B. Farrell**, D. Spence, A. Murphy
- POLY 359.** Optimization silk-polypropylene composite films for use as electromechanical actuators. **J. Larson**, N. Bradshaw, C. Klemke, S. Severt, J. Leger, A. Murphy
- POLY 360.** Molecular weight changing polymers via Diels-Alder chemistry. **M.R. Martinez**, M. Markmann, P.J. Costanzo
- POLY 361.** Investigation of spin coating a thiol-ene/acrylate shape memory polymer for application in thin film flexible devices. **H. Guduru**
- POLY 362.** Investigation of thermally induced microphase separation in dicarboximide functionalized oxanorbornyl diblock copolymers by atomic force microscopy. **T. Kolibaba**, D.A. Waldow

- POLY 363.** Biobased replacements of bisphenol A diglycidyl ether in epoxy resins. **C. Sago**, A. Maiorana, S. Spinella, R.A. Gross
- POLY 364.** Investigation of self-assembled nanomorphologies of functionalized dicarboxide oxanorbornyl diblock copolymers via small angle X-ray scattering and optical birefringence. **J. Rosales**, D.A. Waldow
- POLY 365.** Characterization and toxicity of alanine-based polymeric nanoparticles in *D. tigrina* planarian flatworms. **J.P. Wade**, S. Kumar, S. Taylor, E. Economou-Petrovits, R. Lidberg, P. De, L. Ramakrishnan
- POLY 366.** Synthesis and characterization of novel ethylene oxide functionalized dicarboxide oxanorbornyl polymers for use as a lithium-ion electrolyte support. **D. Smith**, D.A. Waldow

- POLY 367.** Reactivity ratio controlled polycondensation as a route to functional poly(arylene ether ketone)s. **K. Geremia**, E. Fossium
- POLY 368.** Energy efficient, closed-loop, water-free protocol for processing of cellulose with quantitative recovery of an ionic liquid solvent. **D. Smith**, R. Carrazzone, M. Schloder, T.W. Smith
- POLY 369.** Multilayered nanocomposites with high aspect ratio graphene platelets: Controlled interdiffusion and improved gas barrier properties. **M. Otto**, K. Meyers, S.I. Nazarenko

- POLY 370.** Performance evaluation of variable nitrogen containing five membered ring vinyl monomers and acrylonitrile copolymer. **K.L. Denson**, B. Batchelor, S. Mahmood, D. Yang
- POLY 371.** Analysis of thiolene network compatibility with photolithographic solvents. **M. Seymour**, R. Reit, B.R. Lund, W. Voit
- POLY 372.** Modeling of block copolymer thin film behavior between neutral and preferential interfaces. **M. Carlson**, W. Durand, G. Blachut, M. Maher, C.J. Ellison, C.G. Willson

- POLY 373.** Self-assembly of size tagged triblock copolymer brushes via DNA hybridization. **A.H. Spring**
- POLY 374.** Multifunctional polyurethane hydrogels for biomedical applications. **C. Seitz**, M. Nguyen-Kim, J. Borghs, J. Wallenborn
- POLY 375.** Synthesis of jeffamine-based organogels and subsequent characterization using cavitation rheology. **S. Walley**, K.C. Bantz, D.A. Savin
- POLY 376.** Rheological characterization of cementitious mixtures with excess polyethylene oxide. **E. Soltys**, L. Murray, K.A. Erk

Joint PMSE/POLY Poster Session

Sponsored by PMSE, Cosponsored by POLY†

WEDNESDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels
Cosponsored by PMSE†

E. B. Berda, J. Foster, *Organizers*

Y. C. Simon, *Organizer, Presiding*

D. Balkenende, *Presiding*

8:30 Introductory Remarks.

- 8:35 POLY 377.** Thermoresponsive supramolecular hydrogels based on diblock methylcellulose derivatives. **H. Kamitakahara**, A. Nakagawa, T. Takano
- 8:55 POLY 378.** Hollow nanogels and double-shell nanogels with advanced temperature responsiveness. **W. Richtering**, J. Dubbert, M. Karg, J. Pedersen
- 9:15 POLY 379.** Reversible aggregation of smart PEG-PDMAEMA diblock copolymers in aqueous solution. **P. Conor**, E. Stubbs, M. Schneider, D. Karis, E.M. Glogowski
- 9:35 POLY 380.** Shape memory polymer foams through emulsion-templating. **I. Gurevitch**, C. Warwar, M.S. Silverstein
- 9:55 Intermission.**

† Cooperative Cosponsorship

- 10:15 POLY 381.** Bioderived poly(*N*-acryloyl-2-pyrrolidone)s: Structure/property correlations of a novel class of smart materials. R. Bhat, X. Sun, A. Pietrangelo
- 10:35 POLY 382.** Luminescent organoborane polymers for anion detection. F. Jaekle, F. Cheng, F. Guo, P. Chen, F. Pammer
- 10:55 POLY 383.** Liquid infused surfaces assembled by the layer-by-layer process. N. Zacharia, G. Zhu, C. Zhang
- 11:15** Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

- S. Clarson, *Organizer*
S. T. Iacono, A. Sellinger, *Organizers, Presiding*
- 8:30 POLY 384.** Design, synthesis, and characterization of new sulfonated aromatic polyamides as proton exchange membranes for fuel cells. F. Liu, D.M. Knauss
- 8:50 POLY 385.** Effect of hydration on mechanical properties of anion exchange membranes. M. Vandiver, B. Caire, Y. Li, D.M. Knauss, A.M. Herring, **M.W. Liberatore**
- 9:10 POLY 386.** Original blend membranes of partially fluorinated copolymers bearing azole functions with sulfonated PEEK for PEMFC operating at low relative humidity. B.M. Ameduri
- 9:40** Intermission.
- 9:55 POLY 387.** Foldable supercapacitors from triple networks of macroporous cellulose fibers, single-walled carbon nanotubes, and polyaniline nanoribbons. D. Ge, L. Yang, L. Fan, C. Zhang, X. Xiao, Y. Gogotsi, **S. Yang**
- 10:15 POLY 388.** Polymer materials for energy applications: Structure-function studies of porous polymers. S. Sivaram, S. Chatterjee, M. Arukkani
- 10:35 POLY 389.** Synthesis of perfluoropolyether-based electrolytes for lithium-ion battery applications. D. Wong, **J.M. DeSimone, N.P. Balsara**
- 10:55 POLY 390.** Design principles for constructing conducting redox polymer based battery materials. C. Karlsson, H. Huang, L. Yang, X. Huang, M. Stromme, R. Emanuelsson, A. Gogoll, M. Sjödin
- 11:15 POLY 391.** Mechanisms of self-discharge in p-doped conducting polymers. H. Olsson, C. Strietzel, Z. Qiu, M. Stromme, **M. Sjödin**
- 11:35 POLY 392.** Designer nanoporous materials for energy storage and energy conversion applications. A. van Buuren, J. Lee, M. Bagege-Hansen, T. Willey, P.G. Allen, B. Wood, J. Biener

Section C

Sheraton Denver Downtown Hotel
Directors Row E

General Topics: New Synthesis & Characterization of Polymers

- B. Barkakaty, D. Garcia, *Organizers*
Y. A. Elabd, M. R. Van De Mark, *Presiding*
- 8:00 POLY 393.** Mechanochemical degradation of three-arm star polymers: Kinetics and modeling. G.I. Peterson, D. Church, A.J. Boydston
- 8:20 POLY 394.** Impact of alkyl chain length on ion conduction and morphology in polymerized ionic liquid diblock copolymers. J.R. Nykaza, S. Sharick, E. Davis, Y. Ye, K.A. Page, A. Jackson, F.L. Beyer, K.I. Winey, Y.A. Elabd
- 8:40 POLY 395.** Investigating the crystallinity of polytetrafluoroethylene (PTFE) by using terahertz time-domain spectroscopy (THz-TDS). F. Senna Vieira, C. Pasquini
- 9:00 POLY 396.** Application of single-chain polymer nanoparticles from consecutive ROMP-RCM process. Y. Bai, H. Xing, X. Phang, Y. Lu, S.C. Zimmerman

- 9:20 POLY 397.** High stiffness in aromatic-aliphatic poly(tyrosol carbonate) by hierarchical control over isomer sequence, phase behavior, and chain orientation. S.D. Sommerfeld, S.N. Murthy, Z. Zhang, M. Guvendiren, K. Dube, J.B. Kohn
- 9:40 POLY 398.** Electronic and spintronic properties of poly(3-methylthiophene) polymer brushes. T.W. LaJoi, W. You
- 10:00 POLY 399.** Middle and end labeled PMMA-d3: The effect of chain ends on polymer dynamics. U.N. Arua, F.D. Blum
- 10:20 POLY 400.** Dynamic surface tension comparison of colloidal unimolecular polymers with different hydrophilic groups: Sulfonate, carboxylate, and quaternary amine. M.R. Van De Mark
- 10:40 POLY 401.** Modified ABS for fused filament fabrication 3D printing with improved interlayer adhesion. K. Yang, B. Lund, D. Sydney, C. Thompson, R. Smaldone, W. Voit
- 11:00 POLY 402.** Anomalous thermal characteristics of poly(ionic liquids) derived from 1-butyl-2,3-dimethyl-4-vinylimidazolium salts. T.W. Smith, M. Zhao, F. Yang, D. Smith
- 11:20 POLY 403.** Coordinated experimental and theoretical study of a polydisperse polymer thin film. B.S. Lokitz, R. Kumar, M. Kilbey, S.W. Sides, J. Ankrner, J.F. Browning, B. Sumpter
- 11:40 POLY 404.** Probing the interior of dendronized polymers with solvatochromic *p*-nitroanilino groups. C. Gstrein, A. Schüller, B. Zhang
- 12:00 POLY 405.** Preparation of antibacterial surfaces by liquid-infused nanoporous polymer. M. Okuom, D. Sabatka, **A.E. Holmes**

Section D

Sheraton Denver Downtown Hotel
Directors Row I

Polymer Composites and High Performance Materials

- J. W. Gilman, M. Meador, S. E. Morgan, D. Savin, *Organizers*
M. Meador, *Organizer, Presiding*
- 8:30 POLY 349.** Soft, lightweight conductors from nanoscale carbon. N. Pasquale
- 9:00 POLY 406.** Composites of graphene oxide and poly(vinyl acetate) — Implications for enhanced mechanical behavior. B.K. Khaitwada, K. Bastola, R. Vaidyanathan, F.D. Blum
- 9:30 POLY 407.** Covalent functionalization of graphene-based platelets for tailored solubility and assembly. B. McGrail, B. Rodier, E. Pentzer
- 10:00 POLY 408.** Polymer grafted nanoparticle hybrids: Applications to gas separations and biomimetic materials. S. Kumar, C.J. Durning, B. Benicewicz
- 10:30 POLY 409.** Assemblies of conjugated polymers on carbon nanotubes. L. Zhai
- 10:50 POLY 410.** Improved carbon nanotube fibers through crosslinking and surface modification. R. Rippy, X. Lu, N. Kang, J.W. Mays
- 11:10 POLY 412.** Facile synthesis of controlled, high molecular weight polyacrylonitrile via low temperature RAFT polymerization. J.D. Moskowitz, B. Abel, A.J. Varni, J. Welch, C.L. McCormick, J.S. Wiggins
- 11:30 POLY 413.** Polymer matrix composites using covalently modified carbon nanotube sheets. J.S. Baker, M.A. Meador

Section E

Sheraton Denver Downtown Hotel
Governor's Square 14

Interacting with the Immune System using Polymeric Systems

Molecular Adjuvants

B. De Geest, A. P. Esser-Kahn, *Organizers, Presiding*

8:30 Introductory Remarks.

- 8:40 POLY 414.** Application of multi-agonist scaffolds to modulate antigen presentation and adaptive immunity. J. Tom, A. Esser-Kahn
- 9:00 POLY 415.** NIAID Adjuvant Program: Lessons and insights from the frontiers of vaccine adjuvant research. W. Leitner
- 9:50 POLY 416.** Syntheses and biological evaluation of toll-like receptor-7 agonistic macromolecules. N. Shukla, S.A. David, A. Izzo, C. Hamilton, C. Mutz, D.B. Salunke, P. Gao, R. Balakrishnan, R. Ukani, S. Malladi, T. Day, T. Lewis
- 10:20** Intermission.
- 10:50 POLY 417.** Programming immune responses with polymer carriers of Toll-like receptor (TLR) agonists. G. Lynn, R. Laga, B. Seder, L. Seymour
- 11:20 POLY 418.** Controlling the immune system with light: photo-active TLR agonists. A.P. Esser-Kahn, R. Mancini, L. Stutts, K. Ryu

WEDNESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Next Generation Smart Materials Smart Nanomaterials, Composites, and Gels

- Cosponsored by PMSE†*
- E. B. Berda, J. Foster, Y. C. Simon, *Organizers*
M. A. Ayer, N. Zacharia, *Presiding*
- 1:30** Introductory Remarks.
- 1:35 POLY 419.** New opportunities in viral nanoparticle protein:polymer conjugates. J.D. Wallat, S. Isarov, J. Zhang, **J.K. Pokorski**
- 1:55 POLY 420.** Functionalized macro to micro shape memory materials. V.S. Ashby, K.R. Houston, S. Turner, S.M. Brosnan
- 2:15 POLY 421.** Single-chain nanoparticles via reversible acetal crosslinks. C.K. Lyon, E.B. Berda
- 2:35 POLY 422.** Optically responsive supramolecular glasses. D. Balkenende, C. Monnier, G. Fiore, C. Weder
- 2:55** Intermission.
- 3:15 POLY 423.** Thermally-responsive azo-containing polymeric materials. M.A. Ayer, Y.C. Simon, C. Weder
- 3:35 POLY 424.** Synthesis and phase behavior of alkyne-functionalized di- and triblock copolymers and their cobalt carbonyl adducts. B. Jiang, B. Qian, P. Yu, R.B. Grubbs
- 3:55 POLY 425.** Responsive hydrogels for cells in culture. S. Patil, P. Chaudhury, L. Clariuz, M.J. McDonald, E. Reynaud, P. Gaines, **D.F. Schmidt**
- 4:15 POLY 426.** Helical polypeptides mediated nonviral gene and siRNA delivery. L. Yin, N. Zheng, H. Lu, N. Gbrilsson, K. Kim, X. Deng, R. Zhang, J. Cheng
- 4:35** Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

- S. Clarson, *Organizer*
S. T. Iacono, A. Sellinger, *Organizers, Presiding*
- 1:30 POLY 427.** Organic photovoltaics: Materials microstructure and its effects on device parameters. A. Salleo
- 2:00 POLY 428.** High efficiency BODIPY lamellar organic photovoltaics. J. Chen, S.M. Conron, P. Erwin, M. Dimitriou, K. McAlahney, M.E. Thompson
- 2:20 POLY 429.** Role of linking chemistry on charge separation and photovoltaic performance of all-conjugated block copolymers. J. Mok, Y. Lin, K. Smith, K. Yager, S.B. Darling, D.J. Gosztola, Y. Lee, R. Schaller, E. Gomez, **R. Verduzco**
- 2:40 POLY 430.** Development of a DBfA Ttpe block copolymer for solar energy harvesting. M. Hasib, T.H. Nguyen, S.S. Sun
- 3:00** Intermission.

- 3:15 POLY 431.** All-polymer solar cells. Z. Bao
- 3:45 POLY 432.** Supramolecular polymer/fullerene composite nanofibers for organic photovoltaics. Y. Qin
- 4:05 POLY 433.** Toward conjugated polymer photovoltaic cells from low-cost starting materials. M. Jeffries-El, M. Ewan, A. Bhuwanka, B.J. Hale, E.W. Muller, B.M. Kobilka
- 4:35 POLY 434.** Semi-random donor-acceptor copolymers and terpolymers. W.A. Braunecker, Z.R. Owczarczyk, S.D. Oosterhout, N. Kopidakis, D.C. Olson
- 4:55 POLY 435.** Photon upconverting soft materials. F.N. Castellano

Section C

Sheraton Denver Downtown Hotel
Directors Row E

Innovations in Macromolecular Network Chemistry

Self-healing or Magnetic

- Cosponsored by PMSE*
- B. R. Lund, *Organizer*
A. J. Guenther, L. M. Stratton, *Organizers, Presiding*
- 1:30** Introductory Remarks.
- 1:35 POLY 436.** Oxime-functional hydrogels with tunable gelation and degradation behavior. S. Mukherjee, M. Hill, B.S. Sumerlin
- 2:00 POLY 437.** Reversible dynamic urea bond for the design of functional polymers. H. Ying, Y. Zhang, K. Cai, J. Cheng
- 2:20 POLY 438.** Supramolecular motifs in dynamic covalent PEG-hemiaminal organogel networks. J.M. Garcia
- 2:40 POLY 439.** Malleable and self-healing polymer networks based on dynamic imine bond. A. Chao, D. Zhang
- 3:00** Intermission.
- 3:20 POLY 440.** Emergent cure chemistry in the development of aerospace materials. J.M. Mabry, A.J. Guenther, J.C. Marcischak, T.S. Haddad, J.T. Reams, M.D. Ford
- 3:45 POLY 441.** Charged induced formation of crystalline network polymer. C.T. Yavuz
- 4:05 POLY 442.** Magnetically induced free radical polymerization. M. Soucek, K. Miller, Z. He
- 4:30 POLY 443.** New methods for curing thermally stable polycyanurate networks based on magnetic induction heating of coated nanoparticles. A.J. Guenther, C.M. Sahagun, J.M. Mabry
- 4:50** Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel
Directors Row J

Polymer Composites and High Performance Materials

- Biopolymers, Nanocomposites and Bioapplications**
- J. W. Gilman, M. Meador, M. Meador, S. E. Morgan, *Organizers*
D. Savin, *Organizer, Presiding*
- 1:30 POLY 444.** Structural nanocellulose composites. J.P. Youngblood, S. Chen, J. Liu, R. Moon, G. Schueneman
- 2:00 POLY 445.** Sustainable, high-performance fiber composites. C. Kuncho, J. Möller, W. Liu, E. Reynaud, D.F. Schmidt
- 2:30 POLY 446.** Processing and properties of polymeric nanocomposites with cellulose nanocrystals. C. Weder, A. Nicharat, J. Sapkota, J. Foster
- 3:00 POLY 447.** Hierarchically structured nanocomposites. J.R. Dorgan, C. Moran, B. Liu, R. Sosa, L.O. Hollingsworth
- 3:30 POLY 448.** Stick-slip shear phenomenon of interfaces between cellulose nanocrystals. S. Keten, R. Sinko
- 4:00 POLY 449.** Application of natural fiber welding to the fabrication of biopolymer composite materials. E. Fox, E.K. Brown, L. Haverhals, D. Gray, B. Tisserat, T. Price, M. Brusoski, H.C. De Long, P.C. Trulove

4:30 POLY 450. Ultrastiff nanocomposite hydrogels for biomedical applications. M. Jaiswal, J.R. Xavier, J.K. Carrow, P. Desai, A.K. Gaharwar

Section E

Sheraton Denver Downtown Hotel
Governor's Square 14

Interacting with the Immune System using Polymeric Systems

Immunoengineering

B. De Geest, A. P. Esser-Kahn, *Organizers, Presiding*

1:30 POLY 451. NMR and kinetic studies of nitric oxide loading of poly(acrylonitrile-co-1-vinylimidazole) for advanced wound healing. B. Batchelor, A. Lowe, S. Mahmood, K.J. Balkus, B.M. Novak

1:50 POLY 452. Poly(n-acetylglucosamine)-antigen conjugates induce antigen-specific tolerance. D.S. Wilson, M. Damo, S. Kontos, G. Diaceri, J.A. Hubbell

2:15 POLY 453. Biomaterials for recruitment and differentiation of endogenous regulatory T cells. S. Little

2:45 POLY 454. Polymers for tumor immune therapy: In vitro and in vivo results on multifunctional cylindrical brush polymer conjugates. M. Schmidt, S. Gietzen, J. Buehler, C. Hoertz, M. Schinnerer, K. Fischer, A. Birke, M. Barz, C. Kappel, M. Bros, S. Grabbe

3:10 Intermission.

3:40 POLY 455. Using small molecules to engineer and explore human immunity. D.A. Spiegel

4:10 POLY 456. Modulation of the immune response by lymph node targeting. H. Liu

WEDNESDAY EVENING

Section F

Sheraton Denver Downtown Hotel
Plaza Ballroom AB

POLY/PMSE Plenary Lecture and Awards Reception

Cosponsored by PMSE

D. Boday, M. Jeffries-Ei, T. J. White, *Organizers, Presiding*

5:30 Network.

6:10 Introductory Remarks.

6:15 POLY 457. Celebration of the award winners. K.L. Wooley

7:00 Awards Reception.

THURSDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

Cosponsored by PMSE†

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

C. K. Lyon, N. Zacharia, *Presiding*

8:30 Introductory Remarks.

8:35 POLY 458. Size and rigidity dependent pharmacokinetics and biodistribution of cylindrical polymer brushes. M. Mueller, S.J. Dodds, T. Nguyen, D. Senyushyn, C. Porter, B. Boyd, F. Caruso

8:55 POLY 459. Controlling actuation and locomotion: Geometry-composition-humidity gradient correlations for semiautonomic films. R. Vaia, D.H. Wang, P. Buskohl, L. Tan

9:15 POLY 460. Tuning macroscopic properties using stimuli-responsive ionic liquid monomers. J. Texter

9:35 POLY 461. Synthesis and dual-emissive properties of thiophene-substituted difluoroboron β -diketonates in poly(lactic acid). M. Kolpaczynska, C.A. DeRosa, W. Morris, C. Fraser

9:55 Intermission.

10:15 POLY 462. Directed self-assembly of silicon-containing block copolymers for lithography. M. Maher, C. Rettner, C. Bates, G. Blachut, M. Carlson, W. Durand, J. Cheng, D.P. Sanders, C.J. Ellison, C.G. Willson

10:35 POLY 463. Switchable ultrahydrophobic and superhydrophilic polymer surfaces: Synthesis, characterization, and application. T. Hofe

10:55 POLY 464. Reversible single-chain selective point folding via cyclodextrin driven host/guest chemistry in water. J. Willenbacher, B. Schmidt, D. Schulze-Sinninghausen, O. Altintas, B. Luy, G. Delaitre, C. Barner-Kowollik

11:15 POLY 465. Toward self-healing semiconducting polymers. B.C. Schroeder, Z. Bao

11:35 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

S. Larson, *Organizer*

S. T. Iacono, A. Sellinger, *Organizers, Presiding*

8:30 POLY 466. Light harvesting using colloidal quantum dots and hybrid organic-inorganic materials. E. Sargent

9:00 POLY 467. Preparation of P3HT/CdS nanocomposites via in-situ nanocrystal growth in P3HT amphiphilic block copolymers. M. Kern, C. Tian, S.G. Boyes

9:20 POLY 468. Rational material, interface, and device engineering for high-performance polymer and perovskite solar cells. A.K. Jen

9:50 POLY 469. Synthesis, characterization, and properties of selectively fluorinated conjugated polymers for organic photovoltaics. P. Homyak, E. Coughlin

10:10 POLY 470. Novel hierarchical composites of inorganic carbon and polysiloxanes for next-generation energy applications. J.P. Lewicki, M.A. Worsley, T. Baumann, E.B. Duoss, R.S. Maxwell

10:40 Intermission.

10:55 POLY 471. Structure measurements for organic photovoltaics manufacturing. D. DeLongchamp

11:25 POLY 472. Photoinduced charge transfer and thermal recombination dynamics of a ternary cascade heterojunction composed of poly(3-hexylthiophene), titanyl phthalocyanine, and Buckminsterfullerene. J. Park, O. Reid, G. Rumbles

11:45 POLY 473. Expanding use of photovoltaics in the developing world: The Nanopower Africa and Power Ethiopia projects. G. Beauchage

12:05 POLY 474. Withdrawn.

Section C

Sheraton Denver Downtown Hotel
Directors Row E

Innovations in Macromolecular Network Chemistry

Medical: Hydrogels and Particles

Cosponsored by PMSE

L. M. Stratton, *Organizer*

A. J. Guenther, B. R. Lund, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY 475. Polymeric strategies for the encapsulation of cell lysates in view of anticancer immunotherapy. L. Lybaert, B. De Geest

8:55 POLY 476. Natural p(TA) hydrogel and microgel networks for diverse potential biomedical uses. N. Sahiner, S. Sagbas, M. Sahiner, N. Aktas

9:15 POLY 477. Multiresponsive polymer-protein conjugates as immuno-modulating strategy. N. Vanparijs, R. De Coen, B. De Geest

9:35 POLY 478. Tethered-sphere networks: An ideal platform for property control. T.S. Bailey

9:55 Intermission.

10:15 POLY 479. Printing of polymer hydrogels in micron sizes for the Co- and sequential delivery of drugs. B.R. Spears, D. Stevens, E. Harth

10:55 POLY 480. Cyclic defects in tetrafunctional poly(ethylene glycol) networks and networks with mixed junction functionality. K. Kawamoto, M. Zhong, B.D. Olsen, J.A. Johnson

10:35 POLY 481. Withdrawn.

11:15 POLY 482. Development of hydrogels and functionalized silica surfaces utilizing novel fluorocyclic precursors. A.R. Jennings, C. Thrasher, S.T. Iacono

11:40 Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel
Directors Row I

Polymer Composites and High Performance Materials

Nanoparticles & Nanocomposites

J. W. Gilman, M. Meador, D. Savin, *Organizers*

S. E. Morgan, *Organizer, Presiding*

8:30 POLY 483. Hyperbranched epoxy with POSS modification for enhanced toughness polymer composites. S.E. Morgan, Q. Jin, J. Misasi, J.S. Wiggins

9:00 POLY 484. Stacking intumescent multi-layer thin film onto clay-based nanobrick wall to impart self-extinguishing fire retardant behavior to polyurethane. K.M. Holder, M. Huff, M. Cosio, J.C. Grunlan

9:30 POLY 485. Effect of interfacial modification on the morphology and properties of polybenzimidazole/silica nanocomposite proton exchange membrane for use in fuel cells. S. Singha, T. Jana

9:50 POLY 486. Improvement of mechanical properties of methacrylate based composites by latex particles. B. Sandmann, B. Happ, I. Perevyazko, S. Hoepfner, T. Rudolph, F.H. Schacher, M.D. Hager, U. Fischer, P. Burtscher, N. Moszner, U.S. Schubert

10:10 POLY 487. Properties and synthesis of mixed bimodal nanoparticles via RAFT. T.L. Neely, B. Natarajan, L. Schadler, B.C. Benicewicz

10:40 POLY 488. Development of nanosilica thermoset resins for filament winding and prepreg applications. J.M. Nelson

11:10 POLY 489. Photografting random copolymers to nanoparticles for well-dispersed nanocomposites. A.W. Hauser, R.C. Hayward

11:30 POLY 490. Interface-modified multilayer polymer films for high energy density capacitors. M.A. Wolak, M. Mackey, Z. Zhou, J. Carr, L. Zhu, E. Baer

Section E

Sheraton Denver Downtown Hotel
Governor's Square 14

Interacting with the Immune System using Polymeric Systems

Nanoparticulate Vaccination Strategies

B. De Geest, A. P. Esser-Kahn, *Organizers, Presiding*

8:30 POLY 491. Pollen grains for oral vaccination. H. Gill

9:00 POLY 492. mRNA based strategies for steering and amplifying the adaptive immune response. B. De Geest

9:20 POLY 493. Nanoparticles for brain tumor immunotherapy. J.M. Berlin

9:50 Intermission.

10:20 POLY 494. Modulating adaptive immunity with "carrier-free" polyelectrolyte multilayer films. Y. Chiu, L. Tostanoski, C. Jewell

10:50 POLY 495. Engineering lipid-based vaccine nanoparticles for modulation of immune responses. J. Moon

THURSDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

Cosponsored by PMSE†

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*
M. A. Ayer, D. Balkenende, *Presiding*

1:30 Introductory Remarks.

1:35 POLY 496. Concurrent block copolymer polymersome stabilization and bilayer permeabilization by stimuli-regulated "traceless" crosslinking. X. Wang, S. Liu

1:55 POLY 497. Polymeric nanoparticles from cooperative polymerization and their dynamic behaviors. L. Li, C. Yuan, S. Thayumanavan

2:15 POLY 498. Synthesis and characterization of thermoresponsive, biodegradable polyesters. J.P. Swanson, L.R. Montealeone, F. Haso, T. Liu, P.J. Costanzo, A. Joy

2:35 POLY 499. Depolymerization kinetics and gas capture of polycarbidimides. B.L. Batchelor, J.F. Reuther, B.M. Novak

2:55 Intermission.

3:15 POLY 500. Stimuli-responsive micro porous polymer hydrogels for treatment of severe limb wounds. B.C. Streifel, J. Lundin, G. Daniels, J.H. Wynne

3:35 POLY 501. Enhanced dry adhesion from tapered nanorods and their shape effect. Y. Cho, G. Kim, Y. Cho, S. Lee, H. Minsky, K. Turner, D. Gianola, S. Yang

3:55 POLY 502. To randomize or not to randomize: An investigation into the cell-uptake of polymers. J. Moraes, S. Recalcati, G. Gody, R. Peltier, S. Perrier, H.A. Klok

4:15 POLY 503. Polyelectrolyte exceeding ITO capabilities in flexible electrochromics. Y. Zhu, M.T. Otley, X. Zhang, M. Li, G.A. Sotzing

4:35 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

S. Larson, *Organizer*

S. T. Iacono, A. Sellinger, *Organizers, Presiding*

1:30 POLY 504. Conjugated polymers for energy harvesting, storage and modulation. J.R. Reynolds

2:00 POLY 505. Synthesis and characterization of conjugated fulvene chromophores and polymers. S.M. Budy, K.J. Knuths, A. Davidson, G.J. Balaich, D.W. Ball, S.T. Iacono

2:20 POLY 506. Piezoelectric polymer composites: From energy harvesting to artificial muscles. W. Voit, C. Baur, G. Ellison

2:40 POLY 507. Conductance bistability in non-conjugated polymers: Memristors in neuromorphic applications. S.H. Foulger

3:10 Intermission.

3:25 POLY 508. Bioinspired green nanomaterials (GN) design and manufacture for post-combustion carbon capture and sequestration. S.V. Patwardhan

3:55 POLY 509. Microvascular materials for mass and energy transport. A.P. Esser-Kahn, D.T. Nguyen

4:15 POLY 510. Plastron trapping: Fluorinated surface treatment comparison to maintain stable plastrons under flow. J.R. Alston, M.A. Khan, R. Campos, A.J. Guenther, J.M. Mabry

4:35 POLY 511. Self-repairable polymeric networks that consume carbon dioxide and water. Y. Yang, M.W. Urban

4:55 POLY 512. Safer and more energy efficient antifreeze. E.V. Clancy

[†] Cooperative Cosponsorship

Section C

Sheraton Denver Downtown Hotel
Directors Row E

Innovations in Macromolecular Network Chemistry**Click Chemistries**

Cosponsored by PMSE

A. J. Guenther, *Organizer*

B. R. Lund, L. M. Stratton, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY 513. Functional polymer nanoparticles via thiol-ene nanoemulsion photopolymerization. D.A. Amato, D.N. Amato, A.S. Flynt, D.L. Patton

1:55 POLY 514. Raising the glass transition temperature of thiol-ene networks for dental applications. J. Li, T.F. Scott

2:15 POLY 515. Wide bicontinuous compositional windows from co-networks made with telechelic macromonomers. G.N. Tew

2:35 POLY 516. In situ polymerization of thiol-acrylate nanocomposite polymers with encapsulated stem cells. L.A. Garber, A. Forghani, J.A. Pojman, D. Hayes, R. Daviredly

2:55 Intermission.

3:15 POLY 517. Softening polymer substrates for chronically soft neural interface. W. Voit

3:35 POLY 518. Ester-free thiol-X resin: A new material with enhanced mechanical properties. E. Becka, M. Podgorski, C. Bowman

3:55 POLY 519. Photoinitiated Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC) based networks. A.D. Baranek, H. Song, M. McBride, P. Finnegan, T. Gong, C. Bowman

4:15 POLY 520. High temperature cyanate ester resins from renewable feedstocks: Upgrading through deoxygenation or conversion to hybrid resins. B.G. Harvey, A.J. Guenther, W.W. Lai, A. Chafin, M. Garrison, J. Reams, L. Cambrea, H.A. Meylemans, M.C. Davis

4:35 POLY 521. Renewable furan-based epoxy-amine thermosets. G.R. Palmese

4:55 Concluding Remarks.**Section D**

Sheraton Denver Downtown Hotel
Directors Row J

Polymer Composites and High Performance Materials**Computation and Characterization**

J. W. Gilman, M. Meador, M. Meador, S. E. Morgan, D. Savin, *Organizers*

A. L. Fogel, *Presiding*

1:30 POLY 522. Dielectric spectroscopic analysis of cure behavior and relaxation processes in polymer composites. M.K. Hassan, C.H. Childers, K.A. Mauritz, J.S. Wiggins

2:00 POLY 523. Aligned CNT composites: Quantitative analysis by TEM tomography. J. Liddle, B. Natarajan, T. Lam, R. Sharma, N. Lachman, D. Jacobs, B. Wardle

2:30 POLY 524. Mapping the lyotropic phase behavior of diblock copolymer ionogels. T. Bennett, I. Blakey, K.J. Thurecht, K. Jack

2:50 POLY 525. Spectroscopic Investigations of polyethylene-carbon nanofibers composites. R. Benitez, I. Elamin, B. Jones, L. Jianhua, D. Chipara, K. Lozano, M. Chipara

3:10 POLY 526. Computational design of next generation aerospace material systems. E. Sapper, I. Cole, M. Breedon, D. Winkler, F. Chen, C. Chu

3:40 POLY 527. Connecting molecular to continuum: A multiscale modeling approach using molecular dynamics and finite element analysis to predict composite failure. S.J. Tucker, S. Christensen

4:10 POLY 411. Lignin expanded acrylonitrile-butadiene-styrene (ABS) thermoplastic for composite applications. A.K. Naskar, S.K. Akato, D.L. Erdman

Section E

Sheraton Denver Downtown Hotel
Governor's Square 14

Interacting with the Immune System using Polymeric Systems**Macromolecular Engineering of the Immune Response**

B. De Geest, A. P. Esser-Kahn, *Organizers, Presiding*

1:30 POLY 528. Supramolecular peptide immunomodulators. C. Mora Solano, R.R. Pompano, T. Sun, J. Chen, A.S. Chong, J.H. Collier

2:10 POLY 529. Engineering amphiphiles that target lymphoid tissues and optimally engage immune cells for more effective vaccines. D.J. Irvine

2:50 Intermission.

3:20 POLY 530. Designing novel protein mimics from simple synthetic polymers. G.N. Tew

3:50 POLY 531. Effect of 3D presentation of glycomimetic polymers on lectin interaction. A.M. Kasko, W. Liu, K. Lin

PMSE**Division of Polymeric Materials Science and Engineering**

A. H. Tsou, Q. Lin, C. M. Stafford and M. Becker, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Smart and Responsive Composites from Renewable Building Blocks (*see CELL, Tue, Wed*)

Integrating Chemistry and Polymer Science Research into the Classroom (*see CHED, Mon*)

Energy and Materials (*see POLY, Tue, Wed, Thu*)

POLY/PMSE Plenary Lecture and Awards Reception (*see POLY, Wed*)

Nanotechnology: Delivering on the Promise (*see PRES, Sun, Mon*)

WCC Rising Stars Awards Symposium (*see WCC, Mon*)

SOCIAL EVENTS:

Social Hour: Tue
Reception: Wed

BUSINESS MEETINGS:

Business Meeting: Sun, Mon

SUNDAY MORNING**Section A**

Sheraton Denver Downtown Hotel
Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology**Tutorial: Learnings & Developments**

Y. Men, *Organizer*

R. Jones, A. I. Norman, *Organizers, Presiding*

9:15 Introductory Remarks.

9:30 PMSE 1. Synchrotron facility for characterization of hierarchical structures — from microns to Angstroms in less than 3 minutes. J. Ilavsky

10:00 PMSE 2. Travels in reciprocal space: A tutorial on images, microstructures, scattering, and Fourier transforms. A. Bous, J. Butler

10:30 Intermission.

10:45 PMSE 3. Newest developments and adaptive strategies in laboratory SAXS (and WAXS) for polymer research. S.W. Barton, K. Joensen, S. Skou

11:15 PMSE 4. Size, shapes, and crystalline structure of polymeric materials with a SAXS/WAXS instrument. S. Rodrigues, S. Desvergne-Bleneau, P. Panine, M. Fernandez-Martinez, F. Bossan

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

ACS Award in Applied Polymer Science: Symposium in Honor of Geoffrey W. Coates

W. Dichtel, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 PMSE 5. Polymer brushes: Versatile 2D materials for interface engineering. D. Calabrese, M. Welch, C.K. Ober

9:00 PMSE 6. Fun with block copolymers: New materials and processes using directed self assembly for nanoscale patterning. P.D. Hustad

9:30 PMSE 7. Dynamic complex emulsion droplets. T.M. Swager, L. Zarzar

10:00 Intermission.

10:15 PMSE 8. New strategies for living radical polymerization. C.J. Hawker

10:45 PMSE 9. Pushing the limits of β -diimine-based catalysts for olefin polymerization. B.K. Long, J. Rhinehart, N. Mitchell, L. Brown

11:15 PMSE 10. Controlling sequence, stereochemistry, and functionality in linear polymers prepared by ring-opening metathesis polymerization. M.A. Hillmyer

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC: Journal of Materials Chemistry A, B & C, Soft Matter and Chemical Science

A. J. Boydston, L. M. Campos, K. L. Wooley, *Organizers*

E. Pentzer, *Organizer, Presiding*

8:00 PMSE 11. Challenges facing directed assembly of block copolymers: Nanopatterning at the sub-10 nm scale. J.M. Buriak

8:30 PMSE 12. Efficient intramolecular singlet fission in organic molecules. M. Sfeir, E. Busby, J. Xia, Q. Wu, J. Low, R. Song, J.R. Miller, X. Zhu, L.M. Campos

9:00 PMSE 13. Putting side chains to work in conjugated materials. S.W. Thomas

9:20 Intermission.

9:35 PMSE 14. Functional electronic polymer design. Z. Bao

10:05 PMSE 15. Precursor conversion, nucleation, and growth of colloidal metal phosphide quantum dots. B.M. Cossairt, D. Gary, B. Glassy

10:35 PMSE 16. Efficient syntheses of π -conjugated semiconducting polymers. C.K. Luscombe

11:05 PMSE 17. Chemical transformations in bimetallic nanoparticle alloys. J. Millstone, L. Marbella, C.M. Andolina

Section D

Sheraton Denver Downtown Hotel
Directors Row H

Nanostructured Porous Polymers: Synthesis, Properties Applications**Nanostructured Porous Polymers for Membrane Application**

B. D. Freeman, *Organizer*

D. L. Gin, H. Lin, *Organizers, Presiding*

8:30 PMSE 18. Ion sorption and transport in ion-exchange membranes. B.D. Freeman

9:00 PMSE 19. Controlled assemblies of cyclic peptide-polymer conjugates toward sub-nanometer porous membrane. T. Xu

9:30 PMSE 20. Influence of nanoimprint lithography on the structure and permeability of ultrafiltration membranes. H. Park, H. Kim, H. Yoon, B. Yoo, Y. Cho

10:00 Intermission.

10:30 PMSE 21. CO₂-philic graphene oxide thin film composite membranes. H. Park, H. Kim, H. Yoon, B. Yoo, Y. Cho

11:00 PMSE 22. Iptycene-containing polymeric membranes for efficient gas separation. R. Guo, J. Wiegand, S. Luo

11:30 PMSE 23. Advanced materials and membranes for gas separations. C. Liu

Section E

Sheraton Denver Downtown Hotel
Governor's Square 17

Stimulus-Responsive Assemblies and Materials**Chemical Control of Materials Properties**

J. Cha, A. P. Goodwin, *Organizers*

C. Bowman, *Organizer, Presiding*

8:30 PMSE 24. Supramolecular concepts for patterning hydrogels. A. Nelson

9:00 PMSE 25. Dynamic hydrazone-crosslinked hydrogels provide an adaptable matrix for 3D cell culture. D. Domaille, D. McKinnon, K.S. Anseth, J. Cha

9:30 PMSE 26. Synthesis and evaluation of the thermally-responsive coatings based upon Diels-Alder chemistry and renewable materials. D.N. Amato, G.A. Strange, J.P. Swanson, K.L. Varney, D.V. Amato, P.J. Costanzo

9:50 PMSE 27. "Scaffolded" thermally remendable polymers with improved self-healing capabilities. G. Berg, A.D. Baranek, C. Bowman

10:10 PMSE 28. Incorporation of dithioamide mechanophores into polymeric materials. M. Karman, Y.C. Simon

10:30 Intermission.

10:45 PMSE 29. Optically programmed buckling of polymer nanocomposite gels. R.C. Hayward

11:15 PMSE 30. Damage precursor detection in polymer matrix composites. E.M. Nofen, J. Wickham, J. Zou, A. Chattopadhyay, L. Dai

11:35 PMSE 31. Photolabile layer-by-layer films. S.W. Thomas

Section F

Sheraton Denver Downtown Hotel
Governor's Square 15

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications**Energy Harvesting and Storage**

A. D. Taylor, *Organizer*

G. S. Tulevski, *Organizer, Presiding*

8:30 PMSE 32. Harvesting energy with semiconducting single-walled carbon nanotubes: From photovoltaics to thermoelectrics. J. Blackburn, A. Ferguson, A. Avery, A. Dowgiallo, R. Ihly, K. Mistry, J.C. Johnson

9:00 PMSE 33. Few-walled carbon nanotubes for energy storage. J. Liu

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.

9:30 PMSE 34. Ultrafast spectroscopic signature of charge transfer between single-walled carbon nanotubes and C₆₀. A. Dowgiallo, K. Mistry, J.C. Johnson, J. Blackburn

9:50 Intermission.

10:10 PMSE 35. Influence of nanotube polydispersity on SWCNT-Si solar cells. E. Hobbie

10:40 PMSE 36. Porous graphene from polymer templates and their use in energy storage applications. K. Liu, Y. Chen, Y. Zhu

11:10 PMSE 37. Time resolved microwave conductivity on single-walled carbon nanotube fullerene heterojunctions. R. Ihly, K. Mistry, T. Clikeman, B. Larson, O.V. Boltalina, S.H. Strauss, G. Rumbles, J. Blackburn

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Sponsored by POLY, Cosponsored by PMSE

Macromolecular and Nanoparticle Separation Science

Sponsored by POLY, Cosponsored by ANYL and PMSE

SUNDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

Tutorial: Learnings & Developments

A. I. Norman, Organizer
R. Jones, Y. Men, Organizers, Presiding

1:15 Introductory Remarks.

1:30 PMSE 38. Basics of small-angle neutron scattering. B. Hammouda

2:00 PMSE 39. Small angle X-ray scattering for morphological analysis of semicrystalline polymers: Modeling of the interface distribution function. T. Thurn-Albrecht, A. Seidltz

2:30 Intermission.

2:45 PMSE 40. New methods for measuring nanostructures: Grazing-transmission and variance scattering. K. Yager

3:15 PMSE 41. Recent developments in high intensity high resolution in-house SAXS. L. Jianhua, A. Takase

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

ACS Award in Applied Polymer Science: Symposium in Honor of Geoffrey W. Coates

W. Dichtel, Organizer, Presiding

1:30 PMSE 42. Targeted applications as inspirations to develop strategies toward polymer materials and nanoscopic devices derived from natural products. K.L. Wooley

2:00 PMSE 43. Stille catalyst-transfer polycondensation of thiophene. K.J. Noonan

2:30 PMSE 44. Development of epoxide/CO₂ copolymerization technology. S. Allen

3:00 Intermission.

3:15 PMSE 45. Polymerization in 2- and 3D. W. Dichtel, B.J. Smith, G. Hwang, R.P. Bisbey, A.D. Chavez

3:45 PMSE 46. Synthesis of functional materials using ROMP initiators. R.H. Grubbs

4:15 PMSE 47. Catalysis for polymer synthesis. R.M. Waymouth

4:45 PMSE 48. Award Address (ACS Award in Applied Polymer Science sponsored by Eastman Chemical). Advances in polymer chemistry enabled through catalyst design and discovery. G.W. Coates

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC: Journal of Materials Chemistry A, B & C, Soft Matter and Chemical Science

A. J. Boydston, L. M. Campos, E. Pentzer, K. L. Wooley, Organizers
P. McGrier, Presiding

1:00 PMSE 49. Mega-supramolecules for energy conservation and fire safety using long end-associative telechelics in fuel. J.A. Kornfield

1:30 PMSE 50. Block copolymer templates for functional nanostructured materials. H. Tan, L.M. Campos

1:55 PMSE 51. Dual stimuli responsive hydrogels. A. Nelson

2:25 PMSE 52. Manipulating morphological characters with architecturally diverse block polymers for lithographic applications. H. Minehara, L.M. Pitet, S. Kim, E.W. Meijer, C.J. Hawker

2:45 Intermission.

3:00 PMSE 53. Controlling molecular conformations of functional macromolecular materials. L. Fang

3:25 PMSE 54. Cyano substituted benzothiadiazoles: Novel acceptor units allowing systematic lowering of conjugated polymer LUMO levels. A. Casey, Y. Han, Z. Fei, A.J. White, T.D. Anthopoulos, M.J. Heaney

3:45 PMSE 55. Overcoming chirality-selected phase behavior in polypeptide complexes. D. Priftis, L. Leon, Z. Song, S. Perry, K.O. Margossian, A. Tropnikova, J. Cheng, M.V. Tirrell

4:05 PMSE 56. Triggered delivery of therapeutic hydrogen sulfide from macromolecular and supramolecular carriers. J.B. Matson, J. Foster

Section D

Sheraton Denver Downtown Hotel
Directors Row H

Nanostructured Porous Polymers: Synthesis, Properties Applications

Nanostructured Porous Polymers for Membrane Application

D. L. Gin, H. Lin, Organizers
B. D. Freeman, Organizer, Presiding
R. Guo, Presiding

1:30 PMSE 57. Nanoporous block copolymer membranes for ultrafiltration: A simple approach to size tunability. H. Ahn, T.P. Russell

2:00 PMSE 58. Pore-size tuning in self-assembled block copolymer membrane. K. Peinemann, X. Qiu, H. Yu, S. Nunes

2:30 PMSE 59. Membranes with artificial free-volume enabled by block copolymer self-assembly. N. Petzetakis

3:00 Intermission.

3:30 PMSE 60. Recent advances in the design of nanoporous polymers based on lyotropic liquid crystals for membrane applications. D.L. Gin, B.M. Carter, S.M. Dischinger, L.A. Robertson, M.G. Cowan, X. Feng, M.E. Tousley, S. Neijati, Y. Choo, R.D. Noble, M. Elmelech, C.O. Osuji

4:00 PMSE 61. Nanoparticle-embedded water filtration membranes. H.A. Weinstein, N.S. Rentz, L.F. Greenlee

4:30 PMSE 62. Synthesis of passive polymeric membranes for CO₂ separation. S. Chatterjee, T. Hong, S.M. Mahum, J.W. Mays, A.P. Sokolov, T. Saito

Section E

Sheraton Denver Downtown Hotel
Governor's Square 17

Stimuli-Responsive Assemblies and Materials

Functional Materials and Surfaces

C. Bowman, J. Cha, Organizers
A. P. Goodwin, Organizer, Presiding

1:30 PMSE 63. Remotely controlled stimuli-responsive materials. S. Minko

2:00 PMSE 64. Self-healing electronic materials. Z. Bao

2:30 PMSE 65. Composite organic conducting polymers with multiple (thermally accessible) conducting phases. J. Galan-Mascaros, Y. Koo, P. Maldonado-Illescas

2:50 PMSE 66. Remarkable pressure responses of metal-organic frameworks: Proton transfer, linker coiling, order-to-disorder transition. A. Ortiz, A. Boutin, K.J. Gagnon, A. Clearfield, F. Couderc

3:10 PMSE 67. UV-responsive organic thin-film transistors with a benzothiophene semiconductor dispersed in a polymer matrix. C. Smithson, D. Ljubic, Y. Wu, S. Zhu

3:30 Intermission.

3:45 PMSE 68. Origami and kirigami nanocomposites. N. Kotov, T. Shyu, P. Damasceno, S.C. Glotzer

4:15 PMSE 69. Color control in stimuli-responsive cholesteric liquid crystal composites. T.J. White, K. Lee, V. Tonjigila

4:45 PMSE 70. Liquid crystal elastomers with a reversible and multistimulus response. H. Kim, T. Adetiba, A. Agrawal, B. Zhu, H. Chen, J. Jacot, R. Verduzco

5:05 PMSE 71. Responsive liquid crystal/polymer aperiodic and periodic composites. T.J. Bunning, S. Serak, L. De Sio, E. Ouskova, R. Vergara, C. Umeton, N. Tahirian, T.J. White

Section F

Sheraton Denver Downtown Hotel
Governor's Square 15

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications

Chemistry and Materials Science of 2-D Materials

A. D. Taylor, Organizer
G. S. Tulevski, Organizer, Presiding

1:00 PMSE 72. Carbon nanomaterial heterostructure devices. M. Hersam

1:30 PMSE 73. Flexible and conductive MXene-based nanocomposites with high volumetric capacitance. Y. Gogotsi, M. Zhao, Z. Ling, C.E. Ren, M.R. Lukatskaya, M.W. Barsoum

2:00 PMSE 74. Synthesis of novel aromatic architectures through the benzannulation of aryl acetylenes. W. Dichtel, S. Hein, H. Arslan

2:30 PMSE 75. Self-folding polymer-graphene bilayer sensors. T. Deng, C. Yoon, Q. Jin, M. Li, Z. Liu, D.H. Gracias

2:50 Intermission.

3:10 PMSE 76. Hydrogenated graphene: Formation, stability, and applications. P.E. Sheehan, K.E. Whitener, W.K. Lee, J. Felts, J. Robinson, P. Campbell

3:40 PMSE 77. Synthesis of polybenzoquinolines as graphene nanoribbon precursors. Y. Park, D.J. Dibble, M. Umerani, A. Mazaheripour, A.A. Gorodetsky

4:00 PMSE 78. Nematic order drives macroscopic patterns of graphene oxide in drop drying. S. Zhang

4:20 PMSE 79. Protein adsorbed graphene oxide nanosheets for intracellular protein and vaccine delivery. H. Li, B. De Geest

Section G

Sheraton Denver Downtown Hotel
Governor's Square 10

General Papers/ New Concepts in Polymeric Materials

Polymer Nanotechnology

Q. Lin, Organizer
D. Zhang, S. Zhou, Presiding

1:30 PMSE 80. Formation of sub-10 nm features with modified PS-PMMA. S. Zhou, D. Janes, C.G. Willson, C.J. Ellison

1:50 PMSE 81. Photolithographic control of nanostructures in cross-linkable block copolymers. G. Chado, C. He, M.P. Stoykovich

2:10 PMSE 82. Interfacial interactions between conjugated polymers and carbon nanotubes. S. Zhang

2:30 PMSE 83. Graphene fiber induced polymer transcrystallization. J. Abdou, S. Zhang

2:50 PMSE 84. ROMP-derived stimuli-responsive organoboron nanostructures. G. Pawar, J.B. Sheridan, F. Jaekle

3:10 Intermission.

3:30 PMSE 85. Designing the porosity of bacterial cellulose nanopapers. A. Mautner, K. Lee, K. Li, A. Bismarck

3:50 PMSE 86. Alternating donor-acceptor conjugated polymers entailing amide/imide-based accepting moieties toward semiconducting materials. D. Zhang

4:10 PMSE 87. Nanothermometer: Measuring temperature change in nanometer scale on photothermal Au nanoparticles. H. Sakalak, H. Cavusoglu, B. Buyukbekar, G. Demirel, M. Citir, M. Yavuz

4:30 PMSE 88. Microfabrication of microfluidic devices via reaction-diffusion. M. Kleiman, K. Brubaker, D.T. Nguyen, A. Esser-Kahn

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Sponsored by POLY, Cosponsored by PMSE

Macromolecular and Nanoparticle Separation Science

Sponsored by POLY, Cosponsored by ANYL and PMSE

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

Thin Films, Membranes & Fibrous Polymers

R. Jones, Organizer
Y. Men, A. I. Norman, Organizers, Presiding

8:30 PMSE 89. Functional Group Depth Profiling with Resonant Soft X-ray Reflectivity. D. Sunday, E. Chan, C.M. Stafford

8:50 PMSE 90. Simultaneous SAXS/WAXS investigation of out-of-equilibrium polymer films. P. Panine, S. Desvergne, M. Fernandez-Martinez, S. Rodrigues, F. Bossan

9:20 PMSE 91. Resonant soft X-ray scattering for soft materials. C. Wang, A. Young, A. Hexemer, H. Padmore

9:50 PMSE 92. Structure and morphology of P3HT and P3HT-containing donor-acceptor block copolymers as elucidated by x-ray scattering methods. T. Thurn-Albrecht

10:20 Intermission.

10:35 PMSE 93. Structure studies of natural cellulose microfibrils by synchrotron small-angle X-ray scattering. B.S. Hsiao, B.T. Chu, Y. Su

11:05 PMSE 94. Structure evolution of polymer grafted nanoparticle assemblies by selective solvent annealing of the canopy. J. Che, C.A. Grabowski, H. Koerner, R.A. Vaia

11:25 PMSE 95. Small-angle X-ray studies of the morphological change of anion exchange membranes under uniaxial extensional strain. B.R. Caire, M. Vandiver, S. Seifert, M.W. Liberatore

11:45 PMSE 96. Infrared and neutron reflectometry of sulfonated poly(ether ether ketone) interfaces with Pt and SiO₂. J.H. Doan, J.A. Dura, E.S. Smotkin

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

Cooperative Research Award: Symposium in Honor of Andy Tsou and Benjamin Hsiao

Financially supported by ExxonMobil

B. T. Chu, D. Schulz, *Organizers, Presiding*

8:30 Introductory Remarks.

8:30 PMSE 97. Crystallization of polyolefins under flow and deformation. B.S. Hsiao, A.H. Tsou

9:00 PMSE 98. Miscibility and crystallization in hydrocarbon block and block-random copolymers. R.A. Register, B.S. Beckingham, A.B. Burns

9:30 PMSE 99. Supramolecular assembly: Giant polyhedrons and giant surfactants based on "nanotoms". S.Z. Cheng

10:00 PMSE 100. Fluorinated block copolymers: New materials as environmentally benign anti-fouling coatings. B. Wenning, D. Calabrese, C.K. Ober

10:30 PMSE 101. Electrospun fibrous membrane for reducing postoperative peritoneal adhesion and for targeted drug delivery. C.C. Han

11:00 PMSE 102. Cellulose nanofibers as a key component in separation membranes. B.T. Chu, B. Hsiao

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC: Journal of Materials Chemistry A, B & C, Soft Mater and Chemical Science

A. J. Boydston, L. M. Campos, E. Pentzer, K. L. Wooley, *Organizers*

J. B. Matson, *Presiding*

8:30 PMSE 103. Understanding mechanochemistry from first principles. T. Martínez

9:00 PMSE 104. Linking molecular design of the polymer functionalization to tune grafted particle assembly or dispersion within domains and interfaces of polymer matrices. A. Jayaraman

9:25 PMSE 105. Isophthalic acid - pyridine H-bonding: A simple yet versatile supramolecular synthon for the design of functional polymers. L. Montero de Espinosa, S. Balog, C. Weder

9:45 PMSE 106. Synthesis and spontaneous segregation of functional bottlebrush polymer additives. S.L. Pesek, X. Li, I. Mitra, G. Stein, R. Verdusco

10:05 Intermission.

10:20 PMSE 107. Design principles for charge storage within redox-active covalent organic frameworks. C.R. DeBlase, H.D. Abruna, W. Dichtel

10:50 PMSE 108. Ring-opening metathesis oligomerization (ROMP) via electroorganic synthesis. K. Ogawa, A. Goetz, A.J. Boydston

11:15 PMSE 109. Polymer mechanochemistry at surfaces. H. Klok

11:35 PMSE 110. Flow IEG: A scalable route to sequence and architecturally defined unimolecular macromolecules. F.A. Leibfarth, J.A. Johnson, T.F. Jamison

Section D

Sheraton Denver Downtown Hotel
Directors Row H

Nanostructured Porous Polymers: Synthesis, Properties Applications

Nanostructured Porous Polymers for Sorbents

H. Lin, *Organizer*

B. D. Freeman, D. L. Gin, *Organizers, Presiding*

8:30 PMSE 111. Porous organic polymers: synthesis and absorption/transport properties. S.T. Nguyen

9:00 PMSE 112. Directing structural features and gas sorption properties of nanoporous polymers. O. Buyukkakar, A. Coskun

9:30 PMSE 113. Nanoporous selective absorbents based on semicrystalline syndiotactic polystyrene. S. Nazarenko

10:00 Intermission.

10:30 PMSE 114. Porous organic polymers for electrocatalysis and photoresponsive gas adsorption. W. Zhang, Y. Zhu, G. Lu, H. Yang, Y. Jin

11:00 PMSE 115. Rational design of porous organic polymers for decontamination. G. Barin, J.R. Long

11:30 PMSE 116. Effect of cross-link density on carbon dioxide separation in PDMS norbornene membranes. T. Hong, Z. Niu, S.M. Mahurin, D. Jiang, B.K. Long, J.W. Mays, A.P. Sokolov, T. Saito

Section E

Sheraton Denver Downtown Hotel
Governor's Square 17

Stimulus-Responsive Assemblies and Materials

Tunable Particles and Surfaces

C. Bowman, A. P. Goodwin, *Organizers*

J. Cha, *Organizer, Presiding*

8:30 PMSE 117. One-step preparation of thermo/photosensitive nanogels and their use as stabilizers of Pickering high internal phase emulsions. F.M. Winnik, X. Zhang

9:00 PMSE 118. Building responsive materials from compartmentalized microparticles. J. Lahann

9:30 PMSE 119. Polymer directed self assembly of pH-responsive antioxidant nanoparticles. R.K. Prudhomme

9:50 PMSE 120. Responsive porous polymers through emulsion-templating. M. Oviada, I. Gurevitch, M.S. Silverstein

10:10 PMSE 121. Nanogel-based stimulus-responsive capsules with tunable wall permeability. A. Pich

10:30 Intermission.

10:45 PMSE 122. Responsive nanomaterials: Combining nanostructures, cells, and ultrathin polymer films. V.V. Tsukruk

11:15 PMSE 123. Reversible tuning of pore size and CO₂ adsorption in a series of azobenzene functionalized porous organic polymers (POPs). Y. Zhu, W. Zhang

11:35 PMSE 124. Star polyelectrolytes based microcapsules with multiresponsiveness to ionic strength, pH, and temperature. W. Xu, P.A. Ledin, F. Plamper, C. Synatschke, A. Mueller, V.V. Tsukruk

Section F

Sheraton Denver Downtown Hotel
Governor's Square 9

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications

Low-D Carbon Devices and Materials

G. S. Tulevski, *Organizer*

A. D. Taylor, *Organizer, Presiding*

8:30 PMSE 125. How will carbon nanotubes impact the next generation of electronics? A. Franklin

9:00 PMSE 126. Materials science and applications of exceptionally electronic-type sorted semiconducting carbon nanotubes in field effect transistors and photovoltaics. M. Arnold

9:30 PMSE 127. Synthesis and photophysical investigation of a series of porphyrin-containing polymers that helically wrap single-walled carbon nanotubes. M.G. Glesner, H. Yoo, J. Olivier, P. Deria, M.J. Therien

9:50 Intermission.

10:10 PMSE 128. Semiconducting SWCNT enrichment via conjugated polymer extraction. P.R. Malenfant, J. Ding, Z. Li, J. Lefebvre, F. Cheng, C. Homenick, J. Dunford, N. Du, G.P. Lopinski, R. James, C. Kingston, B. Simard, J. Humes, J. Kroeger

10:40 PMSE 129. Graphene photonics and plasmonics. F. Xia

11:10 PMSE 130. Dose-controlled, floating evaporative self-assembly and alignment of semiconducting carbon nanotubes (SWCNTs) from organic solvents. Y. Joo, G.J. Brady, M. Arnold, P. Gopalan

11:30 PMSE 131. Novel route to fabricate graphene oxide quantum dots (GOQDs) and graphene quantum dots (GQDs). T. Fan, C. Yuan, W. Tang, S. Tong, S. Mo, C. Zhao, Y. Liu, Y. Min

Section G

Sheraton Denver Downtown Hotel
Governor's Square 10

General Papers/New Concepts in Polymeric Materials

Polymeric Biomaterials and Applications

Q. Lin, *Organizer*

A. K. Gaharwar, P. B. Smith, *Presiding*

8:50 PMSE 132. Elastomeric and mechanically stiff nanocomposite for bone tissue engineering. P. Keratitivayan, A.K. Gaharwar

9:10 PMSE 133. Biobased composites for tissue engineering from tung oil and collagen. R.L. Quirino, D.B. Page, A. Stewart, A. Scholz

9:30 PMSE 134. Enhanced bone cell functions on poly(ϵ -caprolactone) networks grafted with polyhedral oligomeric silsesquioxane nanocages. L. Cai, C.H. Sprague, C. Foster, S. Wang

9:50 PMSE 135. Poly(ϵ -caprolactone) networks tethered with dangling poly(L-lysine) chains for promoting smooth muscle cell functions. X. Liu, S. Wang

10:10 Intermission.

10:30 PMSE 136. Derivatives of chitin and chitosan for biomedical applications bearing nitric oxide-releasing S-nitrosothiol substituents. A. Lutzke, A. Pegalajar-Jurado, B.H. Neufeld, M.M. Reynolds

10:50 PMSE 137. Producing lignin-based polyols through microwave-assisted liquefaction for rigid polyurethane foam production. B. Xue, R. Sun

11:10 PMSE 138. Glycerol based hyper-branched poly(ester)s for the controlled release of the plant growth regulator naphthalylacetic acid. T. Zhang, B.A. Howell, P.B. Smith

11:30 PMSE 139. Design of biobased hyper-branched polyesters: Structure and molecular weight. P.B. Smith, T. Zhang, B.A. Howell, S.J. Martin

Next Generation Smart Materials

Materials with Special Optical, Electronic and Mechanical Behavior

Sponsored by POLY, Cosponsored by PMSE

Integrating Chemistry and Polymer Science Research into the Classroom

Sponsored by CHED, Cosponsored by PMSE

and POLY

Macromolecular and Nanoparticle Separation Science

Sponsored by POLY, Cosponsored by ANYL and PMSE

MONDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

Block Copolymers & Polymer Blends

A. I. Norman, *Organizer*

R. Jones, Y. Men, *Organizers, Presiding*

1:30 PMSE 140. Thermodynamic interactions and shear-aligned structures in triblock copolymers derived from vegetable oils. S. Wang, S. Vajjala Kesava, E. Gomez, M.L. Robertson

2:00 PMSE 141. Characterizing the distribution and thermodynamics of selectively associating additives in polymer blends. D. Sunday, Y. Tein, R. Kline

2:30 PMSE 142. Structure transitions in symmetric crystalline-crystalline diblock copolymers with synchrotron simultaneous SAXS/WAXS investigations. F. Xue, S. Jiang

3:00 Intermission.

3:15 PMSE 143. Co-solvency and co-non-solvency of polymers in mixed solvents. B. Hammouda

3:45 PMSE 144. Microstructural origins of yield, strain hardening and hysteresis in thermoplastic elastomers under uniaxial deformation: an in situ tensile-SANS study. C. Lopez-Barron, A. Eberle

4:15 PMSE 145. SANS study on the phase behaviors of responsive star polyelectrolytes. W. Xu, I. Choi, F. Plamper, C. Synatschke, A. Mueller, Y. Melnichenko, V.V. Tsukruk

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

Polymeric Biomaterials

Novel Polymeric Biomaterials: Synthesis, Modification and Fabrication

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

1:20 PMSE 146. Responsive materials for the directing and delivering stem cells and therapeutics. M.S. Rehmann, P.M. Kharkar, A.M. Kloxin

1:50 PMSE 147. Withdrawn.

2:10 PMSE 148. Efficient syntheses of polysaccharides and their biomedical applications. W. Du, L. Li, J. Wang, M. Obrinske

2:30 PMSE 149. Tailoring the activity of lysozyme by combining grafting-from and grafting-to RAFT polymerization. R. Falatach, C. McGlone, S. Averick, R.C. Page, D. Konkolewicz, J. Berberich

2:50 Intermission.

3:10 PMSE 150. Silk proteins for stabilization and drug delivery systems. D.L. Kaplan

3:40 PMSE 151. Conjugated polymer nanoparticles for intracellular organelle specific drug delivery. M. Kumar, T. Yokata, E. Mendez, J. Moon

4:00 PMSE 152. Improving network crosslinking of peptide-immobilized hydrogels formed by visible light-initiated thiol-acrylate photopolymerization. C. Lin, J. Bragg

4:20 PMSE 153. Multifunctional polyesters and polyurethanes with peptide-like pendant functional groups. A. Joy, Y. Xu, J.P. Swanson

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC; Journal of Materials Chemistry A, B & C, Soft Mater and Chemical Science

A. J. Boydston, L. M. Campos, E. Pentzer, K. L. Wooley, *Organizers*
Y. Xia, *Presiding*

1:00 PMSE 154. Structural evolution of polyelectrolyte-complex-core micelles and ordered-phase bulk materials. M.V. Tirrell

1:30 PMSE 155. Design of functional materials to tailor glycan interactions at the cell-matrix interface. K. Godula

1:55 PMSE 156. Designing dynamic rearrangement of polymeric structures using the principles found in lungs. A.P. Esser-Kahn, M. Kleiman, D.T. Nguyen, K. Brubaker

2:20 PMSE 157. Kinetic control of modulus properties in peptide functionalized hydrogels. M. Becker, B.D. Vogt, G. Hua, Z.K. Zander, C. Wiener

2:45 Intermission.

3:00 PMSE 158. Sustainable and degradable thermosets and polyesters from sugar-derived dilactones. J. Gallagher, M.A. Hillmyer, T.M. Reineke

3:30 PMSE 159. Design of hydrogels as synthetic extracellular matrix mimics using modular building blocks and facile techniques. A.M. Kloxin

4:00 PMSE 160. Poly(oligonucleotide): Development and biomedical utility of nucleic acid-programmed polymers and nanoparticles. N.C. Gianneschi

Section D

Sheraton Denver Downtown Hotel
Directors Row H

Nanostructured Porous Polymers: Synthesis, Properties Applications**New Approaches and Applications of Nanostructured Porous Polymeric Materials**

D. L. Gin, *Organizer*

B. D. Freeman, H. Lin, *Organizers, Presiding*

1:30 PMSE 161. Hierarchically porous conductive hydrogels as a novel material platform for energy storage and biosensor technologies. G. Yu

2:00 PMSE 162. Surface modification of metal-organic framework nanoparticles using random polymer. T. Li, S. Darnall, I. Lee, T. Xu

2:20 PMSE 163. Photocrosslinked honeycomb-patterned films with submicron pores fabricated using monodisperse silica nanoparticles as templates for regulating MC3T3-E1 cell functions. X. Wu, S. Wang

2:40 PMSE 164. Grafting of poly(oligoethylene glycol) (meth)acrylate brushes on the surface of cylindrical mesopores of ordered silica via activator regenerated by electron transfer ATRP. A.S. Manchanda, M. Kruk

3:00 PMSE 165. Block copolymer packing limits and interfacial reconfigurability in the assembly of periodic mesoporous organosilicas. B.A. Helms, A.W. Wills, P. Ercius, E.R. Rosenberg, R. Runser

3:20 Intermission.

3:40 PMSE 166. High surface area methylsilsesquioxane polymer gels made by fluoride catalyzed rearrangement. J. Furgal, H. Yamane, Y. Chujo, R.M. Laine

4:00 PMSE 167. Nanoporous materials from crosslinked gemini surfactant lyotropic liquid crystal network phases. J. Jennings, M. Mahanthappa

4:20 PMSE 168. Microporous inorganic/organic hybrids via oxyfunctionalization of a cubic symmetry nanobuilding block [(H₂Me₂SiOSiO₂)_n] with R₂Si(OEt)₂ in Hydrophobic media. D. Pan, E. Yi, J. Furgal, M. Schwartz, P. Doan, R.M. Laine

4:40 PMSE 169. Biomimetic amphiphobic surfaces on paper. S. Oyola-Reynoso, I. Tevis, Z. Li, J. Halbertsma-Black, M. Thuo

5:00 PMSE 170. Hierarchical porosity in emulsion-templated polymers. S. Israel, M.S. Silverstein

Section E

Sheraton Denver Downtown Hotel
Governor's Square 17

Stimulus-Responsive Assemblies and Materials**Inspiration from Biology**

C. Bowman, A. P. Goodwin, *Organizers*

J. Cha, *Organizer, Presiding*

1:30 PMSE 171. Peptide supramolecular polymerizations. S.J. Stupp

2:00 PMSE 172. Phase behavior and self-assembly of stimulus response peptide polymers. A. Chilkoti

2:30 PMSE 173. Molecular description of LCST behavior of elastin-like peptides poly(VPGVG) and poly(VGPVG). N.K. Li, Y.G. Yingling

2:50 PMSE 174. Temperature-triggered self-assembly of nanovesicles from collagen-like peptide-containing diblock bioconjugates. T. Luo, L. He, P. Theato, K.L. Kllick

3:10 PMSE 175. Regulating supramolecular polymerization of polypeptide-grafted macromolecules. H. Xia, Y. Zhang, H. Fu, Y. Ren, J. Cheng, Y. Lin

3:30 Intermission.

3:45 PMSE 176. Responsive, switchable, and self-assembled properties of zwitterionic biomaterials. S. Jiang

4:15 PMSE 177. Stimulus-responsive polymer-lipid assemblies as biomolecule-activated imaging contrast agents. A.P. Goodwin

4:45 PMSE 178. Infrared invisibility stickers inspired by cephalopods. L. Phan, D. Ordinario, E. Karshalev, M. Shenk, A.A. Gorodetsky

5:05 PMSE 179. Photoresponsive mussel-derived surgical tissue glue. E. Jeon, B. Hwang, Y. Yang, H.J. Cha

Section F

Sheraton Denver Downtown Hotel
Governor's Square 9

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications**Composite Materials**

G. S. Tulevski, *Organizer*

A. D. Taylor, *Organizer, Presiding*

1:30 PMSE 180. Graphene/polymer derived ceramics with anisotropic properties. L. Zhai

1:50 PMSE 181. Efficient, low-cost, simple method to enhance the thermal efficiency of ceramic by spray deposition of silane-modified graphene. S. Tong, J. Wang, S. Mo, C. Yuan, Y. Liu, Y. Min

2:10 PMSE 182. Conductive nanocomposites of polyethylene/oxidized polyethylene (PE/OPE) blends with thermally reduced graphene and carbon black. M.Z. Iqbal, A.A. Abdala, M.W. Liberatore

2:30 PMSE 183. 3D graphene/58 S bioactive glass scaffolds as a biocompatible scaffold for retinal ganglion cells. Q. Yao, S. Yu, Y. Liu

2:50 PMSE 184. Antibacterial surface acting via photothermal effects. H. Liwei, Y. Linhua

Section G

Sheraton Denver Downtown Hotel
Governor's Square 10

General Papers/New Concepts in Polymeric Materials**Polymer Synthesis**

Q. Lin, *Organizer*

X. Guo, S. Zavada, *Presiding*

1:30 PMSE 185. Polymerization of N-NCAs in ionic liquids: Heterophase synthesis of polypeptides. S.M. Brosnan, C. Secker, H. Schlaad, K. Tauer, M. Antonietti

1:50 PMSE 186. Design and synthesis of a degradable triblock copolymer, poly(ethylene glycol)-block-polyphosphoester-block-poly(L-lactide) for biomedical applications. R. Li, F. Zhang, S. Zhang, H. Wang, K.L. Wooley

2:10 PMSE 187. Synthesis of silver oxide nanoparticles in spherical polyelectrolyte brushes. A. Ahmad, X. Liu, Y. Xu, X. Guo

2:30 PMSE 188. Proton-transfer polymerization (HTP): Converting methacrylates into polyesters by an N-heterocyclic carbene. M. Hong, E.Y. Chen

2:50 PMSE 189. Synthesis and polymerization of substituted oxazine ring of polybenzoxazine. F.P. Cassidy, K. Chiou, H. Ishida

3:10 Intermission.

3:30 PMSE 190. Rapid, puncture-initiated, autonomous healing via oxygen-mediated polymerization. S.R. Zavada, K.L. Gordon, N.R. McHardy, T.F. Scott

3:50 PMSE 191. Biodegradable comb-dendritic tri-block copolymers consisting of poly(ethylene glycol) and poly(L-lactide) or poly(β -caprolactone) and pre-osteoblastic cellular response to the spherulitic surfaces. X. Wu, J. Dou, S. Wang

4:10 PMSE 192. Self-assembly of giant polymer capsules with purely hydrophilic polymers: The hydrophilic effect. S.M. Brosnan, H. Schlaad, M. Antonietti

4:40 PMSE 193. Elucidating the relationships between polyethylene architecture and mechanical properties. A. Kannan, D. Bucknall, A. Eberle, T. Shaffer, A.I. Norman, S. Weigand

5:00 PMSE 194. Molecular weight dependency of crystallization, recrystallization and melting lines in isotactic polypropylene and polybutene-1. Y. Lu, Y. Wang, Y. Men

5:30 PMSE 195. Investigating the crystallization kinetics and structure development of hybrid polymer-nanocomposite materials using SAXS/WAXS and thermal techniques. E.L. Heeley, P.G. Taylor, Y. El Aziz, A. Basindale, D. Hughes

6:00 Intermission.

6:15 PMSE 196. Topology of soft materials using neutron and X-ray scattering. G. Beaucage

6:45 PMSE 197. Morphological origin of the embrittlement of polymers upon crystallization: The case of PET. L. Balzano

7:15 PMSE 198. Phase behavior of polymer-grafted nanoparticles in a polymer matrix. K. Mongcopa, R. Ashkar, P. Butler, R. Krishnamoorti

7:45 PMSE 199. Degradable porous polymer biomaterials through emulsion-templating. T. Bialystocki, D. David, L. Perry, D. Rosenfeld, S. Levenberg, M.S. Silverstein

8:15 PMSE 200. Cell encapsulating tough hydrogel materials. A.P. Dove

8:45 PMSE 201. Development of flexible and elastic, biodegradable and bioactive polycarbonates. Z. Zhang, S.D. Sommerfeld, J. Bushman, M. Guendiren, D. Zunger, P. Mishra, H. Kaplan, J.B. Kohn

9:15 PMSE 202. Advanced biocompatible and high strength underwater tissue bioadhesive. H. Kim, S. Lim, B. Hwang, H.J. Cha

9:45 Intermission.

10:05 PMSE 203. Molecular understanding, design, and development of zwitterionic biomaterials. S. Jiang

10:35 PMSE 204. Antimicrobial coatings for biomedical applications: Challenges and opportunities offered by natural polymers. K. Neoh, M. Li, R. Wang, E. Kang, E. Chiong

11:05 PMSE 205. Low-temperature plasma surface modification of porous polymeric materials for environmental and medical applications. M.N. Mann, A. Pegalajar-Jurado, E.R. Fisher

11:35 PMSE 206. Highly selective antibacterial activity through control of polymer amphiphilicity based on the exploration of non-ionic hydrophilic counts. A. Punia, N. Yang

TUESDAY MORNING**Section A**

Sheraton Denver Downtown Hotel
Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology**High Strength Polymers and Composites**

Y. Men, *Organizer*

R. Jones, A. I. Norman, *Organizers, Presiding*

8:30 PMSE 193. Elucidating the relationships between polyethylene architecture and mechanical properties. A. Kannan, D. Bucknall, A. Eberle, T. Shaffer, A.I. Norman, S. Weigand

9:00 PMSE 194. Molecular weight dependency of crystallization, recrystallization and melting lines in isotactic polypropylene and polybutene-1. Y. Lu, Y. Wang, Y. Men

9:30 PMSE 195. Investigating the crystallization kinetics and structure development of hybrid polymer-nanocomposite materials using SAXS/WAXS and thermal techniques. E.L. Heeley, P.G. Taylor, Y. El Aziz, A. Basindale, D. Hughes

10:00 Intermission.

10:15 PMSE 196. Topology of soft materials using neutron and X-ray scattering. G. Beaucage

10:45 PMSE 197. Morphological origin of the embrittlement of polymers upon crystallization: The case of PET. L. Balzano

11:15 PMSE 198. Phase behavior of polymer-grafted nanoparticles in a polymer matrix. K. Mongcopa, R. Ashkar, P. Butler, R. Krishnamoorti

11:45 PMSE 199. Degradable porous polymer biomaterials through emulsion-templating. T. Bialystocki, D. David, L. Perry, D. Rosenfeld, S. Levenberg, M.S. Silverstein

12:15 PMSE 200. Cell encapsulating tough hydrogel materials. A.P. Dove

12:45 PMSE 201. Development of flexible and elastic, biodegradable and bioactive polycarbonates. Z. Zhang, S.D. Sommerfeld, J. Bushman, M. Guendiren, D. Zunger, P. Mishra, H. Kaplan, J.B. Kohn

1:15 PMSE 202. Advanced biocompatible and high strength underwater tissue bioadhesive. H. Kim, S. Lim, B. Hwang, H.J. Cha

1:45 PMSE 203. Molecular understanding, design, and development of zwitterionic biomaterials. S. Jiang

2:15 PMSE 204. Antimicrobial coatings for biomedical applications: Challenges and opportunities offered by natural polymers. K. Neoh, M. Li, R. Wang, E. Kang, E. Chiong

2:45 PMSE 205. Low-temperature plasma surface modification of porous polymeric materials for environmental and medical applications. M.N. Mann, A. Pegalajar-Jurado, E.R. Fisher

3:15 PMSE 206. Highly selective antibacterial activity through control of polymer amphiphilicity based on the exploration of non-ionic hydrophilic counts. A. Punia, N. Yang

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

[†] Cooperative Cosponsorship

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC; Journal of Materials Chemistry A, B & C, Soft Matter and Chemical Science

A. J. Boydston, L. M. Campos, E. Pentzer,
K. L. Wooley, *Organizers*
B. M. Cossairt, *Presiding*

8:30 PMSE 207. Modeling block copolymer thin film orientation in the presence of neutral and preferential interfaces. W. Durand, M. Carlson, G. Blachut, M. Maher, C.J. Ellison, C.G. Willson

8:55 PMSE 208. Design rules for membranes in artificial solar fuels generators. N.A. Lynd

9:15 PMSE 209. Functional degradable poly(carbonate)s: Design, synthesis, and self-assembly. R.J. Williams, R.K. O'Reilly, A.P. Dove

9:35 PMSE 210. Efficient synthesis of rigid ladder polymers via palladium catalyzed annulation. Y. Xia

10:00 PMSE 211. Photolithographic olefin metathesis polymerization. R. Weitekamp, H. Atwater, R.H. Grubbs

10:20 Intermission.

10:35 PMSE 212. Synthetic polymer anion exchange membranes. W. Zhang, Y. Liu, M.W. Liberatore, A.M. Herring, E. Coughlin

10:55 PMSE 213. Synthesis and design of functional porous organic polymers. P. McGrier

11:20 PMSE 214. Designing a hydrophobic monomer library with LogP values. R.T. Mathers

11:40 PMSE 215. Structural design principles for high performance polysaccharide binders in silicon anodes. T. Kwon, Y.K. Jeong, J. Choi, A. Coskun

Section D

Sheraton Denver Downtown Hotel
Directors Row H

Nanoscale Spectroscopic and Microscopic Characterization

Hybrid SPM/AFM

Financially supported by ExxonMobil Chemicals; Bruker; Nanosurf

A. H. Tsou, D. Yablou, *Organizers*
J. Hobbs, *Presiding*

8:30 PMSE 216. AFMIR: A powerful tool for Infrared Nanoscopy. A. Dazzi, A. Deniset-Besseau, C.A. Marcott, K. Kjoller

9:00 PMSE 217. Investigation of microscopic properties of polymer surface in contact with liquids: A combined SFM-Raman study. S. Hild

9:30 PMSE 218. Infrared nanoimaging and nano-FTIR spectroscopy. R. Hillenbrand

10:00 Intermission.

10:15 PMSE 219. Multimodal and multispectral nano-imaging: Accessing the structure underlying the function in molecular and soft-matter. M.B. Raschke

10:45 PMSE 220. Nanoscale chemical, mechanical and thermal analysis of polymers using AFM-IR. K. Kjoller, M. Lo, Q. Hu, C. Prater

11:05 PMSE 221. Bimodal AFM for elucidation of polyolefin morphology. A.H. Tsou, D. Yablou, H. Bradshaw, E.J. Blok, R.N. Dharamarajan

Section E

Sheraton Denver Downtown Hotel
Governor's Square 17

Stimulus-Responsive Assemblies and Materials

Biomedical Applications of Stimulus-Responsive Assemblies

C. Bowman, J. Cha, A. P. Goodwin, *Organizers*
D. Domaille, *Presiding*

8:30 PMSE 222. Facile synthesis of clickable, pH responsive functional polyphosphoramidates. H. Wang, F. Zhang, R. Li, S. Zhang, K.L. Wooley

8:50 PMSE 223. Dual-triggered polymeric nanoparticles as activatable fluorescent probes for the detection of inflammation and tumors. J. Lux, M.L. Viger, V.A. Nguyen Huu, G. Collet, M. Guma, A. Foucault-Collet, B. Bartok, G.S. Firestein, A. Almutairi

9:10 PMSE 224. Carrier-free, light-activated nanoparticle system for the simultaneous delivery of nucleic acids and cancer drug. K. Zhang, B. Li, J.J. Zhao, X. Tan

9:30 PMSE 225. Enzyme-responsive nanoparticles for tissue targeting. N.C. Gianneschi

10:00 PMSE 226. Stimuli-responsive anisotropic colloidal nanoparticles. C. Lu, M.W. Urban

10:20 Intermission.

10:35 PMSE 227. Light/magnetic responsive polymer/inorganic hybrid assemblies for cancer theranostics. Z. Nie, Y. Liu, J. Lin, X. Chen

11:05 PMSE 228. Magnetic field triggered drug release from polymersomes for cancer therapeutics. H. Oliveira, J. Thévenot, O. Sandre, S. Lecommandoux

11:25 PMSE 229. Versatile platform to temperature-responsive PEG-based materials: Facile post-polymerization functionalization of PEO-co-PAGE with n-alkane thiols. T. Kawamori, D. Klingner, J. Gopez, T. Murakami, C.J. Hawker

Section F

Sheraton Denver Downtown Hotel
Governor's Square 15

ACS Award in Polymer Chemistry: Symposium in Honor of Nikos Hadjichristidis Well-Defined Polymers: From Design to Applications

Financially supported by ExxonMobil

Y. Gnanou, *Organizer*
J. Frechet, *Organizer, Presiding*

8:30 PMSE 230. Branched polymers: Stars, grafts, and gels by ATRP. K. Matyjaszewski

9:00 PMSE 231. Advance of sequential controlled polymerizations for the design of molecular brush block copolymers: Sophisticated functional single molecule materials and hierarchically-assembled cluster properties. K.L. Wooley

9:30 PMSE 232. Model thermoplastic polyurethanes with sequence controlled monodisperse hard segments. L. Ren, P. Shah, N. Kang, R. Faust

10:00 Intermission.

10:30 PMSE 233. Tailored block copolymers and their processing for self-assembled thin films applications. D. Calabrese, B. Wenning, M. Chavis, C.K. Ober

11:00 PMSE 234. Synthesis of star and star-block copolymers by living radical polymerization. D.M. Haddleton

11:30 PMSE 235. Photoinduced ATRP and CuAAC click reactions and their combinations for macromolecular syntheses. S. Doran, E. Murtezi, S. Dadashi-Silab, M. Ciftci, G. Yilmaz, M. Tasdelen, Y. Yagci

Section G

Sheraton Denver Downtown Hotel
Governor's Square 10

Polymer Modeling: Structure, Dynamics and Function

Solutions, Melts and Surfaces

Financially supported by ExxonMobil; Dow Chemical

R. Locker, G. C. Rutledge, *Organizers*
M. A. Pasquinelli, *Presiding*

8:30 PMSE 236. Equilibration of high molecular-weight polymer melts: A hierarchical universal strategy. G. Zhang, L. Moreira, T. Stuehn, K.C. Daoulas, K. Kremer

9:00 PMSE 237. Molecular simulation of polymer adsorption on rough surfaces. A. Venkatakrishnan, A. Frost, J. Lewnard, A. Shim, K. Anderson, V.K. Kuppaa

9:20 PMSE 238. Effects of ionic liquid structure on the thermodynamics of cellulose dissolution. B. Rabideau, A.E. Ismail

9:40 PMSE 239. Threading of ring poly(ethylene oxide) molecules by linear chains or other rings in the melt: molecular dynamics simulations followed by a geometric analysis. D.G. Tsalkalis, V.G. Mavrantzas

10:00 PMSE 240. Tubes, topology, and entangled rings. S. Milner

10:30 PMSE 241. Molecular dynamics study on the influence of copolyester composition on adhesion with soda-lime glass. B. Hanson, J.G. Ray, M.A. Pasquinelli

10:50 PMSE 242. Deformation of poly(amido amine) dendrimers at surfaces. K.A. Maerzke, N. Henson, P. Welch, C.F. Welch

11:10 PMSE 243. Hydrogen bond organization and related structural order in bis-MPA based dendrimers versus hyperbranched polymers. M. Syed, B. Olson, S.I. Nazarenko

Energy and Materials

Sponsored by POLY, Cosponsored by PMSE

Smart and Responsive Composites from Renewable Building Blocks

Cues from Nature: Environmentally-Triggered Functionality in Biopolymers

Sponsored by CELL, Cosponsored by PMSE

Macromolecular and Nanoparticle Separation Science

Sponsored by POLY, Cosponsored by ANYL and PMSE

TUESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

High Strength Polymers and Composites

R. Jones, *Organizer*

Y. Men, A. I. Norman, *Organizers, Presiding*

1:30 PMSE 244. Studying the nonequilibrium nature of extension-induced nucleation in polymer melts with ultrafast X-ray scattering. L. Li

2:00 PMSE 245. Characterization of crystallinity in polyolefins by wide angle X-ray diffraction. R. Ortega, J. Butler, D. Winter

2:30 PMSE 246. Switching Chirality of hybrid left-right crystalline helicoids built of achiral polymer chains: When right-to-left becomes left-to-right. M. Rosenthal, M. Burghammer, A.P. Melnikov, D.V. Anokhin, G. Bar, E.T. Samulsky, D. Ivanov

3:00 Intermission.

3:15 PMSE 247. Depth-sectioning method for X-ray diffraction: isolating the real-time structure development in pressure driven flows. L. Fernandez-Ballester

3:45 PMSE 248. Neutron scattering characterization of amino-polymer/silica composite CO₂ adsorbents: Morphology, mobility, and consequences for performance. A. Holewinski, M. Sakwa-Novak, C.W. Jones

4:15 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

Polymeric Biomaterials

Drug Delivery and Controlled Release

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

1:25 PMSE 249. Lanthanide-containing polycarbonates for imaging and monitoring polyplex dynamics. L. Xue, S. Kelkar, T.M. Reineke

1:55 PMSE 250. Synthesis and evaluation of peptide-based polymers for biomedical applications. L. Chan, C. Ngambenjwong, D. Chu, M. Cieslewicz, X. Wang, H. Wei, Y. Cheng, N. White, P. Horner, S. Pun

2:25 PMSE 251. Gene-delivering non-viral systems from PEI-g-PEG and PEI-functionalized telechelic PEG: Effect of polymer architecture on gene transfection efficiency and cyto-toxicity. L. Cedrone, M. George, V. Mityushin, W. Holmes, R. Bellin, S. Granados Focil

2:45 PMSE 252. Self-assembly of PEGylated poly(amino acids) and their use in DNA complexation. C. Scholz, D. Ulkoski, A. Meister, J. Kressler

3:05 Intermission.

3:20 PMSE 253. Designer antimicrobial materials. A. Shukla

3:50 PMSE 254. Phenylboronic acid-installed polycarbonates: synthesis and use as drug carriers. Y. Aguirre-Chagala, J.L. Santos, M. Herrera-Alonso

4:20 PMSE 255. Temporal control over multiple biological signals using photochemical reactions. M.A. Azagarsamy, K.S. Anseth

4:40 PMSE 256. Comb polymers for non-viral gene delivery. R. Lettieri, S. Parellar, R. Elder, A. Jayaraman, T. Emrick

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Drug Delivery and Drug Device Combination Products

Nanotechnology for Oncology

A. S. Kulshrestha, P. Timmins, *Organizers*

S. Sriharan, *Organizer, Presiding*

S. R. Raghavan, *Presiding*

1:30 PMSE 257. Polyacrylamide nanogels for potential cancer therapy. K. Neoh, S. Lu, E. Kang, R. Mahendran, E. Chiong

1:55 PMSE 258. Development and evaluation of CD44-targeted lipid-based nanoparticles in an orthotopic non-small cell lung cancer xenograft mouse model. S.R. Benhabbour, J.M. DeSimone, R. Mumper, A. Webster, C. Luft

2:20 PMSE 259. Bio-inspired cocoon-like DNA-nanoclew for anticancer drug delivery. W. Sun, R. Mo, Y. Lu, Z. Gu

2:45 PMSE 260. Invertible micellar polymer assemblies for targeted delivery of curcumin to osteosarcoma cells. O. Kudina, K.L. Shogren, C.T. Gustafson, M.J. Yaszemski, A. Maran, A.S. Voronov

3:10 PMSE 261. Modulation of immune response along with bax and bcl-2 mediated enhanced apoptosis in breast cancer cells via paclitaxel loaded vitamin E nanoemulsion. V.K. Pawar, M.K. Chourasia

3:35 PMSE 262. Nanogels from metal-chelating crosslinkers applied to copper-64 PET imaging of tumors and metastases. J. Lux, A.G. White, M. Chan, C.J. Anderson, A. Almutairi

Section D

Sheraton Denver Downtown Hotel
Directors Row H

Nanoscale Spectroscopic and Microscopic Characterization**Nanomechanical Characterization**

Financially supported by ExxonMobil Chemicals; Bruker; Nanosurf

A. H. Tsou, D. Yablou, *Organizers*
M. B. Raschke, *Presiding*

1:30 PMSE 263. Nanomechanical characterization of polymers by atomic force microscopy: dynamic and quasi static approaches. C. Dietz, A. Voss, M. Schulze, R. Stark

2:00 PMSE 264. AFM-based viscoelasticity measurement for polymeric materials. K. Nakajima

2:30 PMSE 265. Molecular scale imaging of semicrystalline polymers. J.K. Hobbs, N. Mullin, R. Savage

3:00 PMSE 266. Deformation rate dependence of nanomechanical properties as measured by atomic force microscopy. B. Pittenger, T. Mueller

3:20 Intermission.

3:30 PMSE 267. Viscoelastic AFM nanomechanics in non-ambient environments. J. Killgore

4:00 PMSE 268. Advances in nanomechanical characterization of polymer materials with scanning probe microscopy. D. Yablou

4:20 PMSE 269. Studies of stimuli responsive polymer composites grafts by colloidal probe microscopy. S.L. Skiles, J. Spear, D. Bergbreiter, J.D. Batteas

4:40 PMSE 270. Photothermally excited contact resonance imaging in air and water. M. Kocun, A. Labuda, A. Gannepalli, R. Proksch

Section E

Sheraton Denver Downtown Hotel
Governor's Square 17

Stimulus-Responsive Assemblies and Materials**Biomedical Applications of Stimulus-Responsive Assemblies**

C. Bowman, J. Cha, *Organizers*
A. P. Goodwin, *Organizer*, *Presiding*

1:30 PMSE 271. Maltodextrins image bacterial infections and drug resistance by positron emission tomography. N. Murthy

2:00 PMSE 272. Tailored supramolecular structures for the controlled release of therapeutics and for polymeric antimicrobials. J.L. Hedrick

2:30 PMSE 273. Photocleavable linkers for cell and protein micropatterning. S.V. Wegner, O. Senturk, J.P. Spatz

2:50 PMSE 274. Stimuli-responsive self-folding soft-grippers for drug delivery. H. Kwag, K. Malachowski, J. Breger, M.O. Wang, J. Fisher, F.M. Selaru, D.H. Gracias

3:10 PMSE 275. Light-responsive strategy for reversible control of elastic modulus in PEG-based hydrogels. A. Rosales, K. Mabry, E. Nehls, K.S. Anseth

3:30 Intermission.

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.

3:45 PMSE 276. Squeezable tubules from self-assembly of amphiphilic macrocycles. M. Lee

4:15 PMSE 277. Triggering the de novo synthesis of phospholipid membranes. N.K. Devaraj

4:45 PMSE 278. Stimuli-responsive uptake and release of polyelectrolytes by amphiphilic microgels. W. Richtering, A. Gellissen, F. Plamper, A. Schmid, D. Pergushov, I. Potemkin, A. Pich

5:05 PMSE 279. Molecular-level interactions in the design of reversible and recyclable flocculants. K.L. Morrissey, R.Z. Chapman, L. Zolnierowski, M. Keirn, G. Henry, M.P. Stoykovich

Section F

Sheraton Denver Downtown Hotel
Governor's Square 15

ACS Award in Polymer Chemistry: Symposium in Honor of Nikos Hadjichristidis**Well-Defined Polymers: From Design to Applications**

Financially supported by ExxonMobil

J. Frechet, Y. Gnanou, *Organizers*
M. Moller, *Presiding*

1:00 PMSE 280. Hypersonic phononic particle brush materials. G. Fytas

1:30 PMSE 281. Regular highly branched polymers: From polymeric to colloidal properties. D. Vlassopoulos

2:00 PMSE 282. Dynamic covalent polymers as viscosity modifiers. T. Nguyen, R. Nicolay, L. Leibler

2:30 Intermission.

3:00 PMSE 283. Ring opening metathesis polymerization for the synthesis of complex macromolecular architectures. M. Pitsikalis

3:30 PMSE 284. Smart hybrid nanocarriers to treat pancreatic cancer. H. Iatrou

4:00 PMSE 285. Synthesis, structure-property studies in lactic acid derived polymers: Multiarm branched polymers and copolymers of by "core-first" and "arm-first" approach. S. Sivaram

4:30 PMSE 286. Polymeric surfaces exhibiting photocatalytic activity and controlled wettability with anisotropic features. S.H. Anastasiadis, M.A. Frysali, L. Papoutsakis, G. Kenanakis, E. Stratakis, M. Vamvakaki, S. Pispas

5:00 PMSE 287. Directed self-assembly of block copolymers. A. Avgeropoulos

Section G

Sheraton Denver Downtown Hotel
Governor's Square 10

Polymer Modeling: Structure, Dynamics and Function**Self-Assembly and Structure Development**

Financially supported by ExxonMobil; Dow Chemical

R. Locker, G. C. Rutledge, *Organizers*
V. K. Kuppala, *Presiding*

1:00 PMSE 288. Ultracoarse-grained simulation of biopolymers. G.A. Voth

1:30 PMSE 289. Multiresolution modeling of polymers: Wavelet-based reconstruction. C.S. Adorf, A. Agarwal, B. Rabideau, C.R. Iacobella, A.E. Ismail

1:50 PMSE 290. Computational analysis of solvent effects on electron transfer in organic radical battery cathode materials. R.E. Larsen, T.W. Kemper, W. Braunecker, B.K. Hughes, D. Bobela, A. Ferguson, T. Gennett

2:10 PMSE 291. Effect of short chain branching on the properties of semi-crystalline polyethylene. V. Kumar, R. Locker, G.C. Rutledge

2:30 PMSE 292. Usage of Poly(NIPAm) in the biofuel production. J.V. Ribeiro, R.C. Bernardi, K. Schulten

3:00 PMSE 293. Coarse-grained simulations of solvent-assisted self-assembly of block copolymer thin films. S. Hur, M. Mueller, P.F. Nealey, J.J. De Pablo

3:20 PMSE 294. Folding behavior of polypeptide-grafted comb-like macromolecules. Y. Ren, Y. Zhang, H. Xia, J. Cheng, Y. Lin

3:40 PMSE 295. Molecular dynamics simulations of structure and effective interactions of diblock copolymer grafted nanoparticles in a homopolymer blend matrix. C. Estridge, A. Jayaraman

Energy and Materials

Sponsored by POLY, Cosponsored by PMSE

Macromolecular and Nanoparticle Separation Science

Sponsored by POLY, Cosponsored by ANYL and PMSE

TUESDAY EVENING**Section A**

Colorado Convention Center
Hall D

Joint PMSE/POLY Poster Session

Cosponsored by POLY†

Q. Lin, *Organizer*

6:00 - 8:00

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications.

PMSE 296. Synthesis, characterization of graphene incorporated polyamide resin. A. Musa, A. AlSheikh, T.A. Saleh

PMSE 297. Graphene filler and graphenated nanogels. I. Yaghoobi Rad, J.W. Stansbury

Nanoscale Spectroscopic and Microscopic Characterization of Polymers.

PMSE 298. Quantitative modulus mapping of polymer thin films using tapping mode. M. Kocun, A. Labuda, R. Proksch

Polymeric Biomaterials.

PMSE 299. Structure and properties of bisoxalamide-based segmented block-copolymers with controlled crystal thickness. D. Anokhin, M. Rosenthal, Y. Odarchenko, N. Sijbrandi, P. Dijkstra, J. Feijen, D. Ivanov

PMSE 300. Synthesis and characterization of anorganic bone/polyglycolide composites. L. Gauza, K. Papke, K. Thorpe, J. Redepinning

PMSE 301. Influence of nanocarbons on collagen molecular ordering and fibril alignment. E.C. Green, M.L. Minus, D. Aishanjiang

PMSE 302. Folding graft copolymer with pendant drug segments for co-delivery of anticancer drugs. W. Tai, Y. Lu, R. Mo, Z. Gu

PMSE 303. Plasma modification of 3D, bioresorbable, polymeric scaffolds: Customizing surface chemistry to fabricate bioactive and bioinert materials. M.J. Hawker, A. Pegalajar-Jurado, E.R. Fisher

PMSE 304. Solute stabilization via amphiphilic polymers possessing different architectures. H. Luo, J.L. Santos, M. Herrera-Alonso, B.A. Aguilar-Castillo

PMSE 305. 4D printing for spatially and temporally dynamic bioscaffolds. J.M. McCracken, R.G. Nuzzo

PMSE 306. Positive effect of biaxial stretching on the mechanical behavior of PLA-Talc nanocomposites. S. Ouchiar, G. Stoclet, C. Cabaret, J. Gloaguen, V. Gloaguen, J. Lefebvre

PMSE 307. Development of a hyperbranched polymer theranostic for prostate cancer. A. Pearce, B.E. Rolfe, A.V. Fuchs, P.J. Russell, A.K. Whittaker, K.J. Thurecht

PMSE 308. Synthesis, characterization, and antibacterial activity evaluation of a water-soluble chitosan derivative and its application on paper. G. Rodriguez Galindo, R. Manriquez Gonzalez, J. Andrade Ortega, J. Casas Solis, E. Delgado

PMSE 309. Impact of cross-linking on rate of release of pyridoxine from Zein fibers and films. G.W. Selling, E. LaFont, K.D. Utt

PMSE 310. Targeted CT imaging of human hepatocellular carcinoma using low-generation dendrimer-entrapped gold nanoparticles modified with lactobionin acid. Y. Cao, Y. He, H. Liu, Y. Luo, M. Shen, J. Xia, X. Shi

PMSE 311. Withdrawn.

PMSE 312. Thermomechanical properties of poly(L-lactide)/poly(D-lactide) blends. G. Stoclet

Stimulus-Responsive Assemblies and Materials.

PMSE 313. In situ functionalization of azlactone-based polymer brushes. B.M. Aden, B.S. Lokitz, M. Kilbey

PMSE 314. Single-molecule resolution of polymer diffusion on a thermo-responsive polymer brush. H. Chin, D.K. Schwartz

PMSE 315. CO₂ adjustable and magnetic recyclable catalyst-supports based on "smart" hybrid nanoparticles. A. Feng, J. Yuan

PMSE 316. Thermally-responsive phosphorus-filled nanobrick wall multilayer thin film eliminates polyurethane melt dripping and reduces heat release associated with fire. A. Cain, Y. Li, R.D. Davis, C. Nolen, M. Huff, J.C. Grunlan

PMSE 317. Surface charge generation in nanogels for activated cellular uptake at tumor-relevant pH. L. Li, K. Raghupathi, C. Yuan, S. Thayumanavan

PMSE 318. Ketal-containing polyacrylates and polyacrylamides as building blocks for multi-responsive nanomedicines. B. Louage, B. De Geest

PMSE 319. Biocompatible mesoporous carbon nanocapsule as a nanoreactor: In situ synthesis of imaging nanoparticles and surface modifications for stimuli responsive theranostic applications. G. Mishra, A. Rammohan, A. Mukhopadhyay, S. Sivakumar, A. Sharma

PMSE 320. Diffusion of photoabsorbing degradation byproducts in photodegradable polymer networks. S. Norris, A.M. Kasko, T. Chou

PMSE 321. Light-triggered chemical amplification to accelerate degradation and release from polymeric particles. J. Olejniczak, V. Nguyen Huu, J. Lux, M.R. Grossman, A. Almutairi

PMSE 322. Swellable polysiloxane elastomers as substrates for passive radio frequency identification (RFID) gas sensors. C. Rumes, M. Ziai, K. Belsey, J. Batchelor, S.J. Holder

PMSE 323. Strong attraction among the carboxylic acid-functionalized hydrophilic fullerene giant anions and the spontaneous, reversible self-assembly in dilute solution. P. Yin, T. Liu

Well-Defined Polymers: From Design to Applications — ACS Award in Polymer Chemistry Symposium in Honor of Nikos Hadjichristidis.

PMSE 324. Phosphazene-catalyzed ring-opening polymerization of ε-caprolactone and epoxide. H. Alamri

PMSE 325. Synthesis and characterization of poly(vinyl ether)-based graft polymers by combination of living polymerization techniques. R. Alghamdi, H. Boucheff, N. Hadjichristidis

PMSE 326. Triblock and pentablock terpolymers of functionalized vinyl ethers by base-assisted living cationic polymerization. A. Al-sulami, H. Boucheff, N. Hadjichristidis

PMSE 327. Withdrawn.

PMSE 328. Ruthenium N-heterocyclic carbene star polymer. K. Bukhriakov, C. Muegmana, V. Rodionov

PMSE 329. Anion-conducting block copolymer membranes for artificial photosynthesis. P. Cotanda, N.P. Balsara

PMSE 330. Methyl methacrylate polymerization by Frustrated Lewis Pairs (FLPs): Polymerization and termination mechanism. L. Falivene, L. Caporaso, L. Cavallo

† Cooperative Cosponsorship

- PMSE 331.** Organopolymerization of acrylic monomers by N heterocyclic carbenes. I. **Falivene, L. Caporaso, L. Cavallo**
- PMSE 332.** Mechanistic insight into the ethylene reactivity promoted by phosphine-sulfonamide palladium(II) complexes. I. **Falivene, L. Caporaso, L. Cavallo**
- PMSE 333.** Carbon dioxide based building blocks for polycarbonate synthesis by polycondensation and ring opening polymerization. **D. Pati, X. Feng, N. Hadjichristidis, Y. Gnanou**
- PMSE 334.** Development of nanoporous membranes by block copolymer self-assembly for biofuel production. **N. Petzetakis**
- PMSE 335.** Enzyme-inspired soft materials for catalysis by design. **V.O. Rodionov**
- PMSE 336.** Synthesis of macromolecular architectures with a high hydrophobic/hydrophilic contrast by ring-opening metathesis polymerization. **V.O. Rodionov, C. Jehanno, K. Bukhariakov**
- PMSE 337.** Facile metal-free “grafting-from” route from acrylamide-based substrate toward complex macromolecular combs. **J. Zhao, H. Alamri, N. Hadjichristidis**
- General Papers/New Concepts in Polymeric Materials.
- PMSE 338.** Nitric oxide releasing polymeric systems for wound healing applications. **K.A. Arabea, A. Pegalajar-Jurado, K.A. Wold, M.M. Reynolds**
- PMSE 339.** Design, surface modification, and evaluation of cell-growth directive properties of 3D hydrogel scaffolds. **A. Badea, J.M. McCracken, R.G. Nuzzo**
- PMSE 340.** Study of antibacterial properties of silver chloride/poly (3-hydroxybutyrate-co-3-hydroxyvalerate) (AgCl/PHBV) composite: A potential scaffold for bone tissue regeneration. **R.A. Bakare**
- PMSE 341.** Crystallinity determination of poly(3-hexyl thiophene) thin films by means of fast scanning calorimetry. **J. Balko, A. Rinscheid, A. Wurm, C. Schick, R. Lohwasser, M. Thelakkat, T. Thurn-Albrecht**
- PMSE 342.** Role of PEO-segment lengths in surface properties of antiogelling PEG-silane amphiphile. **M. Barry, M.A. Ruffin, P.A. Adair, M. Grunlan**
- PMSE 343.** Synthesis of highly swellable functional poly(dimethylsiloxane) composites for use as selective gas and solvent sensors. **K. Belsey, C. Rumens, S.J. Holder**
- PMSE 344.** Determining temperature change on photothermal Au nanorod and Au nanocage using smart polymers. **B. Buyukbekar, H. Cavusoglu, H. Sakalaki, M. Citir, G. Demirel, M. Yavuz**
- PMSE 345.** MALDI MS results for organotin polyamines from reaction of 3-amino-1,2,4-triazole and organotin dihalides. **C.E. Carraher, Jr., V. Suresh, R. Crichton, M.R. Roner**
- PMSE 346.** Synthesis of organotin polyamines from reaction of 3-amino-1,2,4-triazole and organotin dihalides. **C.E. Carraher, Jr., R. Crichton, M.R. Roner**
- PMSE 347.** Inhibition of cancer cell lines by organotin polyesters synthesized from reaction of the salt of D-camphoric acid and organotin dihalides. **M.R. Roner, C.E. Carraher, Jr., A. Moric-Johnson, L. Miller, A. Campbell**
- PMSE 348.** Initial study of the ability of organotin polyethers derived from the anticoagulant dicumaryl to inhibit cancer cell lines. **M.R. Roner, C.E. Carraher, Jr., A. Moric-Johnson, L. Miller, N. Sookedo**
- PMSE 349.** Inhibition of cancer cell lines by the organotin polyether esters synthesized from reaction of the salt of alpha-cyano-4-hydroxycinnamic acid and organotin dihalides. **C.E. Carraher, Jr., M.R. Roner, A. Moric-Johnson, L. Miller, V. Suresh**
- PMSE 350.** Use of the diocetyl tin polyether ester synthesized from reaction of alpha-cyano-4-hydroxycinnamic acid and diocetyl tin dichloride itself acting as the MALDI MS matrix. **C.E. Carraher, Jr., V. Suresh, M.R. Roner**
- PMSE 351.** Interfacial profile control in cross-linkable block copolymers for improved pattern transfer. **G. Chado, C. He, M.P. Stoykovich**
- PMSE 352.** Behavior of compatibilizers with different chemical structure in polyethylene-MMT nanocomposites. **C. Chapple, N. Shabestary**
- PMSE 353.** Carbon nanotube polymer nanocomposites for potential solder application. **C. Chen, S. Ganguli, A.K. Roy**
- PMSE 354.** Tuning of the glass transition temperature of epoxy polymer. **C. Chen, S. Ganguli, A.K. Roy**
- PMSE 355.** Cyclopentadiene-Based π-Conjugated Polymers. **L. Chen**
- PMSE 356.** Fully physical double network hydrogels with high strength and fatigue resistance. **Q. Chen, L. Zhu, H. Chen, J. Zheng**
- PMSE 357.** Redox active polymers for size-exclusion transport in nonaqueous redox flow batteries. **N. Gavvalapalli, J. Hui, K.J. Cheng, T. Lichtenstein, M. Shen, J.S. Moore, J. Rodriguez-Lopez**
- PMSE 358.** Step-growth dental composites with improved mechanical performance from photopolymerized thiol-vinyl sulfone resins. **M.J. Claudino, P.K. Shah, M. Podgoriski, E. Becka, J.W. Stansbury, C. Bowman**
- PMSE 359.** Nonviral gene therapy applications of multifunctional fluorescent quantum dots. **J.M. Davis, M. Ellis, N. Mundt, K. Fichter**
- PMSE 360.** Controlling transport through a cubic-phase lyotropic liquid-crystalline polymer nanofiltration membrane via anion exchange. **S. Dischinger, B.M. Carter, D. Gin, R.D. Noble**
- PMSE 361.** Shape memory polyurethane aerogels. **S. Donthula, F. Zheng, C. Sotiropoulos, N. Leventis**
- PMSE 362.** Synthesis of Gd-doped quantum dots for theranostic applications with multiple imaging modalities. **M.A. Ellis, N. Mundt, K. Fichter**
- PMSE 363.** Chemically modified dendritic starch: A novel nanomaterial for siRNA delivery. **S.A. Engelberth, N. Hempel, M. Bergkvist**
- PMSE 364.** Mechanical properties and electromagnetic interference shielding effect of epoxy composite reinforced with Ni-plated basalt chopped fiber. **W. Eom, H. Kim**
- PMSE 365.** Synthesis of highly gas-selective triptycene-based polymers of intrinsic microporosity (TPIMs). **B.S. Ghanem, R. Swaidan, E. Litwiller, I. Pinnau**
- PMSE 366.** Synthesis of poly(2-methacryloxy ethyltrimethyl ammonium chloride) brushes by ATRP on magnetic nanoparticles. **L. Qin, H. Han, Y. Xu, L. Li, X. Guo**
- PMSE 367.** In situ preparation of Ag/Au nanoparticle bilayer via layer-by-layer assembly in spherical polyelectrolyte brushes. **F. Zhao, J. Wang, Y. Tian, L. Li, X. Guo**
- PMSE 368.** Phase behavior of spherical polyelectrolyte brushes solution in supercritical carbon dioxide. **L. Liu, Y. Wen, Y. Cang, J. Zhang, Z. Yu, X. Hou, R. Zhang, X. Guo**
- PMSE 369.** Influence of compressed gas on the solubility of inorganic salt in reverse micelle. **J. Zhang, Y. Cang, Y. Wen, L. Liu, X. Hou, Z. Yu, R. Zhang, X. Guo**
- PMSE 370.** Assessment of subcutaneous injection pads as acceptable skin mimics. **R. Gupta, D. Karvani, C. Clawson, S. Pansare, S. Patel, S. Dutta Ray**
- PMSE 371.** Characterization of the distribution of deuterium as a function of molecular weight in D-labeled commercial polyolefins. **B.M. Habersberger**
- PMSE 372.** Functional β-sheet stabilized polypeptide microspheres by NCA-ROP and noncovalent entrapment. **S. Harris Wibowo, G. Qiao**
- PMSE 373.** Pyrene-modified polyelectrolytes/MWNT LbL assemblies extinguish flames on polyurethane foam. **A. Cain, M. Plummer, B. Stevens, T. Smith, P. Odenborg, K.M. Holder, J.C. Grunlan**
- PMSE 374.** Intumescent nanocoating extinguishes flame on fabric using aqueous polyelectrolyte complex deposited in single step. **A. Cain, S. Murray, K.M. Holder, C. Nolen, M. Huff, J.C. Grunlan**
- PMSE 375.** Extending soft lithography methods to generate patterned hydrogels. **H.G. Jayasinghe, Y. Vasquez**
- PMSE 376.** Investigation of effect of bulky and hydroxyl groups in the polyimide membrane for gas separation. **S. Nam, D.J. Kim, H. Koh, S. Ha**
- PMSE 377.** Reversible transformation of planar sheets into nanocapsules by host-guest trigger. **Y. Kim, M. Lee**
- PMSE 378.** Elastomeric microfluidic reactors for use with 2D and 3D surfaces. **A. Konda, M.A. Stoller, S.A. Morin**
- PMSE 379.** Withdrawn.
- PMSE 380.** Can we tune the color of organic charge transfer systems by varying their donor-acceptor interaction geometry? **P. Li, J. Hwang, J.M. Maier, M.D. Smith, K.D. Shimizu**
- PMSE 381.** Design, synthesis, and gas transport properties of spirobifluorene-based intrinsically microporous polyimides (SPIM-PI). **X. Ma, B. Ghanem, R. Swaidan, E. Litwiller, I. Pinnau**
- PMSE 382.** Assessment of freeze drying as a technique to obtain silver nanoparticles and easing its incorporation in silver/chitosan composites for its potential use as an antibacterial film in medical devices. **G. Madrigal, P. Zuniga, A. Dickerman, C. Chaves-Villarreal**
- PMSE 383.** Synthesis and characterization of robust terephthalaldehyde-phloroglucinol (TPOL) aerogels as precursors for nanoporous carbons. **H. Majedifar, M.A. Saeed, S. Donthula, N. Leventis, C. Sotiropoulos**
- PMSE 384.** Donor-acceptor core-shell nanoparticles for organic photovoltaics. **K. McKenna, J. Ferguson, H.P. Rathnayake**
- PMSE 385.** Highly specific quantum dot bioconjugates for single molecule imaging. **N. Mundt, M. Butts, K. Fichter**
- PMSE 386.** Comparison of ion transport property of the ion exchange membrane by molecular dynamic simulation. **S. Nam, C. Park, D.J. Kim**
- PMSE 387.** Alginate microspheres with encapsulated *lactobacillus* for potential bladder cancer therapy. **K. Neoh, L. Shi, E. Kang, R. Mahendran, E. Chiong**
- PMSE 388.** Plasma surface modifications of nitric oxide releasing polymer films for increased hydrophilicity. **B.H. Neufeld, A. Pegalajar-Jurado, M. Hawker**
- PMSE 389.** Crystallization kinetics and interfacial behavior of multiwalled carbon nanotubes based polypropylene composites. **S. Parjia, A.R. Bhattacharyya**
- PMSE 390.** Glass transitions of individual microdomains in phase-mixed poly(urethane urea) elastomers investigated by solid-state NMR. **N.V. Patil, W. Hu, A. Hsieh**
- PMSE 391.** Thiol-ene/anhydride networks for tunably degradable neural substrates. **R. Reit, V. Agrawal, B.R. Lund, W. Voit**
- PMSE 392.** Ferrocene-based polyamide aerogels: Graphitization, transmetalation, and use in heterogeneous catalysis. **M.A. Saeed, C.A. Wisner, S. Donthula, A. Mumtaz, C. Sotiropoulos, N. Leventis**
- PMSE 393.** Self-healing potential of triazole-pyridine based metallopolymers. **B. Sandmann, B. Happ, S. Kupfer, S. Gräfe, F.H. Schacher, M.D. Hager, U.S. Schubert**
- PMSE 394.** Metal-free cycloaddition of internal alkynes and multifunctional azides under solvent-free conditions. **B. Sandmann, B. Happ, M.D. Hager, J. Vitz, R. Paulus, P. Bartscher, N. Moszner, U.S. Schubert**
- PMSE 395.** In vivo evaluation of mithramycin analog nanoformulations. **D. Scott, P. Cao, J. Rohr, Y. Bae**
- PMSE 396.** Effect of different fillers on the durability and mechanical properties of LDPE and PVC composites. **M.N. Siddiqui, H.H. Redhwi, M. Younas, S. Hussain**
- PMSE 397.** Synthesis of donor-acceptor conjugated copolymers via acyclic diene metathesis (ADMET) and Suzuki polycondensation (SPC). **G. Singh, H. Ardolic, M. Montano, R.M. Peetz**
- PMSE 398.** Synthesis and characterization of PTT using novel catalyst. **G. Song, M. Huang, X. Li, W. Zhou, W. Yang**
- PMSE 399.** Applications of addition fragmentation chain transfer. **N. Sowan, L. Cox, Y. Ding, C. Bowman**
- PMSE 400.** Computational design of polyethylene glycol (PEG) brushes for display of biofunctional molecules for delivery applications. **F. Stanzone, A. Jayaraman**
- PMSE 401.** Increasing hydrophobic interactions in a polyelectrolyte for improved oxygen barrier in multilayer nanocomposite thin films. **B. Stevens, J.C. Grunlan**
- PMSE 402.** Programmed shape change of 2D thermoplastic structures into 3D components. **M. Vannoy, A. Konda, S.A. Morin**
- PMSE 403.** Synthesis and structure-property relationship of novel azobenzene-containing diamines and polyimides. **D.H. Wang, M.L. Baczkowski, J. Wie, T.J. White, L. Tan**
- PMSE 404.** Controlled formation and dissolution of polymer suspension with visible light. **Z. Wang, Y. Liao**
- PMSE 405.** Microfluidic encapsulation and photopolymerization of single cell-laden microgel. **B. Xia, J. Oakley, K. Krutkramelis**
- PMSE 406.** pH-responsive polymeric microspheres for micronutrients fortification of salt. **X. Xu, Y. Zeng, E. Rosenberg, R. Langer, A. Jablekene**
- PMSE 407.** Withdrawn.
- PMSE 408.** Biodegradable nitric oxide-releasing S-nitrosated derivatives of citrate elastomer for biomedical applications. **P. Yapor**
- PMSE 409.** Shape memorizing micro and nano polymer particles. **L. Cox, Y. Ding, J. Xiao, M.P. Stoykovich, Z. Zhang, Z. Li, J. Killgore**
- PMSE 410.** Arylene-ethylene polymer with high ethylene/ethane adsorption selectivity. **C. Yu, M.G. Cowan, R.D. Noble, W. Zhang**
- PMSE 411.** Effects of substrate on the gradient structure and surface properties of fluorinated polycarylates latex blends film. **H. Yuanyuan, Z. Chaoan, C. Yanjun**
- PMSE 412.** Capillary instability of polymer lithographic structures: Influence of viscosity, substrate confinement and local curvature. **Z. Zhang, G. Hilton, Y. Ding**
- Energy and Materials**
Sponsored by POLY, Cosponsored by ENFL and PMSE
- Innovations in Macromolecular Network Chemistry**
Sponsored by POLY, Cosponsored by PMSE
- Next Generation Smart Materials**
Sponsored by POLY, Cosponsored by PMSE

WEDNESDAY MORNING

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

Polymeric Biomaterials

Sensors and Medical Devices

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

8:25 **PMSE 413.** Synthesis and characterization of poly(N-acryloylamino-Ethoxyethanol)-based antifouling materials. **H. Chen, M. Zhang, R. Hu, C. Zhao, J. Zheng**

Section F

Sheraton Denver Downtown Hotel
Plaza Court 8

General Papers/New Concepts in Polymeric Materials

New Concepts in Polymeric Materials

Q. Lin, Organizer
H. Dong, A. Shirke, Presiding

8:30 PMSE 536. Efficient Cu(I) acetate-catalyzed cycloaddition of multifunctional alkynes and azides under solvent-free conditions. **B. Sandmann**, B. Happ, M.D. Hager, J. Vitz, R. Paulus, E. Rettler, P. Burtscher, N. Moszner, U.S. Schubert

8:50 PMSE 537. Withdrawn.

9:10 PMSE 538. Toughening a glassy polymer with naturally derived cellulose nanofibrils. **H. Dong**, J. Steele, J.F. Snyder, J.A. Orlicki, G. Napadensky, R.S. Reiner, A.W. Rudie

9:30 PMSE 539. Surfactant-direct assembly of water soluble conjugated polyelectrolytes. **G. Braggini**, S. Zhang

9:50 PMSE 540. Sustainable large-scale solvent driven actuation by self-healable polyelectrolyte multilayers. **Y. Gu**, X. Huang, N. Zacharia

10:10 Intermission.

10:30 PMSE 541. Preparation of poly(methyl methacrylate/butyl acrylate) nanoparticles by miniemulsion polymerization in the presence of commercially available hydrophobized TiO₂ nanoparticles. **E.S. Adurahim, M.A. Bahattab**, A. Schoth, K. Landfester, R. Munoz-Espi

10:50 PMSE 542. Cutinase paradigm: Sustainable biocatalysis for polymer surface modifications and plastic recycling. **A. Shirke**, D. Basore, A. Su, S. Holton, G. Butterfoss, C. Bystruff, R.A. Gross

11:10 PMSE 543. Chain mobility and penetrant transport in poly(ethylene furanolate) compared to poly(ethylene terephthalate). **S.K. Burgess**, R.M. Kriegel, W.J. Koros

11:30 PMSE 544. Proton conduction in a cephalopod structural protein. **D.D. Ordinario**, L. Phan, W.G. Walkup, J. Jocsion, E. Karshalev, N. Hüskken, A.A. Gorodetsky

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels
Sponsored by POLY, Cosponsored by PMSE†

Innovations in Macromolecular Network Chemistry

Medical: Hydrogels and Particles

Sponsored by POLY, Cosponsored by PMSE

PROF

Division of Professional Relations

R. D. Libby, Program Chair

BUSINESS MEETINGS:

PROF Division Business Meeting, 3:00 PM:
Tue

SUNDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 6

Native American Women Chemists of Color

Cosponsored by CMA and WCC

L. M. Watkins, Organizer
N. B. Jackson, G. Thomas, Presiding

8:30 Introductory Remarks.

8:40 PROF 1. Otakuye Conroy-Ben: University of Utah. **O. Conroy-Ben**

8:50 PROF 2. Robyn Hannigan, University of Massachusetts Boston. **R. Hannigan**

9:00 PROF 3. Joslynn Lee, University of Minnesota Medical School. **J. Lee**

9:10 PROF 4. Naomi Lee, National Institutes of Health. **N. Lee**

9:20 PROF 5. Amy Paris, Kimberly-Clark Corporation. **A.K. Paris**

9:30 Panel Discussion.

10:30 Intermission.

10:45 Questions and Answers.

11:45 Concluding Remarks.

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored by CHED, PROF and YCC

SUNDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 6

Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations

Cosponsored by BMGT, SCHB and WCC

J. L. Bryant, Organizer, Presiding
A. S. Hinkle, Presiding

1:00 Introductory Remarks.

1:15 Moderated Panel I.

2:00 Hands-On Working Sessions.

2:45 Report Out from Working Groups.

3:00 Intermission.

3:15 Introductory Remarks.

3:20 Moderated Panel II.

4:00 Hands-On Working Sessions.

4:45 Report Out from Working Groups.

4:55 Concluding Remarks.

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored by CHED, PROF and YCC

Starting a Successful Research Program at a Predominantly Undergraduate Institution

Sponsored by YCC, Cosponsored by PROF

MONDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 6

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in Honor of E. Ann Nalley

Championing the Empowerment of Women in Chemistry

Cosponsored by WCC

Z. M. Lerman, Organizer

F. K. Wood-Black, Organizer, Presiding

8:30 Introductory Remarks.

8:35 PROF 6. Ann Nalley: A teacher — a colleague — a legacy. **D.G. McGuire**

9:00 PROF 7. The importance of mentoring in developing female leaders. **M. Jeffries-El**

9:25 PROF 8. Inspiration for generations. **K. Galindo**

9:50 PROF 9. Paying it forward: Small actions and encouragement result in a grand legacy. **F.K. Wood-Black**

10:15 PROF 10. Chain reaction—the smallest things have the biggest impact: A window into how Ann Nalley changed my life. **C.J. Siddons**

10:40 Intermission.

10:50 PROF 11. Ann Nalley: Consummate and tireless teacher, friend, mentor, scholar, and international leader in promoting women in science. **T. Conley**

11:15 PROF 12. NanoExplorers: A high school summer science academy and applied mathematics and aerospace engineering summer academy for middle school girls. **J.L. Gesell**, E.A. Nalley, M. Polson

11:40 PROF 13. How to get buy in the: Woodall Nalley theory. **R.A. Woodall**

12:05 Concluding Remarks.

Diversifying STEM: Uniting through our Differences for a Brighter Scientific Future

Sponsored by CMA, Cosponsored by CHED and PROF

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 6

Chemical Angel Network: Chemists Investing in Chemical Companies

Cosponsored by SCHB

J. L. Bryant, M. Vreeke, Organizers

S. S. White, Organizer, Presiding

1:30 Introductory Remarks.

1:35 PROF 14. News and updates from the Chemical Angel Network (CaN). **M. Vreeke**, S.S. White, J.C. Giordan

2:00 PROF 15. Angel Investing 101. **J.C. Giordan**

2:30 Company Presentations.

3:30 Investment Discussion.

4:00 Open Forum.

4:30 Concluding Remarks.

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 6

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in Honor of E. Ann Nalley

Championing the Empowerment of Women in Chemistry

Cosponsored by WCC

F. K. Wood-Black, Organizer

Z. M. Lerman, Organizer, Presiding

8:30 Introductory Remarks.

8:35 PROF 16. Ann Nalley, the female trail-blazer. **A. Pavlath**

9:00 PROF 17. Experiences with Ann Nalley Spanning 30 years. **D.J. Nelson**

9:25 PROF 18. Honoring Ann Nalley, a friend, mentor, and champion for women in science. **M.P. Wu**

9:50 Intermission.

10:00 PROF 19. Woman of valor: More precious than pearls. **Z.M. Lerman**

10:25 PROF 20. The Legacy of Dr. E. Ann Nalley. **O.D. Nelson**

10:50 PROF 21. What women can do (WWCD©): The future is really up to us. **J.C. Giordan**

11:15 PROF 22. Award Address (ACS Award for Encouraging Women into Careers in the Chemical Sciences sponsored by the Camille and Henry Dreyfus Foundation). Inspiring women in chemistry: Leading by example. **E.A. Nalley**

11:40 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 6

Proposing and Administering a Successful REU Program

L. M. Watkins, Organizer
G. Thomas, Presiding

1:00 Introductory Remarks.

1:05 PROF 23. REU site focusing on regional 2-yr community college students. **W. Jang**, **A.D. Headley**, **S.D. Starnes**

1:30 PROF 24. Hosting an REU at a PU: Benefits and challenges. **S.B. Braun-Sand**, **A.M. Schoffstall**

1:55 PROF 25. Description of an inaugural Research Experiences for Undergraduates (REU) program. **A.M. Powe**

2:20 PROF 26. Chemistry REU program at the University of Kansas. **D.R. Benson**

2:45 PROF 27. CheMIE REU chemistry research community with a focus on molecular innovation and entrepreneurship. **W.M. David**, **W.J. Brittain**

3:10 Intermission.

3:25 PROF 28. Exploring the unknown with the REU program at the University of Oregon. **G.L. Richmond**

3:50 PROF 29. Mentoring experience behind successful iREU participants. **R. Duran**, **D. Spivak**, **G. Thomas**

4:15 PROF 30. International multisite REU program. **T.A. Nile**

4:40 Panel Discussion.

5:20 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Capitol Ballroom 6

Hands-on STEM Enrichment Programs for Persons with Disabilities

A. A. Hill, C. A. Supalo, Organizers, Presiding

1:30 Introductory Remarks.

1:35 PROF 31. Enriching the discourse of equity in the globalized knowledge economy. **J. Bhattacharya**

1:55 PROF 32. Hands-on laboratory experiences for the visually impaired. **A.A. Hill**

2:15 PROF 33. 2014 "Summer Science Spectacular": A model for successful partnerships between the NFB and post-secondary institutions. **C.A. Supalo**

2:35 PROF 34. Summer research experience for undergraduate students with disabilities at the University of Delaware. **K.S. Booksh**

2:55 Intermission.

3:10 PROF 35. Exemplars of summer enrichment programs for students with disabilities hosted around the world. **H. Wohlers**

3:30 PROF 36. Cal Poly laboratory chemistry workshops for blind and visually impaired high school students. **D.M. Fantin**

3:50 PROF 37. Outreach and educational programs for deaf and hard-of-hearing students in the sciences. **A.D. Ross**, **S.B. Smith**, **T. Pagano**

4:10 PROF 38. Research and cooperative work experiences for deaf and hard-of-hearing undergraduate students in the sciences. **T. Pagano**, **A.D. Ross**, **S.B. Smith**

4:30 Concluding Remarks.

RUBB

Rubber Division

T. R. DeLapa, Program Chair

MONDAY EVENING

STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum

Polymer Science Education and the NGSS

Sponsored by CHED, Cosponsored by PMSE, POLY, RUBB and SCC†

SCHB

Division of Small Chemical Businesses

J. Sabol, Program Chair

OTHER SYMPOSIA OF INTEREST:

Water Our Most Critical Resource (see AGFD, Wed, Thu)

Colorado Biotechnology: The Science of Colorado's Craft Beer, Wine & Spirits Industries (see BIOT, Sun)

Citizens First: Communicating Climate Science to the Public (see CHED, Tue)

Transitioning between Academic Research into Practical Use: Solar-Energy and Advanced Materials (see COMSCI, Mon)

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment (see ENVR, Wed)

Hydraulic Fracturing Impacts on Water, Soil and Air Quality (see ENVR, Mon, Tue)

SOCIAL EVENTS:

Breakfast, 7:30 AM: Sun

Luncheon, 12:00 PM: Sun

SCHB Hach Award Luncheon, 12:00 PM: Mon

SCHB Hach Award Reception, 5:30 PM: Mon

Social Hour, 5:30 PM: Mon

BUSINESS MEETINGS:

SCHB Division Executive Committee Meeting, 8:30 AM: Sun

SCHB Division Business Meeting, 1:15 PM: Sun

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 2

SCHB Entrepreneurs' Poster Session

Cosponsored by YCC

G. Ruger, Organizer, Presiding

1:30 - 3:30

SCHB 1. Thirty-five years and going strong: SCHB offers resources and networking opportunities for small and growing chemical businesses. **M. Chorghade**, A. Rahman, S.S. Seelig, P. Kearney, D.J. Deutsch, S.V. Verocellotti, J.E. Sabol, J.L. MacLachlan, C.A. Burton, K. Hylton-Rodic, J. Lee, G. Ruger, N.A. Vaidya

SCHB 2. Chemical Angel Network chemists investing in chemical businesses. **S. White**, M. Vreeke, J.C. Giordan

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 2

Best Practices for Success with SBIR & STTR Grants

Cosponsored by PROF and YCC

P. Kearney, Organizer, Presiding

2:00 Introductory Remarks.

2:05 **SCHB 3.** ThruPore Technologies LLC: Experiences in NSF's I-Corps and SBIR programs. **M.G. Bakker**, F.M. Saylor

2:30 **SCHB 4.** Chemical entrepreneur's first time NIH SBIR grant application submission. **P.C. Kearney**

2:55 Panel Discussion.

Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations

Sponsored by PROF, Cosponsored by BMGT, SCHB and WCC

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 2

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of Terry L. Brewer

Cosponsored by PROF and YCC

P. Kearney, Organizer

J. E. Sabol, Organizer, Presiding

8:00 Coffee & Networking.

8:30 Introductory Remarks.

8:50 **SCHB 5.** Entrepreneurs: Locally born to accept the global challenges. **S. Moles**

9:20 **SCHB 6.** Innovation and entrepreneurship: Advantages of private companies. **J. Mooney**

9:50 Intermission.

10:20 **SCHB 7.** Small business in a big industry. **K. Savala**

10:50 **SCHB 8. Award Address** (Kathryn C. Hach Award for Entrepreneurial Success sponsored by the Kathryn C. Hach Award Fund). Small business (chemistry) in a big world (technology). **T.L. Brewer**

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 2

Water is the Next Oil: Small Businesses Percolating to the Top

Cosponsored by YCC

A. Boal, Organizer, Presiding

2:00 Introductory Remarks.

2:05 **SCHB 9.** Surface-modified carbon electrodes for long-life capacitive deionization processes. **J.R. Landon**, C. Lippert

2:35 **SCHB 10.** Innovating water treatment with on-demand chemistry. **A.K. Boal**

3:05 **SCHB 11.** Evolution of Hach Chemical Company to Hach Lange: Success and growth through customer focus. **C.C. Johnson**

3:35 Concluding Remarks.

Chemical Angel Network: Chemists Investing in Chemical Companies

Sponsored by PROF, Cosponsored by SCHB

MONDAY EVENING

Section A

Colorado Convention Center Halls C/D

Sci-Mix

J. Sabol, Organizer

8:00 - 10:00

1-2, 9. See previous listings.

CCS

Committee on Chemical Safety

E. Howson, Program Chair

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Legalized Marijuana & Health & Safety

Sponsored by CHAS, Cosponsored by CCS

TUESDAY MORNING

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

Sponsored by CHAS, Cosponsored by AGFD, CCS and PRES

TUESDAY AFTERNOON

Safety in Undergraduate Teaching

Sponsored by CHAS, Cosponsored by CCS

CCPA

Committee on Chemistry and Public Affairs

S. Butts, Program Chair

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

TUESDAY MORNING

DOE Nanoscience Research Centers

National Resources for the Nanoscience Community

Sponsored by PRES, Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG

CORP

Committee on Corporation Associates

D. Mason, Program Chair

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

DAC

Committee on Divisional Activities

M. J. Morello, Program Chair

MONDAY MORNING

Frontiers in Glycoscience

Synthesis and Functions

Sponsored by CELL, Cosponsored by CARB† and DAC†

MONDAY AFTERNOON

Frontiers in Glycoscience

Control of Sequence and Regiochemistry

Sponsored by CELL, Cosponsored by CARB† and DAC†

TUESDAY MORNING

Frontiers in Glycoscience

Characterization and Applications

Sponsored by CELL, Cosponsored by CARB† and DAC†

TUESDAY AFTERNOON
Frontiers in Glycoscience**Medicine**

Sponsored by CELL, Cosponsored by DAC†

CEI**Committee on Environmental Improvement**

C. Middlecamp, Program Chair

SUNDAY MORNING**Green Chemistry and the Environment**

Sponsored by ENVR, Cosponsored by CEI, MPPG† and NUCL

Uranium in Seawater**The Chemistry**

Sponsored by I&EC, Cosponsored by CEI and MPPG†

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG†

SUNDAY AFTERNOON**Green Chemistry and the Environment**

Sponsored by ENVR, Cosponsored by CEI and MPPG

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG†

Uranium in Seawater**The Sorbents**

Sponsored by I&EC, Cosponsored by CEI, MPPG† and NUCL

MONDAY MORNING**Green Chemistry and the Environment**

Sponsored by ENVR, Cosponsored by CEI

Uranium in Seawater**Sorbents and Analysis**

Sponsored by I&EC, Cosponsored by CEI, MPPG† and NUCL

MONDAY AFTERNOON**Uranium in Seawater****Analysis and Toxicity/Cost**

Sponsored by I&EC, Cosponsored by CEI, MPPG† and NUCL

TUESDAY MORNING**DOE Nanoscience Research Centers****National Resources for the Nanoscience Community**

Sponsored by PRES, Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG

ACS-CEI Award for Incorporating Sustainability into Chemistry Education

Sponsored by CHED, Cosponsored by CEI

Technical program information known at press time.

The official technical program for the 249th ACS National Meeting is available at:

www.acs.org/denver2015**Citizens First: Communicating Climate Science to the Public**

Sponsored by CHED, Cosponsored by CEI†

WEDNESDAY MORNING**Green Chemistry: Theory and Practice**

Sponsored by CHED, Cosponsored by CEI†

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Sponsored by ENVR, Cosponsored by CEI and MPPG†

WEDNESDAY AFTERNOON**Green Chemistry: Theory and Practice**

Sponsored by CHED, Cosponsored by CEI†

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Sponsored by ENVR, Cosponsored by CEI and MPPG†

WEDNESDAY EVENING**Water Sustainability in Oil and Gas Exploration: Treatment Issues**

Sponsored by ENVR, Cosponsored by CEI and MPPG†

CMA**Committee on Minority Affairs**

J. Sarquis, Program Chair

OTHER SYMPOSIA OF INTEREST:**ACS Award for Encouraging Disadvantaged Students in Chemistry: Symposium in Honor of Catherine H. Middlecamp** (see CHED, Mon)**SOCIAL EVENTS:****Diversity Reception**, 5:00 pm: Sun
CMA Luncheon (Tickets Required), 11:30 AM: Mon**BUSINESS MEETINGS:****CMA Open Meeting**, 12:00 PM: Sun**SUNDAY MORNING****Native American Women Chemists of Color**

Sponsored by PROF, Cosponsored by CMA and WCC

MONDAY MORNING**Section A**

Hyatt Regency Denver at Colorado Convention Center

Mineral Hall F

Diversifying STEM: Uniting through our Differences for a Brighter Scientific Future

Cosponsored by CHED and PROF

C. P. Frazier, S. A. Lopez, Organizers, Presiding

8:00 Introductory Remarks.

8:05 **CMA 1.** Peer-led activities in STEM based on values affirmation. L.M. Campos8:30 **CMA 2.** Alliance for Diversity in Science and Engineering: A graduate-student centered approach to diversify STEM. S.A. Lopez8:55 **CMA 3.** NSF AGEP California Alliance: A community of practice to increase diversity in the physical sciences and engineering. R.L. Garrell9:20 **CMA 4.** Future faculty workshop. T.M. Swager

9:45 Intermission.

9:55 **CMA 5.** Chancellor's Science Scholars program: Adapting the Meyerhoff model to UNC-Chapel Hill. J.L. Templeton, M. Peifer, A. Panter, W. Marzluff, M. Patil10:20 **CMA 6.** STEM Posse: Recruiting and retaining underrepresented students in the STEM disciplines. I.R. Epstein10:45 **CMA 7.** Building a STEM community for the next generation. E. Patridge

11:10 Panel Discussion.

11:40 Concluding Remarks.

MONDAY AFTERNOON**ACS Award for Encouraging Disadvantaged Students in Chemistry: Symposium in Honor of Catherine H. Middlecamp****Four-Part Harmony (or Disharmony)**

Sponsored by CHED, Cosponsored by CMA and WCC

CPRC**Committee on Public Relations and Communications**

D. Gottfried, Program Chair

TUESDAY MORNING**The Interface of Chemical and Biological Sciences International Disarmament Efforts**

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

TUESDAY AFTERNOON**The Interface of Chemical and Biological Sciences International Disarmament Efforts**

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

COMSCI**Committee on Science**

D. Crans, Program Chair

SUNDAY MORNING**The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders**

Sponsored by PRES, Cosponsored by BMGT, COMSCI, IAC and SOCED

SUNDAY AFTERNOON**Nanotechnology: Delivering on the Promise Research & Development**

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING**Section A**

Colorado Convention Center Room 301

Transitioning between Academic Research into Practical Use: Solar-Energy and Advanced Materials

Cosponsored by MPPG† and PRES

D. C. Crans, Organizer, Presiding

8:30 Introductory Remarks.

8:35 **COMSCI 1.** Will solar-driven water splitting devices see the light of day? H.B. Gray

9:05 Discussion.

9:15 **COMSCI 2.** Solar water splitting and the hydrogen economy. J. Turner

9:45 Discussion.

9:55 **COMSCI 3.** Revolutionizing CdTe photovoltaics through industrial research. A. Duggal

10:25 Discussion.

10:35 Intermission.

10:50 **COMSCI 4.** If it works, will it matter? C.A. Martin

11:20 Discussion.

11:30 **COMSCI 5.** Postdoc's perspective on use-inspired academic research. J. McKone

11:50 Discussion.

12:00 Panel Discussion.

Nanotechnology: Delivering on the Promise**Opportunities and Challenges for Health, Safety and the Environment**

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON**Nanotechnology: Delivering on the Promise****Bridging the Gap to a Thriving US Marketplace**

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORR, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

IAC**International Activities Committee**

H.N. Cheng, Program Chair

SUNDAY MORNING**Section A**

Hyatt Regency Denver at Colorado Convention Center

Mineral Hall D

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Cosponsored by CHED, PROF and YCC

H. Cheng, Organizer

S. Hill, Organizer, Presiding

9:00 Introductory Remarks.

9:10 **IAC 1.** Exploring electrochemistry in Düsseldorf, Germany. B. Ferguson, J. Grote, K. Mayrhofer9:30 **IAC 2.** Undergraduate research in Jülich, Germany: Fuel cell systems studies as a catalyst for personal growth and cultural exploration. K. Fong, D. Krekel9:50 **IAC 3.** A summer in Freiburg: Materials chemistry research in Germany. G. Ruehl, M. Benkler10:10 **IAC 4.** My ACS-IREU experience: Science and exploration in Europe. J. Ford, M. Schwillk, H. Werner

10:30 Intermission.

10:40 **IAC 5.** Research along the Ruhr: A chemical and personal excursion in west Germany. T.J. Myers, M. Ulbricht11:00 **IAC 6.** Highlights of an international research experience in Berlin, Germany. L. Hristov, A. Senf11:20 **IAC 7.** Hybrid polymer studies in Germany: Synthesis, surface chemistry, and soccer. D. Brauer11:40 **IAC 8.** ACS international research experience for undergraduates: Kiel, Germany. A. Kim**The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders**

Sponsored by PRES, Cosponsored by BMGT, COMSCI, IAC and SOCED

† Cooperative Cosponsorship

SUNDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Mineral Hall D

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Cosponsored by CHED, PROF and YCC

H. Cheng, *Organizer*
S. Hill, *Organizer, Presiding*

- 1:30 IAC 9.** Organic solar cell active layer synthesis and synopsis of time abroad. T. Range, C. Ping Sen, S. Valiyaveetil
- 1:50 IAC 10.** Electrochemistry in Singapore: Going into the sea lion's den and returning out a more well-versed chemist. G. Panetti
- 2:10 IAC 11.** Reflections on a summer research experience at the National University of Singapore. S.J. Faucher
- 2:30** Intermission.
- 2:40 IAC 12.** My inorganic materials chemistry IREU experience in Italy. C.M. Gentle
- 3:00 IAC 13.** Italian inquiry into alternative energy. S. Barnett
- 3:20 IAC 14.** Italian research experience: Development of a sustainable and efficient protocol for palladium-catalyzed Sonogashira cross-coupling reactions. M.F. McLaughlin, L. Vaccaro
- 3:40** Intermission.
- 3:50 IAC 15.** Summer research in the UK: Unique chemistry in a unique environment. D.G. Mackanic, S. Mabbott, D. Graham
- 4:10 IAC 16.** Investigations into the stability of photosynthetic proteins in Glasgow, Scotland. E.K. Reagan, N. Javid, S.K. Nalluri, R. Uljin
- 4:30 IAC 17.** Solar power in Scotland: Examining new materials for organic photovoltaic devices. L.R. Savagian

TUESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center
Mineral Hall D

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Cosponsored by ANYL, CHAL, CPRC and PRES

L. Brown, *Organizer*
D. J. Phillips, *Presiding*

- 9:00** Introductory Remarks.
- 9:15 IAC 18.** Finding the needle in the haystack: The development of analytical capabilities at the OPCW and partner laboratories in support of verification of the Chemical Weapons Convention. M. Blum
- 9:45 IAC 19.** Chemical Issues in context: The role of intent in nonproliferation and disarmament policy. K. Rodda
- 10:15 IAC 20.** Chemistry, international disarmament and policy in a technologically evolving world. J. Forman
- 10:45** Intermission.
- 11:00 IAC 21.** Eradication techniques for chemical and biological weapons. R. Holmes
- 11:30 IAC 22.** Emerging technologies and diffusion of innovation: Security challenges for the 21st century. M. Kosal
- 12:00 IAC 23.** Finding better therapeutics for chemical poisonings: The NIH Countermeasures against Chemical Threats (CounterACT) program. D. Jett

TUESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Mineral Hall D

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Cosponsored by ANYL, CHAL, CPRC and PRES

- L. Brown, *Organizer*
D. J. Phillips, *Presiding*
- 2:00 IAC 24.** Education and outreach relevant to the Organisation for the Prohibition of Chemical Weapons Chemical Weapons Convention. A. Suárez
- 2:30 IAC 25.** Not in my backyard: Outreach efforts by the Program Executive Office, Assembled Weapons Alternatives (PEO-ACWA) on chemical weapons destruction. G.B. Mohrman
- 3:00 IAC 26.** U.S. Department of State's Chemical Security Program: Challenges, successes, and expanding international disarmament/nonproliferation efforts. D. Verdugo
- 3:30** Intermission.
- 3:45** Panel Discussion.
- 4:30** Concluding Remarks.

SCC

Senior Chemists Committee

G. Heinze, *Program Chair*

MONDAY EVENING

STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum

Polymer Science Education and the NGSS

Sponsored by CHED, Cosponsored by PMSE, POLY, RUBB and SCC†

SOCED

Society Committee on Education

D. Swartling, *Program Chair*

SOCIAL EVENTS:

- Networking Social with Graduate School and Research Opportunity Representatives, 1:00 PM:** Sun
- ACS Student Chapter Awards Ceremony, 7:00 PM:** Sun
- Undergraduate Social, 8:30 PM:** Sun
- Undergraduate Speed Networking with Chemistry Professionals, 3:45 PM:** Mon
- Chemistry and the Environment Film Series, 12:00 PM:** Tue

SUNDAY MORNING

The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders

Sponsored by PRES, Cosponsored by BMGT, COMSCI, IAC and SOCED

High School Program
Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Papers

Organic Chemistry
Sponsored by CHED, Cosponsored by SOCED

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

High School Program

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Papers

Analytical and Environmental Chemistry
Sponsored by CHED, Cosponsored by SOCED

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Grand Ballroom 1

Biomass to Fuel and Products

Cosponsored by CELL, ENFL and MPPG

D. J. Swartling, *Organizer, Presiding*

9:00 SOCED 1. Current state of biofuels in the USA and world. T. Foust

Section A

Sheraton Denver Downtown Hotel
Grand Ballroom 1

Forensic Toxicology of Marijuana

Cosponsored by BMGT and TOXI

D. J. Swartling, *Organizer, Presiding*

10:45 SOCED 2. Forensic toxicology of marijuana. K.M. Allen, D. Wallace Duckworth

Nanotechnology: Delivering on the Promise Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Undergraduate Research Papers

Computational, Physical and Inorganic Chemistry

Sponsored by CHED, Cosponsored by SOCED

MONDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Grand Ballroom 1

Sustainability in the 21st Century: Optimizing Complex Interdependent Systems

Cosponsored by CELL and ENFL

D. J. Swartling, *Organizer, Presiding*

2:30 SOCED 3. Eminent Scientist Lecture: Sustainability in the 21st century: Optimizing complex interdependent systems. H.T. Kohlbrand

Nanotechnology: Delivering on the Promise Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Undergraduate Research Posters

Agricultural and Food Chemistry

Sponsored by CHED, Cosponsored by AGFD, ANYL, BIOL, BIOT, COMP, ENVR, GEOC, INOR, MEDI, PMSE, POLY and SOCED

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Undergraduate Research Papers

Biochemistry and Chemical Education

Sponsored by CHED, Cosponsored by SOCED

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*

SOCIAL EVENTS:

- WCC Breakfast, 7:30 AM:** Mon
- WCC Just Cocktails, 3:30 PM:** Mon
- WCC/Eli Lilly Travel Award Poster Session, 11:00 AM:** Tue
- WCC Luncheon, 12:00 PM:** Tue

BUSINESS MEETINGS:

- WCC Division Business Meeting, 5:30 PM:** Fri
- WCC Division Business Meeting, 7:30 AM:** Sat

SUNDAY MORNING

ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur

Sponsored by FLUO, Cosponsored by WCC

Native American Women Chemists of Color

Sponsored by PROF, Cosponsored by CMA and WCC

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Emily A. Weiss

Sponsored by INOR, Cosponsored by WCC

SUNDAY AFTERNOON

ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur

Sponsored by FLUO, Cosponsored by WCC

Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations

Sponsored by PROF, Cosponsored by BMGT, SCHB and WCC

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Emily A. Weiss

Sponsored by INOR, Cosponsored by WCC

SUNDAY EVENING

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Sponsored by INOR, Cosponsored by WCC

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.

MONDAY MORNING

Section A

Colorado Convention Center
Room 105

WCC Rising Stars Awards Symposium

Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

S. Azad, M. A. Kane, Organizers, Presiding

9:20 Introductory Remarks.

9:30 **wcc 1.** Making science and education gel: Building a career in technical research and pursuing a passion for STEM education outreach. J.L. Curtis-Fisk

9:50 **wcc 2.** Redox-active ligands for the f-block: Promoting multi-electron chemistry at low-valent uranium centers. S.C. Bart

10:10 Intermission.

10:25 **wcc 3.** Tale of two journeys: Protein misfolding in light chain amyloidosis and the career path of a protein biochemist. M. Ramirez Alvarado

10:45 **wcc 4.** Chemical research with fun in new materials design and application. C. Liu

11:05 **wcc 5.** Engineering next-generation porous materials for energy and environmental applications. K.S. Walton

ACS Award for Achievement in Research for the Teaching and Learning of Chemistry: Symposium in Honor of Vickie M. Williamson

Sponsored by CHED, Cosponsored by WCC

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in Honor of E. Ann Nalley

Championing the Empowerment of Women in Chemistry

Sponsored by PROF, Cosponsored by WCC

MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 710

WCC Rising Stars Awards Symposium

Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

S. Azad, M. A. Kane, Organizers, Presiding

1:20 **wcc 6.** Art and Industry: Science takes an artsy turn. M.H. Keefe

1:40 **wcc 7.** Phase-selective synthesis and surface passivation of binary and ternary copper sulfide nanoparticles. K. Plass, N. Freymeyer, C. Kim, Z. Georgieva

2:00 **wcc 8.** Nuclear waste management: Where geology meets nuclear science. F.N. Smith

2:20 Intermission.

2:35 **wcc 9.** Magnetic quantum dots for biomedical applications. J.O. Winter

2:55 **wcc 10.** Overview of the discovery of a potent *Septoria tritici* fungicide. B.A. Lorsbach

3:15 Concluding Remarks.

ACS Award for Achievement in Research for the Teaching and Learning of Chemistry: Symposium in Honor of Vickie M. Williamson

Sponsored by CHED, Cosponsored by WCC

ACS Award for Encouraging Disadvantaged Students in Chemistry: Symposium in Honor of Catherine H. Middlecamp

Four-Part Harmony (or Disharmony)
Sponsored by CHED, Cosponsored by CMA and WCC

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Sponsored by INOR, Cosponsored by WCC

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger

Sponsored by INOR, Cosponsored by WCC

TUESDAY MORNING

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in Honor of E. Ann Nalley

Championing the Empowerment of Women in Chemistry

Sponsored by PROF, Cosponsored by WCC

E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Symposium in Honor of Ruth R. Wexler

Sponsored by MEDI, Cosponsored by WCC

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Sponsored by INOR, Cosponsored by WCC

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger

Sponsored by INOR, Cosponsored by WCC

TUESDAY AFTERNOON

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Sponsored by INOR, Cosponsored by WCC

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger

Sponsored by INOR, Cosponsored by WCC

WEDNESDAY MORNING

National Fresenius Award: Symposium in Honor of Abigail G. Doyle

Sponsored by ORGN, Cosponsored by WCC

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Sponsored by INOR, Cosponsored by WCC

WEDNESDAY AFTERNOON

Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Symposium in Honor of Hilka I. Kenttämää

Sponsored by ANYL, Cosponsored by WCC

YCC

Younger Chemists Committee

T. Matos and A. Gavrilenko, Program Chairs

SUNDAY MORNING

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored by CHED, PROF and YCC

SUNDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Agate B/C

Starting a Successful Research Program at a Predominantly Undergraduate Institution

Cosponsored by PROF

A. V. Gavrilenko, T. D. Matos, Organizers

M. Druelinger, Organizer, Presiding

1:00 Introductory Remarks.

1:15 **ycc 1.** What is undergraduate research and why do research at a predominantly undergraduate institution? T.J. Wenzel

1:25 **ycc 2.** Collaborative research with undergraduates: research project and research group design. G. Van Hecke

1:45 **ycc 3.** Balancing teaching, research, service, and life in the context of primarily undergraduate institutions (PUIs). B.L. Gourley

2:05 **ycc 4.** Art and necessity of gaining internal support from institutional administrators. M. Druelinger

2:25 Intermission.

2:35 **ycc 5.** Undergraduate new investigator grants at the ACS Petroleum Research Fund. B. Lee

3:00 **ycc 6.** Funding opportunities at the National Science Foundation of particular interest to faculty at primarily undergraduate institutions (PUIs). M. Bushey

3:30 **ycc 7.** Writing more competitive grant proposals. T.J. Wenzel

3:50 Panel Discussion.

SCHB Entrepreneurs' Poster Session

Sponsored by SCHB, Cosponsored by YCC

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored by CHED, PROF and YCC

Best Practices for Success with SBIR & STTR Grants

Sponsored by SCHB, Cosponsored by PROF and YCC

Young Investigator in Medicinal Chemistry

Sponsored by MEDI, Cosponsored by YCC

MONDAY MORNING

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of Terry L. Brewer

Sponsored by SCHB, Cosponsored by PROF and YCC

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Water is the Next Oil: Small Businesses Percolating to the Top

Sponsored by SCHB, Cosponsored by YCC

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Centennial H

Chemical Tales of Success: Helpful Tips for Younger Chemists

Cosponsored by NUCL and SCHB

J. C. Braley, Organizer, Presiding

8:30 **ycc 8.** What I wish I had known: You can learn from my mistakes. L.M. Balbes

9:00 **ycc 9.** Professional skills for chemists. R.M. Richards

9:40 **ycc 10.** Balancing entrepreneurship with academic life. A.L. Prieto

10:10 Intermission.

10:30 **ycc 11.** Tales from the home stretch. K.M. Schulz

11:00 **ycc 12.** Tales from the dark side: Alternative careers in administration. P.K. Dorhout

TUESDAY EVENING

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY EVENING

Environmental Chemistry: Pedagogical Models and Practices

Sponsored by ENVR, Cosponsored by CHED, MPPG# and YCC

THURSDAY MORNING

Environmental Chemistry: Pedagogical Models and Practices

Sponsored by ENVR, Cosponsored by CHED, MPPG# and YCC

ACCESS INCLUDED with ACS Membership!

IMMEDIATE: Streaming video of presentations from recent ACS national meetings

CONVENIENT: View presentations anytime, anywhere

PORTABLE: Compatible with mobile devices



AMERICAN CHEMICAL SOCIETY
www.presentations.acs.org

COME BE PART OF THE GROWTH

We are currently seeking the following experienced professionals to join our team

Foster City, CA

Director, Analytical Development Req#16733
Research Scientist II, Analytical Development Req#11491
Sr. Research Scientist II, Process Chemistry Req#15688
Associate Scientist, Process Chemistry Req#20417
Sr. Research Associate, Process Chemistry Req#18045
Sr. Research Associate II, Medicinal Chemistry Req#20405

For more details and to apply: gilead.com/careers



 **GILEAD**
Advancing Therapeutics.
Improving Lives.

CHEMISTRY OF NATURAL RESOURCES



249th ACS National Meeting DENVER, COLORADO • MARCH 22–26, 2015 UNDERGRADUATE PROGRAM

All events are sponsored or cosponsored by the Society Committee on Education Undergraduate Programs Advisory Board.

CHAIR: Matthew J. Mio • University of Detroit Mercy, MI **PROGRAM CHAIR:** Daniel J. Swartling • Tennessee Tech University, Cookeville

SUNDAY, MARCH 22

Undergraduate Hospitality Center

Sheraton Denver Downtown,
Majestic Ballroom
8:00 AM–5:00 PM

Undergraduate Research Oral Session

Sheraton Denver Downtown, Denver Room
8:30 AM–5:00 PM

Making the Most of Your First National Meeting

Sheraton Denver Downtown,
Majestic Ballroom
9:00–9:45 AM

Graduate School Reality Check: Getting In

Sheraton Denver Downtown,
Plaza Ballrooms A&B
10:00–11:15 AM
Cosponsored by the ACS Younger Chemists Committee

Chem Demo Exchange

Colorado Convention Center, Hall B2
11:00 AM–12:30 PM

Graduate School Reality Check: You're In—Now What?

Sheraton Denver Downtown,
Plaza Ballrooms A&B
11:15 AM–12:30 PM
Cosponsored by the ACS Younger Chemists Committee

How to Be a Successful ACS Student Chapter

Sheraton Denver Downtown,
Plaza Ballrooms D&E
1:00–2:30 PM

Networking Social with Graduate School and Research Opportunity Representatives

Sheraton Denver Downtown,
Grand Ballroom
1:00–5:00 PM

Symposium: Can You Have a Life and Career?

Sheraton Denver Downtown,
Plaza Ballrooms D&E
2:45–4:00 PM
Cosponsored by the ACS Women Chemists Committee

Workshop: Improving Scientific Communication Skills

Sheraton Denver Downtown,
Plaza Ballrooms A&B
4:00–5:30 PM

Workshop: Careers in Teaching Chemistry

Sheraton Denver Downtown,
Plaza Ballrooms D&E
4:00–5:30 PM

Student Chapter Awards Ceremony

Colorado Convention Center,
Bellco Theatre
7:00–8:30 PM

Undergraduate Social

Colorado Convention Center,
Four Seasons Ballroom
8:30–11:00 PM
Hosted by the Colorado School of Mines and the University of Colorado at Boulder

MONDAY, MARCH 23

Undergraduate Hospitality Center

Sheraton Denver Downtown,
Majestic Ballroom
8:00 AM–5:00 PM

Undergraduate Research Oral Session

Sheraton Denver Downtown,
Denver Room
8:30 AM–5:00 PM

Symposium: Biomass to Fuel & Products

Sheraton Denver Downtown,
Grand Ballroom I
9:00–10:30 AM
Cosponsored by the ACS Cellulose and Renewable Materials Division and the ACS Division of Energy & Fuels

Workshop: Networking 101

Colorado Convention Center,
Rooms 601/603
9:45–11:00 AM

Workshop: Chemists Celebrate Earth Day

Sheraton Denver Downtown,
Grand Ballroom II
9:45–11:45 AM
Cosponsored by the ACS Committee on Community Activities

Symposium: Forensic Toxicology of Marijuana

Sheraton Denver Downtown,
Grand Ballroom I
10:45–11:45 AM
Cosponsored by the ACS Divisions of Chemical Toxicology and Business Development & Management

Undergraduate Research Poster Session

Colorado Convention Center, Hall C
12:00 NOON–2:00 PM
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

"Sustainability in the 21st Century: Optimizing Complex Interdependent Systems", with Henry Kohlbrand, Dow Chemical Company
Sheraton Denver Downtown,
Grand Ballroom I
2:30–3:30 PM
Cosponsored by the ACS Cellulose and Renewable Materials Division and the ACS Division of Energy & Fuels

Speed Networking with Chemistry Professionals

Hyatt Regency Denver at Colorado Convention Center, Centennial D
3:45–5:15 PM
Cosponsored by ACS Corporation Associates and the ACS Senior Chemists Committee

Kavli Lectures

Colorado Convention Center,
Bellco Theatre
4:00–6:30 PM

Sci-Mix/Successful Student Chapter Posters

Colorado Convention Center, Hall C
8:00–10:00 PM

TUESDAY, MARCH 24

Chemistry and the Environment Film Series

Sheraton Denver Downtown,
Grand Ballroom I
12:00 NOON–2:00 PM
Cosponsored by the ACS Committee on Environmental Improvement

Program format and times are subject to change. Please consult the final program.

EXPOSITION HIGHLIGHTS

SEE WHAT'S NEW INSIDE THE

EXPOSITION. Visit the ACS National Exposition at the Colorado Convention Center, Halls A/F, from Sunday, March 22, through Tuesday, March 24. 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/denver2015 to learn more about exhibiting companies and to 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 Moscone 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. Preregister at www.acs.org/denver2015 to reserve your seat.

Presentations, Prizes & Special Events. Visit the Daily Prize Raffle area (#339) from Sunday through Tuesday for a chance to win a prize. Also, don't forget to join us on Sunday from 6:00 to 8:30 PM for the Attendee Welcome Reception. Take a break, and visit the exposition on Monday and Tuesday from

1:00 to 3:00 PM for treats in the Town Center. Stop by the Town Center on Tuesday, from 2:00 to 4:00 PM to view the Division of Energy and Fuels poster session.

Internet & Technology. Use free Internet access, and leave messages for one another at the Meeting Mail terminals located throughout the exposition and Moscone Center. Also, enjoy free Wi-Fi service at designated areas in the Moscone 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 \$50. Students with school identification can obtain an expo-only badge for \$25. Registration can be handled online or in person at ACS Attendee Registration in the Moscone Center, North Lobby.



ACS Exposition

EXHIBITORS

The following list exhibitors, as of February 20th, and is the property of the American Chemical Society. Any unauthorized use of this list, or any part thereof, either directly or indirectly, is strictly prohibited.

Visit the Online ACS National Exposition at www.acs.org/denver2015 to download the updated exhibitor list and access product information.

AAPS (Amer Assoc. of Pharm Sci.) 2107 Wilson Blvd., Suite 700, Arlington, VA 22201, 703-243-2800, Internet: www.aaps.org AAPS provides an international forum for the exchange of knowledge among scientists to enhance their contributions to health. We offer scientific programs, ongoing education, networking opportunities, and professional development. Join AAPS and gain access to customized journal searches, pharmaceutical news and discounts on meetings, conferences and more. **1311**

ACS Career Navigator™ is your source for career resources and training at the ACS National Meeting in San Francisco. Visit us in the ACS Booth to discover the resources you need to achieve your goals and advance your career. **624**

ACS Committee on Chemical Safety, P.O. Box 152329, CA, United States 92195, 619-990-4908, The ACS Committee on Chemical Safety (CCS) and the Division of Chemical Health and Safety (CHAS) provide leadership and technical guidance to all ACS members and the community regarding the safe and proper handling of chemicals. Chemical safety practices are supported across the entire chemical enterprise from K-12 through college and graduate school into the industrial and academic workplace. **425**

ACS Division of Small Chemical Businesses (SCHB), 4344 Moorpark Ave. Ste # 1San Jose, CA 95129 United States, 408-834-8597, Fax: 408-351-7900 Email: expo-booth@acs-schb.org, Internet: <http://www.acs-schb.org>

The ACS Division of Small Chemical Business (SCHB) has objectives "To aid in the formation, development, and growth of small chemical businesses."

SCHB helps chemists working in small enterprises, including self-employed, with the legal, social, educational, legislative, regulatory, and economic aspects of their unique professional status. SCHB serves as a clearing house of information, a forum for discussion, and a liaison between small businesses and students. **332**

ACS Education, 1155 16th Street, NW, Washington, DC 20036, 202-872-6269, fax: 202-833-7732, e-mail: education@acs.org, Internet: www.acs.org/education The ACS Education Division serves learners and educators by building communities and providing effective chemistry education resources, grants, communities, professional development opportunities, standards and guidelines. Stop by our booth to find information that can support your efforts to provide innovative, relevant, and effective chemistry education from kindergarten through professional education. **624**

ACS Green Chemistry Institute, 1155 16th Street, NW, Washington, DC 20036, 202-872-6102, fax: 202-776-8009, e-mail: gci@acs.org, Internet: www.acs.org/gci The ACS Green Chemistry Institute believes that innovation in sustainable and green chemistry and engineer-

ing (GC&E) is vital to solving environmental and human health challenges. Our mission is to catalyze and enable the implementation of GC&E throughout the global chemical enterprise and empower you to reimagine a sustainable future. **524**

ACS Industry Concierge, 1155 16th Street, NW Washington, DC 20036, 202-872-6326 Email: v_kuruganti@acs.org, Internet: www.acs.org/industry **1331c**

ACS Meetings & Expositions, 1155 Sixteenth Street NW, Washington, DC, United States 20036, 800-227-5558, fax: 202-872-6128, e-mail: m_stevenson@acs.org, Internet: www.acs.org/meetings The ACS Meetings booth displays information on current and future regional meetings also spring and fall National Meetings. Register for a regional meeting or get information on submitting an abstract to a meeting in your region. The programming is diverse and exciting! Meet the volunteers who are planning these meetings at the booth. Visit the regional meetings website at www.acs.org/regionalmeetings for a tour of this year's conferences. Information on future national meetings will be on display. **624**

ACS Member Insurance Program, 1155 16th Street, N.W., Washington, DC 20036, 800-227-5558, ext. 6037, fax: 202-872-4435, e-mail: memins@acs.org, Internet: www.acs.org/insurance The ACS Member Insurance Program is committed to offering quality comprehensive insurance plans to members and their families. Stop by the ACS booth to learn more about the plans available such as Life and Health Insurance, Auto & Homeowners, Long Term Care, Professional Liability, Pet Insurance and more. **624**

ACS Membership, 1155 16th St., NW, Suite OTH420, Washington, DC 20036, 2028726062, Internet: www.acs.org/MemberHandbook Are you a Rockstar of Chemistry? Visit ACS Membership in the ACS Booth and take a Commemorative ACS Rockstar photo at the open air photo booth! Learn about your benefits at the Membership Rocks presentation in the ACS Theater on Monday from 3 to 4 PM. **624**

The ACS Office of Public Affairs (OPA) works with ACS members to help advance the chemical enterprise by encouraging strong member participation in advocacy with legislators as well as in communicating with community leaders and the media. Stop by the OPA booth to learn more about how to get involved with advocacy through the Act4chemistry Network, how to be more effective communicators and advocates through the Chemistry Ambassadors initiative, and how to get involved with, or create, a Local Section Government Affairs and/or Public Relations Committees, and more! **825**

ACS Publications, 1155 16th Street, N.W., Washington, DC 20036, 202-872-6862, fax: 202-872-6005, e-mail: s_jackson@acs.org, Internet: pubs.acs.org ACS Publications introduces ACS Central Science—our first completely open access journal—along with ACS Biomaterials Science & Engineering and ACS Infectious Diseases. Stop in at our booth to ask about redeeming ACS Author Rewards, and see a demonstration of the ACS ChemWorx reference management platform. On Monday at noon, attend our free, live webinar at the booth: "Mastering the Art of Scientific Publication," featuring a panel of 4 ACS journal Editors. And get your C&EN signed by the Priestley Medalist! ACS Publications is the most trusted, most cited, and most read publisher in chemistry and the related sciences. **624**

The ACS Store features limited edition chemistry themed merchandise, such as mole dolls, t-shirts and beaker mugs. **624**

ACS Web Strategy & Operations, 1155 16th Street, NW, Washington, DC 20036, 202-872-4548, e-mail: m_parker@acs.org, Internet: www.acs.org

The ACS web site is becoming more personalized! From subtle changes to My Account to more noticeable changes on the www.acs.org home page, we're striving to deliver the most relevant ACS content, programs, products and services—tailored for YOU! Stop by the ACS Web kiosk to see what we've personalized so far, share your interests and help us take ACS Web Personalization to the next level. In order to develop the best personalized ACS web experience, we want to get to know you better! Take brief survey/quiz get a free gift while supplies last. **624**

AdValue Technology, 3470 S. Dodge Blvd., Tucson, AZ 85713, 520-514-1100, fax: 520-747-4024, Internet: www.advaluetech.com AdValue Technology is a leading supplier of high temperature ceramic products made of alumina, fused quartz, sapphire and zirconia. Our products include crucibles, tubes, plates and discs, sample pans for thermal analysis, quartz cuvettes and various custom components. We also carry other lab supplies such as agate mortar and pestles. **1325**

Advanced Clustering Technologies, 1100 W. Cambridge Circle Drive, Suite 300, Kansas City, KS, United States 66103, 913-643-0307, Internet: www.advancedclustering.com **940**

Advion, 10 Brown Rd., Ithaca, NY 14850, 607-379-4565, fax: 607-257-5761, Internet: www.advion.com **1033**

AGI USA Inc., PO Box 21388, Lehigh Valley, PA, United States 18002-1388, (610) 691-2385, Internet: www.asahiglassplant.com **1007**

Agilent Technologies, 2850 Centerville Rd., Wilmington, DE 19808, 302-636-8108, fax: 302-633-8944, e-mail: alonzo_brown@agilent.com, Internet: www.agilent.com/chem **517**

AIP Publishing – The Journal of Chemical Physics, 1305 Walt Whitman Road, Suite 300, Melville, NY 11747, 516-576-2279, fax: 516-349-9704, e-mail: mgross@aip.org, Internet: jcp.aip.org **831**

AK Scientific, Inc., 30023 Ahern Avenue, Union City, CA 94587, (510)429-8835, Internet: www.aksci.com **536**

Alfa Aesar-A Johnson Matthey Co., 26 Parkridge Rd, Ward Hill, MA 01835, 800-343-0660, fax: 800-322-4757, e-mail: info@alfa.com, Internet: www.alfa.com Alfa Aesar, a Johnson Matthey Company, is a leading international manufacturer and supplier of research chemicals, metals and materials. The Alfa Aesar Catalog has over 46,000 products listed, which include, organic compounds, high purity inorganics, pure metals, alloys, elements, precious metal compounds and catalysts, rare earths, AA/ICP standards and more. **909**

Anasazi Instruments Inc., 4101 Cashard Ave., Suite 103, Indianapolis, IN 46203, 317-783-4126, fax: 317-783-7083, e-mail: sales@ainmr.com, Internet: www.ainmr.com Manufacturers of the highest resolution, highest sensitivity, and largest application base of any permanent magnet based NMR instrument. 60 and 90 MHz Eft are general purpose NMR instruments available as 1H, 1H/13C, and multinuclear instruments. These instruments have very low maintenance requirements and do not require cryogenics. **1027**

Anasys Instruments Corp., 325 Chapala St., Santa Barbara, CA 93101, 805-730-3310, Internet: www.anasysinstruments.com Anasys Instruments is dedicated to delivering innovative products that measure and characterize chemical, thermal and mechanical properties of materials at the nanoscale with high spatial precision. Notably in 2010, Anasys introduced the nano-IR²c Platform which led the field with 100nm IR measurement capabilities; a resolution breakthrough of over 100x. **540**

Anton Paar USA, 10215 Timber Ridge Drive, Ashland, VA 23005, 800-722-7556, fax: 804-550-1057, e-mail:info.us@anton-paar.com, Internet: www.anton-paar.com **324**

Ark Pharm, Inc., 1840 Industrial Drive, Suite 120, Libertyville, IL, United States 60048, 847-367-3680, fax: 847-367-3681, e-mail:sales@arkpharminc.com, Internet: www.arkpharminc.com Ark Pharm, Inc. specializes in design and synthesis of medicinal building blocks, scaffolds and other advanced intermediates. Ark Pharm has over 30,000 compounds in stock. We do contract research, custom synthesis and bulk intermediates. Please visit our website at www.arkpharminc.com for more information. **812**

Aspira Scientific, Inc., 521 Cottonwood Drive, Suite 112, Milpitas, CA, United States 95035, 408-571-1100, fax: 408-571-1123, Internet: www.aspirasci.com **1205**

Asylum Research, an Oxford Instruments Company, 6310 Hollister Avenue, Santa Barbara, CA 93117, 805-696-6466, fax: 805-696-6444, e-mail:sales@asylumresearch.com, Internet: www.AsylumResearch.com **307**

Avantes Inc., 9769 W. 119th Dr. Suite 4, Suite 4, Broomfield, CO 80021, 303-410-8668, fax: 303-410-8669. **411**

Beantown Chemical Corporation, 9 Sagamore Park Road, Hudson, NH, United States 603-402-2231, Fax: 603-402-9713, Internet: www.beantownchem.com Beantown Chemical (BTC) manufactures and distributes a line of specialty chemicals, including organics, inorganics and metals. BTC offers over 7,000 products, which are primarily used for research and development in the pharmaceutical industry, chemical industry, government institutions and academia. **1131**

Bentham Sciences Publishers Ltd., 833 S. Wood Street, Room 539, Chicago, IL 60612, 312-413-5867, fax: 312-996-7107, e-mail:morrisry@bentham.org, Internet: www.bentham.org We are a leading STM publisher of 131 high quality journals which helps to answer the information needs of the pharmaceutical, medical & biomedical research community. FREE online journals and information: www.benthamscience.com Subscribe, Consortia, discounted global licenses and trials: marketing@benthamscience.org To know more about our publications please visit here http://benthamscience.com/journal/browse-by-title.php?alphacode=A&pcount=1 **1309**

Biolin Scientific, 514 Progress Drive Suite G, Linthicum Heights, MD 21090 United States, 877-773-6730, Fax: 866-415-8164, Internet: www.biolinscientific.com. Biolin Scientific develops and provides analytical instrumentation for the nanoscale analysis of interactions and reactions occurring at surfaces, thin films, materials and interfaces. Biolin Scientific consists of the following brands: Q-Sense, KSV NIMA and Attension, that provide expertise in Quartz Crystal Microbalance, Langmuir Blodgett and Contact Angle technologies and instrumentation. **938**

Biotage, 10430 Harris Oaks Blvd, Suite C, Charlotte, NC 28269, 704 654 4900, fax: 704 654 4917, Internet: www.biotage.com Biotage is a leading provider of Instruments and Consumables for use in Analytical Testing, Medicinal Chemistry, Organic Chemistry and Peptide Synthesis. Check out the New Extrahera, simple automation of SLE/SPE plates and cartridges, the New Isolera Dalton, Mass Detection for Flash Systems, and the Isolera™ Spektra with ACI Accelerated Chromatographic Isolation. **1024**


BioTools, Inc., 17546 Bee Line, Jupiter, FL 33458, 561-625-0133, 866-btools1, fax: 561-625-0717, e-mail:info@btools.com, Internet: www.btools.com **340**

Boulder Scientific Co., 598 3rd Street, Mead, CO 80542, 970-535-4494, Internet: www.bouldersci.com Since 1972, Boulder Scientific


Company (BSC) has provided the highest quality organometallic compounds to the polymer, pharmaceutical fine and specialty chemical industries. We offer custom synthesis, scale-up and bulk production of custom for your catalytic and stoichiometric product requirements. **841**

BrandTech Scientific, 11 Bokum Road, Essex, CT 06426, 860-767-2562, fax: 860-767-2563, Internet: www.brandtech.com **419**


Brookhaven Instruments Corp., 750 Blue Point Road, Holtsville, NY 11742-1832, 631-758-3200, fax: 631-758-3255, e-mail:info@brookhaveninstruments.com, Internet: www.brookhaveninstruments.com Brookhaven pioneered modern techniques in characterizing nanoparticles, proteins, and polymers using light scattering techniques such as dynamic, static, electrophoretic, and phase analysis for particle sizing, zeta potential, and absolute molecular weight analysis. New SEC/GPC software, Par-SEC, works with almost any detector on the market. New particle characterization software, Particle Solutions, is a unique, database approach with unsurpassed search features that combines all the techniques under one umbrella to ensure maximum productivity. For dispersion stability problems, we offer zeta potential instruments using electrophoretic as well as phase analysis light scattering, the latter technique first introduced by Brookhaven. **1424**

 **Bruker**, 5465 E Cheryl Pkwy, Madison, WI 53711, 888-4BRUKER, e-mail:info@bruker.com, Internet: www.bruker.com Welcome to the world's most comprehensive range of scientific instrumentation available under one brand—a brand synonymous with excellence, innovation and quality. Bruker offers a wide range of applications for molecular characterization in chemistry and life sciences as well as solutions for materials research and nanotechnology. **916,917**

Camag Scientific, Inc., 515 Cornelius Hamett Drive, Wilmington, NC 28401, 9103431830, fax: 9103431834, Internet: www.camagusa.com CAMAG is the world leader in High Performance Thin Layer Chromatography (HPTLC) instrumentation which features the automatic TLC sampler for sample application, the Automatic Developing Chamber for plate development, the Visualizer for Documentation/Camera system and our TLC scanning densitometer for the most versatile densitometer evaluation available, including variable spectra recording and multi-wavelength scanning. We are presenting also our new instruments: the manual and fully-automated DBS (Dried Blood Spots) extraction devices connected to any Mass Spectrometer; in addition to the TLC-MS Interface: TLC plate extraction device to any MS. **409**

 **Cambridge Crystallographic Data Ctr.**, 12 Union Road, Cambridge, United Kingdom CB2 1EZ, 44-1223-336408, fax: 44-1223-336033, e-mail:admin@ccdc.cam.ac.uk, Internet: www.ccdc.cam.ac.uk The CCDC is the world's leading structural chemistry research organisation, and a Cambridge University Partner Institute. We produce the Cambridge Structural Database (CSD), the only comprehensive resource of small-molecule crystal structures, containing over 750,000 quality-checked entries, each available for free download. We serve communities in industry, academic research and teaching. **604**

Career Fair Recruiters Row: **140**
Brewer Scientific, Inc. **140**
Ecolab **137**
EURAXESS Links North America, **141**
Kaust **143**
Sabir **144**

 **CAS**, 2540 Olenangy Road, Columbus, OH 43210, 614-447-3600, fax: 614-447-3713, e-mail:help@cas.org, Internet: www.cas.org Visit CAS, the world's authority for chemical information, at the ACS booth today! See how our databases meet

your research needs using the power of SciFinder and STN. Experience SciFinder, learn more about our collaboration with Chem-Draw **624**

CDS Analytical, LLC, 465 Limestone Road, P.O. Box 277, Oxford, PA, United States 19363-0277, 610-932-3636, fax: 610-932-4158, Internet: http://www.cdsanalytical.com CDS Analytical is a leading global provider of innovative thermal sample preparation instrumentation for the analytical laboratory. For over 35 years our exclusive focus has been on conceiving, designing, manufacturing, and supporting leading edge instruments. CDS offers a complete suite of diverse front-end GC equipment including pyrolyzers, purge and trap, headspace, and thermal desorption systems. These robust, field-tested products provide the entire range of temperature, heating rate, and multiple step manipulations required by today's most demanding analytical laboratories. **302**

CEM Corp., PO Box 200, Matthews, NC 28106, 704-821-7015, fax: 704-821-7894, Internet: www.cem.com **817**

Cengage Learning, Inc., 500 Terry Francois Blvd., Second Floor, San Francisco, CA, United States 94158, 415-839-2329, Internet: www.cengage.com Cengage Learning is a leading educational content, software and services company for the K12, higher education, professional and library markets with operations in more than 20 countries around the world. The company provides superior content, personalized services and course-driven digital solutions that accelerate student engagement and transform the learning experience. **1114**

Chem21 Labs LLC, 2503 Oakland Drive, Cleveland, TN 37312. **1301**

ChemBridge Corp., 11199 Sorrento Valley Rd., Suite 206, San Diego, CA 92121, 858-451-7400, fax: 858-451-7401, e-mail:sales@chembridge.com, Internet: www.chembridge.com **530**

Chemglass Life Sciences, 3800 North Mill Road, Vineland, NJ 08360, 800-843-1794, fax: 800-922-4361, Internet: www.cglifesciences.com In addition to our wide selection of glassware and equipment for chemistry we have begun adding products for chromatography and cell culture keeping us on the forefront of scientific innovation. CGLS fabricates standard glassware items and components as well as custom glassware. We have the capability to produce not only the most complex glass apparatus, but also intricate electronic equipment and customized machined components. Products include Process Reactors from 10L-100L, Benchtop Reactors from 100mL-5L, Filter Reactors, Huber Unistat Circulators, Chromatography Vials and Closures, NMR Tubes, OptiTherm Blocks, Pie-Blocks, Reaction Blocks, Pressure Vessels, Volumetric Flasks, Schlenk Glassware/Manifolds, Rotary and Fritted Glassware. **514**

Chemical Computing Group, 1010 Sherbrooke St. W, Suite 910, Montreal, QC, Canada H3A 2R7, 514-393-1055, e-mail:info@chemcomp.com, Internet: www.chemcomp.com **1324**

Cehmical Semantics, Inc., Florida Science & Tech Park 1115 NW 4th St., Gainesville, FL 32601, 352-371-7744 Fax: 352-371-3662 **333**

Chemistry At Your Fingertips, PO Box 127, Westerly, RI, United States 02891, 401-935-3534, Chemistry At Your Fingertips will be displaying and selling beautiful chemistry, nature and engineering inspired t-shirts and jewelry created by talented artists. Our booth has unique items celebrating the 2014 International Year of Crystallography. Our shirts feature chemistry and biology inspired postage stamps from around the world. **443**

ChemPartner, 965 Halei Road #10 Pudong New Area, Shanghai, China 21203, Internet: www.chempartner.com **429**

EXPOSITION

Chemrus Inc., P.O. Box 920524, Needham, MA 02492, Chemrus developed the world's first polymer-structured disposable filter funnel for solid-liquid separation. Recently, we developed the world's first reaction flasks, which can keep itself upright without the support of cork ring, perform multi-flask reactions without the use of clamps, and perform solvent concentration under reduced pressure. **334**

Chemshuttle, 29548 Union City Blvd., Union City, CA, United States 94587, 510-999-8909, fax: 510-999-8902, e-mail:sales@chemshuttle.com, Internet: chemshuttle.com *Founded in 2010 by medicinal chemists for chemists, ChemShuttle is a growing chemistry CRO and specialty research chemical supplier, currently serving 100+ global organizations in life science research. ChemShuttle has its business center at San Francisco Bay Area in the US, and its research center at Wuxi, Jiangsu, China.* **1132**

Chengdu Aslee Biopharmaceuticals, Inc., Chengdu High-Tech Zone, Keyuan South Road 88#, Chengdu, Sichuan, China, 86-28-8530 5008, e-mail:sales@asleechem.com, Internet: www.asleechem.com *Catalog synthesis, customer synthesis on API, building block and organic coupling reagents* **1133**

CombiPhos Catalysts, Inc., P.O. Box 220, Princeton, NJ 08542-0220, 609-587-6500, fax: 609-587-6570, e-mail:info@combiphos.com, Internet: http://www.combiphos.com **926**

CRC Press, 6000 Broken Sound Parkway, Suite 300, Boca Raton, FL, United States 33487, 561-361-6000, fax: 561-998-2559, Internet: www.crcpress.com *CRC Press is a premier publisher of scientific and technical content in chemistry, chemical engineering and physics for researchers, academics, professionals and students. Our products include world-class reference books, handbooks, encyclopedias, textbooks, journals and the award-winning netBASE eBook collections. Visit us at Booth 709. Learn more at www.crcpress.com.* **709**

CrystalMaker Software Ltd., Centre for Innovation & Enterprise, Oxford University Begbroke Science Park, Begbroke, Oxfordshire, United Kingdom OX5 1PF, 44-1865-854804, fax: 44-1865-854805, e-mail:info@crystalmaker.com, Internet: http://www.crystalmaker.com *Award-winning software for crystal and molecular modelling and diffraction simulation. Build, display, manipulate chemical structures - fast. Elegant user interface with multi-structure browsing, synchronization and animation - and one-click movie generation. Optional software for single-crystal or powder diffraction, with real-time simulation control and display of observed data.* **233**

De Gruyter, Genthiner Str. 13, Berlin, Germany D-10785, 0049 (0)30 26005 0, fax: 0049 (0)30 26005 251, e-mail:info@degruyter.com, Internet: www.degruyter.com *The independent academic publisher De Gruyter can look back at over 260 years of history. The De Gruyter Group publishes over 1,300 new titles each year in the humanities, medicine, natural sciences and law, more than 650 journals, and a variety of digital media.* **837**

Dotmatics Inc., 11300 Sorrento Valley Rd, Suite 115, San Diego, CA, United States 92121, 619-419-2808, fax: 858-852-7903, e-mail:hayleigh.popplewell@dotmatics.com, Internet: www.dotmatics.com *Dotmatics is a software and services provider for scientific data management. A ready-to-use platform provides data capture, registration, secure externalized collaboration, data querying, visualization and reporting tools, fully configurable ELN for all disciplines (chem, bio, formulations, manufacturing, etc), DMPK. Available on Cloud or on premise. PC, Mac, mobile dev or Linux.* **318**

Edinburgh Instruments, 2 Bain Square, Kirkton Campus, Livingston, United Kingdom EH54 7DQ, +44 (0) 1506 425 300, fax: +44 (0) 1506

425 320, e-mail:sales@edininst.com, Internet: www.edinburghphotonics.com *With unparalleled customer support and instruments with the highest sensitivity, Edinburgh Instruments are the experts in fluorescence. Products include fluorescence spectroscopy (steady-state and TCSPC), laser flash photolysis and TCSPC light sources. Our low cost FS5 Spectrofluorometer is the latest addition to our product range, visit us to find out more.* **1224**

Eicom USA, 7098 Miratech Drive, Suite 100, San Diego, CA, United States 92121, 888-680-7775, fax: 858-560-8040, Internet: www.eicom-usa.com *The Smart Evaporator is a new type of evaporator based on a Vacuum-Assisted Vortex Technology, allowing you to evaporate without worry of bumping or the need to nurse the equipment. It is compact-sized (fits in a fume hood), temperature-controlled, and is compatible with various flasks/vials to avoid unnecessary sample transfer.* **338**

Elsevier, 80 High Street, Sawston, Cambridge, United Kingdom CB22 3HJ, Internet: www.elsevier.com *Elsevier is a leading Science and Technology publisher and provides search and discovery tools in Chemistry, Chemical Engineering and related subject areas. We publish over 125 highly-respected journal titles, all with Open Access options, and a huge range of textbooks, scientific monographs and major reference works. With innovative electronic products and services such as ScienceDirect, for access to scientific papers, and Scopus, for easy searching of abstracts and citations, we continue to refine our portfolio to serve the research needs of educators, researchers and students worldwide. Visit: www.elsevier.com/chemistry* **211**

Extrel CMS, 575 Epsilon Drive, Pittsburgh, PA 15238, Internet: www.extrel.com *Extrel is the world's leading manufacturer of research and process mass spectrometers, residual gas analyzers, and quadrupole mass spectrometry components. For 50 years, Extrel's instruments have been recognized for exceptional performance, reliability, and flexibility complemented by the most comprehensive application, technical, and on-site support in the industry.* **717**

FEI Company, 5350 NE Dawson Creek Drive, Hillsboro, OR 97124, 503-726-7500, fax: 503-726-7509, e-mail:fei_info@fei.com, Internet: www.fei.com *FEI designs, manufactures, and supports the broadest range of high-performance microscopy solutions and workflows. FEI's customers are working to address global challenges. They study materials' structures, quantify elemental composition and distribution, and observe materials' responses to (near) real world environmental influences, at resolutions from sub-micron to sub-Ångström.* **1400**

FlackTek, Inc., 1708 Hwy, 11 Landrum, SC 29356 United States 864-895-7441, Internet: flacktek.net. *FlackTek Inc. will be demonstrating an advanced tool for mixing, grinding/milling and dispersing. This Non-Invasive Mixing™ technology can be used to process any combination of powders, pastes, putties and liquids from 1g to 5kg. The SpeedMixer removes air bubbles while homogenizing the sample, in seconds, and there is ABSOLUTELY NO CLEAUP!* **1302**

Formulation USA, 6660 N High Street, Suite 2A, Worthington, OH, United States 43085, 614-888-0023, fax: 614-987-0045, Internet: www.formulation.com *Formulation offers instrumentation to help formulators characterize dispersions in terms of physical stability as well as micro rheology where viscoelastic properties are easily determined. The range of instrumentation includes the different models of the Turbiscan, the Rheolaser Master and Horus film formation analyzer.* **532**

FRITSCH Milling and Sizing, 2009 Mackenzie Way, Suite 100, Cranberry Township, PA, United States 16066, 412-559-8840, Internet: www.

fritsch-us.com *FRITSCH is an internationally respected German manufacturer of application-oriented laboratory instruments. Our instruments are used worldwide for sample preparation and particle analysis for fast paced industrial process monitoring and critical applications in QA, QC, and R&D.* **1217**

Frontiers, EPFL Innovation Park, Building I, Lausanne, Switzerland 1015, 41 21 510 17 00, fax: 41 21 510 17 01, e-mail:editorial.office@frontiersin.org, Internet: www.frontiersin.org *Frontiers is a community-driven open-access academic publisher and research network. Our grand vision is to build an Open Science platform that empowers researchers in their daily work and where everybody has equal opportunity to seek, share and generate knowledge.* **839**

Gamry Instruments, 734 Louis Drive, Warminster, PA 18974, 877-367-4267, fax: 215-682-9331, e-mail:info@gamry.com, Internet: www.gamry.com *Gamry designs/manufactures high-quality electrochemical instrumentation and accessories. Single and multichannel potentiostats-600 mA to 30 A, fully-integrated spectroelectrochemical setups for UV/Vis and Raman, coin cell and 18650 battery holders and an EOCM that can handle crystals from 1-10 MHz. See our new potentiostats-one specially designed for testing batteries, fuel cells, supercapacitors* **1009**

Gaussian, 340 Quinpiac Street, Building 40, Wallingford, CT 06492, 203-284-2501, fax: 203-284-2521, e-mail:info@gaussian.com, Internet: www.gaussian.com *Gaussian, Inc. is the world leader in electronic structure computational chemistry programs. The Gaussian series of programs is available on every major computing environment, from PCs to supercomputers, and it is currently used in a wide variety of industrial, governmental and academic research settings worldwide. Gaussian, Inc. will be demonstrating the latest versions of Gaussian and GaussView.* **400**

Gilead Sciences, 333 Lakeside Drive, Foster City, CA 94404 United States, 650-522-1275, Internet: www.gilead.com/careers **1317**

Grace Discovery Sciences, 2051 Waukegan Road, Deerfield, IL 60015, 847-948-8600, fax: 847-948-1078, e-mail:discoverysciences@grace.com, Internet: grace.com/pharma-and-biotech/en-us *Grace is a premier manufacturer of silica media for HPLC, flash, and process chromatography. Our extensive offering includes Reveleris® purification systems, Vydac® and Davisil® purification media, and MODcol® Spring® columns, together with a complementary offering of columns, instruments and accessories for all stages of research, from discovery through process.* **1314**

Guizhou Wylton Jinglin Electronic Material Co., Ltd., New Materials Industrial Park, North Baiyun Road, Baiyun District, Guiyang, Guizhou, China 550014, 0851-4350785/4288779, fax: 0851-4350785-8666, e-mail:wyltonchem@wylton.com, Internet: www.wyltonchem.com *Wylton Jinglin is proud to supply Heterocyclic Building Block Products to customers in high end chemical compounds market. It spares no efforts to research and develop Boron Acid and Boron Acid Ester Products to strive to be the best supplier, which features the most complete varieties, most up-to-date products, best R&D efficiency and superior service, for Heterocyclic Building Block Products and Boron Acid and Boron Acid Ester Products.* **929**

Hands-On Learning, 3880 S. Windermere Street, Englewood, CO 80110, United States 720-485-6061, Fax: 720-420-4926, Internet: www.holscience.com. *Hands-On Learning is the world leader in science distance learning. HOL pioneered the way education is conceived and delivered around the world, regardless of location, time zone, or language. Our cutting-edge*

lab kits are self-contained learning portals that allow instructors and students to collaborate anytime, anywhere. **304**

Hayden McNeil Publishing, 14903 Pilot Dr., Plymouth, MI 48170, 734-455-7900, fax: 734-455-3901, e-mail:orders@hmpublishing.com, Internet: www.hmpublishing.com **1036**

HE Chemical, 7-Jia-1701, Jingrui Xicheng, Changzhou, Jiangsu, China 213000, 0086 519 86883102, fax: 0086 519 85104102, Internet: www.hechemical.com Pyridinecarboxylic acids, (Trifluoromethyl)pyridines, Pyridineacetic acids, Fluoro chemicals, Difluoromethyl chemicals, Difluoromethoxy chemicals, Thiophenes, Pyrimidines, Indoles, and other rare products. **1206**

Heidolph North America, 1241 Jarvis Ave., Elk Grove Village, IL, United States 60007, 2242659600, Internet: www.heidolphNA.com Heidolph North America focuses on providing unparalleled sales & support of premium laboratory equipment to the North America scientific community. With a combination of expertise and quality products Heidolph is the category leader in rotary evaporators, overhead stirrers and magnetic stirring hotplates. Other product portfolio highlights are the full line of Tuttnauer sterilizers and innovative productivity equipment from Radleys. With a team of 12 in field sales representatives and service engineers providing onsite product demonstrations, product health day visits, trainings, installations, and product maintenance is an added value to researchers. Heidolph North America's headquarters are based in the Chicago area providing dedicated customer service, shipping, logistics, technical support and sales management to the US and Canadian laboratory market. We believe in our "Research made easy" philosophy of prompt customer service of all Heidolph products and supported by a 3 year warranty you can depend on. For more information on Heidolph North America, visit www.HeidolphNA.com **1201**

Hidden Analytical Inc., 37699 Schoolcraft Road, Livonia, MI 48150, 734-542-6666, fax: 734-542-6030, e-mail:info@hiddeninc.com, Internet: www.HiddenAnalytical.com Hidden Analytical manufactures high performance quadrupole mass spectrometers for precision gas analysis, materials characterization and surface science applications. Showcasing systems for catalysis studies, reaction kinetics, residual and process gas analysis. For quantitative atmospheric pressure gas analysis the new, compact QGA system includes automated gas calibration for spectral deconvolution, sub-ppm detection and fast inlet technology for pulsed gas studies. Also featuring CatLab, a unique, integrated microreactor and mass spectrometer system for characterization and evaluation of catalysts or thermal studies of evolved species. For atmospheric gas studies the SPACI-MS quantifies intra-catalyst channel species transients and distributions with high temporal resolution. **511**

ICE Publishing, Institution of Civil Engineers, 1 Great George Street, Westminster, London, United Kingdom SW1P 3AA, Internet: www.icevirtuallibrary.com/science ICE Science is the innovative multi-disciplinary materials science series from ICE Publishing, the publishing division of the Institution of Civil Engineers, who have been uniting research and practice in science and technology since 1836. Launched in 2012, the ICE Science collection comprises 5 titles: Bioinspired, Biomimetic and Nanobiomaterials; Emerging Materials Research; Green Materials; Nanomaterials and Energy; and Surface Innovations. For further information, visit www.icevirtuallibrary.com/science **1331f**

IIE/Council for International Exchange Of Scholars, 1400 K Street, NW, Washington, DC 20005, 202-686-4017, Internet: www.cies.org The Council for International Exchange of Scholars (CIES) has administered the Fulbright Scholar Program, the U.S. government's flagship aca-

dem exchange effort, on behalf of the United States Department of State, Bureau of Educational and Cultural Affairs. **902**

Indofine Chemical Co., 121 Stryker Lane, Hillsborough, NJ 08844, 908-359-6778, fax: 908-359-1179, e-mail:chemical@indofinechemical.com, Internet: www.indofinechemical.com **1318**

InfoChem GmbH, Landsberger Strasse 408, Munich, Germany 81241, 49-89-583002, fax: 49-89-5803839, e-mail:info@infochem.de, Internet: www.infochem.de InfoChem is a software company focusing on the production and marketing of innovative products for chemical information and cheminformatics. The company's main activities involve the development of software tools to handle, store and retrieve chemical structures and reactions, and to automatically extract scientific information from text and images. **809**

InRedox LLC, P.O. Box 0681, Niwot, CO, United States 80544-0681, 720-352-1715, Internet: www.inredox.com **1028**

Instec, Inc., 5589 Arapahoe Avenue, Ste. 208, Boulder, CO 80303, 303-444-4608, Fax: 303-444-4607, Internet: www.instec.com Precision thermal microscopy stages, plates, and chucks for use with POM, FT-IR, XRD, AFM, etc. Also offering automatic liquid crystal testing equipment, liquid crystal materials and supplies, as well as custom temperature control solutions to fit into any experiment. 30+ years of experience in liquid crystal and material testing applications. **326**

INTAVIS Bioanalytical Instruments AG, Widdersdorfer Str. 248-252, Cologne, Germany 50933, Internet: http://www.intavis.com/en/ Intavis is a leading manufacturer automated peptide synthesizers. The MultiPep RSi and ResPep SL are fully automated tabletop peptide synthesizers that use exchangeable modules for a wide range of synthesis scales. Modules are available for SPOT synthesis arrays, small scale synthesis of hundreds of peptides in parallel, the affordable production of specialty peptides in micro-columns, up to large scale synthesis of individual peptides. The newly released MultiPep CF utilizes an advanced large scale module that allows for efficient synthesis of long and difficult sequences. **314**

Interchim Inc., 1536 West 25th St., Suite 452, San Pedro, CA 90732, 800-560-8262, fax: 310-802-3877, e-mail:tkorman@interchiminc.com, Internet: www.interchiminc.com **905**

ISS Incorporated, 1602 Newton Drive, Champaign, IL 61822, 217-359-8681, Fax: 217-359-7879, e-mail: iss@iss.com, Internet: www.iss.com ISS manufactures fluorescence instrumentation for time-resolved and steady-state measurements. Including, a line of modular components for fluorimeters (laser diodes, LEDs, high pressure cell and fiber optic sensors amongst an extensive line of accessories) and microscopy (data acquisition cards for FCS and FLIM, laser launchers, galvo-scanning mirrors and detector units). Applications include Fluorescence Resonance Energy Transfer (FRET), Fluorescence Lifetime Imaging (FLIM), Fluorescence Fluctuation Spectroscopy (FCS, FCCS, PCH). Ask about our new NanofImaging packages for Alba and Olympus FV1000/FV1200 for resolving 3D cellular structures down to 20-40 nm with a precision of 2 nm in a matter of a few seconds. **1406**

J-KEM Scientific, 6970 Olive Blvd., St. Louis, MO 63130, 800-827-4849, fax: 314-863-6070, Internet: www.jkem.com Digital temperature controllers regulate any volume (0.1ml to 100L) or piece of equipment to 0.1 degree. Advanced safety features with over & under temperature alarms. Free control, data logging, and ramping software. Programmable syringe pumps deliver multiple reagents to multiple reactors in parallel with no volume restrictions, automatically refill. Digital vacuum regulator controls to 0.1 torr. Infinity Controller automates any lab or bioreac-

tor process, controls temperature, stirring, pressure, pH, oxygen, and reagent addition. Robotic workstations for weighing, synthesis, reformulating and custom applications for \$30,000. Articulating arm and SCARA robots. Accessories include filter stations, capping stations, robotic shakers, centrifuge. **424**

Japan Analytical Industry Co. Ltd., 208 Musashi, Mizuho, Nishitama Tokyo 190-12 JAPAN, Internet: www.jai.co.jp/english/index/html Do you have difficult samples to separate? JAI offers unique purification / separation system called "Recycling" preparative HPLC that can make your purification as easy as possible while saving solvent. JAI offers also offers world first portable pyrolyzer for Py-GC. **241**

JASCO, 28600 Mary's Court, Easton, MD 21601, 800-333-5272, fax: 410-822-7526, e-mail:sales@jascoinc.com, Internet: www.jascoinc.com **928**

JEOL USA, Inc., 11 Dearborn Road, Peabody, MA 01960, 978-535-5900, fax: 978-536-2205, e-mail:salesinfo@jeol.com, Internet: www.jeolusa.com JEOL is a world leader in analytical instrumentation-NMR, GC/MS, DART/MS, SEM, TEM, and more. We recently introduced our ECZ NMR series which has an ultra-compact design and improved performance. Our AccuTOF GCX is the only high-resolution mass spectrometer that combines GCxGC with high-resolution mass spectrometry and a choice of EI, CI, and FI ion sources. New capabilities of our SpiralTOF Maldi-TOF mass spectrometer include Maldi imaging, LC/MALDI-MS, and correlative microscopy. **1101**

John Wiley & Sons, Inc., 111 River St. 4-02, Hoboken, NJ 07030, Phone: 201-748-6000, Internet: www.wiley.com Wiley's product diversity is unique, spanning books, journals, databases, web-portals and workflow tools. Visit Booth #700 and talk to us about our new journal enhancements—you'll be entered in our restaurant raffle! At the booth, browse our books on display-ACS attendees receive 30% off orders and FREE shipping

JoVE, One Alewife Center, Suite 200, Cambridge, MA, United States 02140, Internet: www.jove.com JoVE, the Journal of Visualized Experiments, is a peer reviewed, PubMed indexed journal devoted to the publication of physical and life science research in a video format. **207**

JULABO, 884 Marcon Blvd., Allentown, PA 18109, (800) 458-5226, fax: (610)231-0260, e-mail:info@julabo.com, Internet: www.julabo.com **925**

KBI Biopharma, Inc., 1101 Hamlin Road, Durham, NC, United States 27704, **1414**

Keysight Technologies (formerly Agilent LSCA), 5301 Stevens Creek Blvd., Santa Clara, CA 95051, 800-227-9770, fax: 302-633-8944, e-mail:contact_us@agilent.com, Internet: www.keysight.com/find/nano Keysight Technologies (formerly Agilent) will feature the 7500 AFM that establishes new performance for nanoscale measurement, characterization & manipulation. This next-generation system offers 90µm closed-loop atomic resolution & industry-leading environmental control. The NEW compact, high performance FE-SEM now combines low-voltage imaging with the option of EDS elemental analysis. **503**

Kimble Chase LLC, 234 Cardiff Valley Road, Rockwood, TN, United States 37854, e-mail:info@kimble-chase.com, Internet: www.kimble-chase.com **1215**

Knauer, Hegauer Weg 38, Berlin, Germany D-14163, 49-30-8097-2718, Internet: www.knauer.net KNAUER offers UHPLC/HPLC systems for the analytical up to the preparative range of applications. KNAUER is a competent partner for continuous chromatography using SMB and MCSGP technologies. LC columns, UV/VIS/NIR and RI detection systems, biochro-

EXPOSITION

matography solutions, as well as appropriate software complete the choice of high quality LC products. KNAUER also supplies osmometers for chemistry and clinical use. KNAUER is certified DIN EN ISO 9001:2008 and ISO 14001.

1110

KNF Neuberger, 2 Black Forest Road, Trenton, NJ 08691-1810, 609-890-8600, fax: 608-890-8323, e-mail: knfusa@knf.com, Internet: www.knfusa.com Visit KNF Neuberger to learn why the new RC 900 Rotary Evaporator is "Inspiringly Easy to Use"! Features include easy-to-use remote control, easy flask exchange, and minimal footprint. Also new are SIMDOS 10 liquid dosing/metering pumps and a 12V field filtration vacuum pump

225

Krüss America, LLC, 1020 Crews Road, Suite K, Matthews, NC 28105, 704-847-8933, fax: 704-847-9416, e-mail: mlh@krussusa.com, Internet: www.krussusa.com KRÜSS is the world leading manufacturer of surface science equipment for research, development, educational, and quality control labs. We provide a full line of contact angle meters and tensiometers, for the measurement of contact angle, surface tension, interfacial tension, surface energy, and many other surface properties.

331

Lab Manager/LabX, 478 Bay Street, Midland, ON, Canada L4R 1K9, 888-781-0328, fax: 705-528-0270, e-mail: info@labmanager.com, Internet: www.labxmediagroup.com Lab Manager analyzes the link between business strategy, technological innovation and implementation. It is focused on the lab professional in a leadership role who is responsible for setting the labs direction. LabX (www.labx.com) is an online marketplace and a resource to buy and sell laboratory equipment and high-tech products.

1331a

Late Nite Labs, Ltd., 33 Irvine Place, 9th Floor, New York, NY, United States 44118, 862-596-2325, Internet: latenitelabs.com Late Nite Labs is the leading innovator of digital science labs. Our realistic science labs offer an authentic, accessible experience that moves learning beyond the classroom. Give students the freedom to experiment and learn from their mistakes—at their own pace, at any time or place. Learn more at: <http://latenitelabs.com>

1208

M. BRAUN, Inc., 14 Marin Way, Stratham, NH 03885, 603-773-9333, fax: 603-773-0008, e-mail: info@mbraunusa.com, Internet: www.mbraunusa.com

500

Magritek Inc., 6440 Lusk Blvd., Suite 108, San Diego, CA, United States 92121, 855-667-6835, Internet: www.magritek.com

937

Malvern Instruments, Inc., 117 Flanders Road, Westborough, MA 01581, 508-768-6400, fax: 508-768-6403, e-mail: sales.us@malvern.com, Internet: www.malvern.com Malvern's materials and biophysical characterization technology and expertise enables scientists and engineers to investigate, understand and control the properties of dispersed systems. Used in research, development and manufacturing, Malvern's instruments provide critical information that helps accelerate research and product development, enhance and maintain product quality and optimize process efficiency.

1107

Maruzen Co., Ltd., 110B Meadowlands Parkway, Suite 205, Secaucus, NJ 07094, 201-865-4400, fax: 201-865-4845, Internet: www.maruzen.info/hgs Maruzen International Co., Ltd (MIC) is the leading distributor of globally renowned HGS Molecular Model. The company is located in Secaucus, NJ, with the parent company Maruzen Co., Ltd. in Tokyo. Manufactured in Japan, HGS molecular model has attracted researchers, educators, and students all over the world for over 40 years. This subtle and professionally manufactured model has very wide variety of options, which will suit any type of research/educational activities in the broad fields of chemistry, pharmacology etc.

808

Materials Design, Inc., P.O. Box 2000, Angel Fire, NM 87710, 760-495-4924,

407

Matrix Scientific, P.O. Box 25067, Columbia, SC 29224, 803-788-9494, fax: 803-788-9419, e-mail: sales@matrixscientific.com, Internet: www.matrixscientific.com Over 105,000 research chemical intermediates and building blocks available; many novel to Matrix. Entire catalog updated daily on our website which offers structure search ability. Over 22,000 building blocks! Principals have over 49 years of experience in the manufacture and supply of quality products for research and development.

714

McGraw-Hill Education, Two Penn Plaza, New York, NY 10121-2298, 646-766-2892, fax: 646-766-2208, Internet: www.mheducation.com Chemistry at McGraw-Hill Education offers a variety of digital and print solutions for your course needs. From our suite of adaptive learning and assessment products, such as ALEKS and SmartBook, to our traditional texts, McGraw-Hill provides you with superior content and learning tools to build a strong foundation for your chemistry course. Booth #1124.

1124

Mestrelab Research SL, Feliciano Barrera, 9B-Baixo, Santiago de Compostela, Spain 15706, 34-881-976-775, fax: 34-981-941-079, e-mail: info@mestrelab.com, Internet: www.mestrelab.com

932

Metrohm USA, Inc., 6555 Pelican Creek Circle, Riverview, FL 33578, 866-Metrohm, fax: 813-316-4900, e-mail: info@metrohmusa.com, Internet: www.metrohmusa.com Metrohm offers a complete line of analytical laboratory and process systems for titration, ion chromatography, electrochemistry and spectroscopy. From routine moisture analysis to sophisticated anion and cation quantification, we are ready to help you develop your method and configure the optimum system. Move your analysis from the lab to the production line with our custom process analyzers. At Metrohm we provide systems that find solutions, stop by our booth and meet Metrohm.

416

MicroLAB, Inc., PO Box 7358, Bozeman, MT 59771, 406-586-3274, fax: 406-586-3582, Internet: www.microlabinfo.com MicroLAB equipment will engage your students in learning fundamental chemical principles. MicroLab's FS-524 Lab Interface combines our patented FASTspecTM 360-880 nm scanning spectrophotometer and integrated sensors for an affordable high-quality general purpose lab instrument. Appropriate for chemistry laboratory courses or undergraduate/graduate research. Stop by for mini-workshops on electrochemistry and spectrophotometry.

317

Micromeritics Instrument Corp., 4356 Communications Drive, Norcross, GA 30093, 770-662-3636, fax: 770-662-3696, e-mail: ussales@micromeritics.com, Internet: <http://www.micromeritics.com>

924

Microtrac Inc., 148 Keystone Drive, Montgomeryville, PA 18936, United States 727-507-9770, Fax: 727-507-9774, Internet: www.microtrac.com

316

Midland Scientific, Inc., 1202 S. 11th Street, Omaha, NE, United States 68108, 800-642-5263, fax: 402-346-7694, Internet: www.midlandsci.com

1300

Molbase (Shanghai) Co., Ltd., Floor 5, Building 12, No. 1001 North Qingzhou Rd., Xuhui Dist, Shanghai 201109 China, 647-836-9600, Fax: 647-560-4953 Email: dan.liu@molbase.com

1037

Molymod Models - Spiring Ltd, Spiring Enterprises Ltd., Unite 8E, Gillmans Industrial Estate, West Sussex, United Kingdom RH14 9EZ, 44-1403-782-387, fax: 44-1403-785-215, e-mail: email@molymod.com, Internet: www.molymod.com Spiring Enterprises Ltd the inventor & exclusive manufacturer of molymod® molecular & atomic models & the miniDNA® abstract

system for modelling DNA & RNA. Molymod® range comprises sets kits & spare parts suitable for organic, biochem and general chemistry courses at college or university. Proudly made In Great Britain.

406

Nanalysis Corp., Bay 4, 4500, 5 Street NE, Calgary, AB, Canada T2E 7C3, 403-769-9499, fax: 403-775-6683, Internet: nanalysis.com NMRReady is a revolutionary benchtop NMR spectrometer. As the only all-in-one instrument available, it has a built-in touchscreen with an easy-to-use interface that makes data acquisition & processing simple, even for non-experts, without increasing the footprint of the spectrometer. No matter what your application – teaching, research or industry – the NMRReady offers spectroscopic resolution at the fraction of the size, cost and maintenance of current instrumentation.

1111

NanoMagnetics Instruments, Hacettepe-Ivedik OSB Teknokent, Melih Gokcek Bulvari No:61, 33 Kat:5 Ivedik, Yenimahalle Ankara, Turkey 06370, Internet: www.nanomagnetics-inst.com NANOMAGNETICS INSTRUMENTS is one of the world leading companies in the field of Scanning Probe Microscopes (SPMs) and measurement systems. SPMs are engineered and manufactured to work under various atmospheric conditions(0K-300K). Company is focused on research, development and manufacturing of SPMs including their mechanical parts manufacturing, controller electronics and software.

1418

Nat'l Res. Council/ Nat'l Academies, Fellowship Programs, 500 5th St., NW, Washington, DC 20001, 202-334-2760, fax: 202-334-2759, e-mail: jdellammo@nas.edu, Internet: www.national-academies.org/rap The National Research Council of the National Academies offers awards four times annually to graduate, postdoctoral and senior researchers for independent research to be conducted in residence at participating US federal laboratories and affiliated institutions. Application submission dates are February 1, May 1, August 1, and November 1.

504

Nature Publishing Group, 75 Varick Street, 9th Floor, New York, NY 10013, 212-726-9200, fax: 212-696-9006, Internet: www.nature.com Nature Publishing Group (NPG) produces scientific information for researchers and the scientifically interested general public. Each month our high-impact journals, open access titles, news, apps, conferences and job listings help over 9 million users to advance their research, reputation, careers and knowledge. Part of Macmillan Science and Education.

601

Neaspec GmbH, Bunsenstrasse 5, 82152 Martinsried, Germany, 49 89 4524 206 34, fax: 49 89 4524 206 99, e-mail: miriam.boehmler@neaspec.com, Internet: www.neaspec.com nanoFTIR – the ultimate nanoanalytic microscopy and spectroscopy platform for materials research – enables optical analysis of complex material systems at visible, infrared and terahertz frequencies at a spatial resolution of 10nm. Neaspec is dedicated to delivering innovative solutions for nanoscale optical imaging & spectroscopy for researchers in industry and academic institutions.

927

NIST, 100 Bureau Drive, Stop 2300, Gaithersburg, MD 20899-2300, 301-975-3774, fax: 301-926-0416, e-mail: diane.decker@nist.gov, Internet: www.nist.gov/srm

325


NT-MDT Co., NT-MDT House, National Technological Park, Castletroy, Limerick, Ireland, Internet: www.ntmdt.com From cutting edge scientific research to routine surface investigations, NT-MDT has a unique and unrivalled portfolio of scanning probe microscopes. Our application-focused instruments provide you with a full range of capabilities in AFM-Raman, high-resolution, multi-frequency measurements, and AFM based nanomechanics. As an innovator in SPM for over 20 years, NT-MDT has a specialized high-performance solution for your research needs.

1000

Oakwood Products Inc., 1741 Old Dunbar Road, West Columbia, SC 29172, 803-739-8800, fax: 803-739-6957, e-mail:sales@oakwoodchemical.com, Internet: www.oakwoodchemical.com
Oakwood Chemical, a manufacturer and distributor, supplies research chemicals to the research community. Oakwood's product listing contains over 100,000 items, including many unique building blocks and reactive intermediates, solvents and reagents. Routine synthetic work includes sulfur tetrafluoride chemistry as well as most routine transformations. Oakwood provides custom synthesis services. **600**

Ocean Optics, Inc., 830 Douglas Avenue, Dunedin, FL 34698, 727-733-2447, fax: 727-733-3962, e-mail:info@oceanoptics.com, Internet: www.OceanOptics.com **1209**

On the Avenue Marketing, 391 Totten Pond Road, Waltham, MA 02451 United States, 216-789-8194, Internet: www.ontheavenuemarketing.com Visit The New York Times booth for 50% off of home delivery or digital subscriptions, plus a free gift upon purchase. **215**

 **OpenStax College, Rice University**, 6100 Main Street, MS-375, Houston, TX 77005, Internet: openstax.org OpenStax College is committed to improving student access to quality learning materials. An initiative of Rice University and supported by philanthropic foundations, OpenStax College provides entirely free textbooks, developed and peer-reviewed by educators to ensure they are readable, accurate and meet the scope and sequence requirements of your course. **313**

Optibrium Ltd., 7221 Cambridge Research Park, Beach Drive, Cambridge, United Kingdom CB25 9TL, +44 1223 815900, fax: +44 1223 815907, e-mail:info@optibrium.com, Internet: www.optibrium.com Optibrium creates elegant software solutions for small molecule design, optimisation and data analysis, including: StarDrop™, a comprehensive environment that guides the design and selection of high-quality compounds; Sentira™ a powerful and easy-to-use desktop tool for chemistry data visualisation; and Asteris, an iPad® app for creative compound exploration and design. **1219**

Oxchem Corporation, 1408 E. Arrow Highway, Invaldale, CA, United States 91706, 626-461-2812, Internet: www.ox-chem.com OXCHEM CORPORATION offer Multiple Catalog Service, Efficient Sourcing Service and Specialized Custom Synthesis Services, we provide innovative products to worldwide clients. Our main products lines include alcohols, amines, aldehydes, acids/esters, halo of heterocycles (indole, imidazole, pyrazole, pyridazine, pyridine, pyrimidine, pyrazine, piperazine, piperidine, pyrrolidine, thiazole, triazole). **308**

Oxford University Press, 198 Madison Avenue, New York, NY, United States 10016, Internet: www.oup.com/us **805**

Papers, 236 Gray's Inn Road, Floor 6, London WC1X 8HB United Kingdom, 44 786 741 0264 **315**

Paraza Pharma Inc., Montreal, Quebec, Canada H4S 1Z9, 617-216-9459, Internet: www.parazapharma.com A premium drug discovery service provider with deep expertise in Medicinal Chemistry, Custom Synthesis and DMPK (in vitro/in vivo). Entirely based in N. America (Montreal) in a state of the art building with highly experienced staff from large companies. Established track record of success and unparalleled cost efficiency **1410**

Parr Instrument Co., 211 53rd Street, Moline, IL 61265, 309-762-7716, fax: 309-762-9453, e-mail:parr@parrinst.com, Internet: www.parrinst.com Parr Instrument Company designs and manufactures Laboratory Reactors and Pressure Vessels, stirred and unstirred, used at elevated temperatures and pressures in the catalytic hydrogenation, organic synthesis and the polym-


erization processes. Parr also specializes in providing complete systems for batch, semi-batch and continuous-flow applications. Oxygen Combustion Calorimeters for the determination of the heat of combustion in solid, liquid and refuse derived fuels. **1001**


Particle Sizing Systems, 8203 Kristel Circle, Port Richey, FL 34668, 727-846-0866, fax: 727-846-0865, e-mail:donna@pssnicomp.com, Internet: pssnicomp.com PSS provides solutions with the Nicomp Nano and the AccuSizer particle analyzers. We've grown with the AccuSizer FX and FX Nano, high concentration analyzers that size/count particles over a wide dynamic range starting at 0.15 microns and at concentrations exceeding 10 million particles per mL. A modular design provides applications based solutions so our analyzers can be used in the lab/process environments achieving unprecedented resolution, accuracy and sensitivity. Through corporate relationships we offer instrumentation which measures surface/interfacial tension and characterizes foam properties by using digital image analysis and conductivity. **1127**

PASCO scientific, 10101 Foothills Boulevard, Roseville, CA 95747, 916-786-3800, fax: 916-786-8905, e-mail:sales@pasco.com, Internet: www.pasco.com Help your chemistry students "think science" with PASCO Scientific's award-winning product line. Integrating the latest standards-based content, probeware, and data collection and analysis software, PASCO chemistry solutions are easy to use, affordable, and work on iPad® as well as Mac® and Windows® computers. And don't miss our new Wireless Spectrometer! **219**

Pearson, One Lake Street, Upper Saddle River, NJ, United States 07458, 415-402-2583, Internet: www.pearsonhighered.com Pearson, the world's leading learning company, partners with K-20 institutions and educators to provide educational solutions and services that help to improve learning outcomes. Pearson serves learners of all ages around the globe, employing 41,000 people in more than 70 countries. For more information, visit www.pearsoned.com. **1308**

periodictable.co.uk, 3 Warple Mews, Warple Way, London, United Kingdom W3 0RF, 020 8749 3354, fax: 020 8749 9986, Internet: periodictable.co.uk RGB Research is the company behind periodictable.co.uk and partner in Theodore Gray's The Elements, Molecules and periodictable.com. We make beautiful periodic table displays presenting real element samples. We've installed 50+ displays in science buildings, educational institutions and chemical companies including Dow Chemical, Chemical Heritage Foundation and many universities. **439**

 **PerkinElmer Corp.**, 710 Bridgeport Avenue, Shelton, CT 06484, 1-800-762-4000, fax: 203-944-4950, Internet: www.perkinelmer.com PerkinElmer is a global leader focused on improving the health and safety of people and their environment. PerkinElmer is dedicated to the quality and sustainability of the environment. With our analytical instrumentation, illumination and detection technologies, and leading laboratory services, we focus on improving the integrity and safety of the world. **1104**

 **PerkinElmer Informatics**, 940 Winter Street, Waltham, MA, 02451, 781 663-8011, Fax: 781 663-8080, e-mail:informatics.customer_service@perkinelmer.com, Internet: www.cambridgesoft.com. PerkinElmer delivers a comprehensive suite of scientific informatics and software solutions from instrument generated data, to enterprise solutions to mobile applications, providing scientists with the necessary tools to aggregate, search, mine, analyze and visualize critical data to help turn data into actionable insights in an automated, predictive and scalable way **1106**

Pharmablock USA, Inc., 725 San Aleso Avenue, Suite 8, Sunnyvale, CA, United States 94085, 408-921-9969, Internet: www.pharmablock.com PharmaBlock is a fast growing chemistry service company. We supply innovative and unique building blocks that are specifically designed for today's pharmaceutical R&D. We have >150 chemists and offer >15000 compounds in grams to kilograms quantities. We specialize in custom synthesis for pre-clinical and clinical development. **403**

PharmAgra Labs, Inc., 158 McLean Road, Brevard, NC, United States 28712, 828-884-8656, fax: 828-884-9469, Internet: www.pharmagra.com PharmAgra Labs, Inc. is a chemistry CRO that for fifteen years has been conducting contract Research and Development in organic and medicinal chemistry. We specialize in providing a rapid-response team of organic chemists that can bring their high level of expertise to bear in all areas of discovery, scale-up, process and analytical chemistry. In our FDA inspected kilo suite we offer cGMP preparation of drug substances for use in Clinical Trials as well as low volume API manufacturing. Our company-owned, fully-equipped facility is located in Brevard, NC. **509**

PIKE Technologies, 6125 Cottonwood Drive, Madison, WI 53719, 608-274-2721, fax: 608-274-0103, Internet: www.piketech.com **415**

Pine Research Instrumentation, 2741 Campus Walk Avenue, Building 100, Durham, NC 27705, (919)782-8320, fax: 919-782-8323, e-mail:jgarry@pineinst.com, Internet: www.pineinst.com/echem Pine Research Instrumentation is your reliable source for electrochemical research equipment and accessories. We design, manufacture, and support high quality products for electrochemistry education and electrochemical research. Some of our products include the MSR electrode rotator, the WaveNow potentiostat and WaveDriver 20 bipotentiostat, the Honeycomb spectroelectrochemical cell, quartz photoelectrochemical cells, and disposable screen printed electrodes. **1029**

Poly-Med Inc., 51 Technology Dr., Anderson, SC, United States 29625, 864-328-0008, Internet: www.poly-med.com Bioabsorbable polymers and fibers produced by Poly-Med are used in numerous medical devices. Supplied components exhibit tailored bioabsorption and include granules; micro-, mono-, and multifilament fibers; and textiles. The company has developed and manufactured bioabsorbable constructs for more than 20 years. Poly-Med is ISO 9001 and 13485 certified and FDA registered. **904**

Precision Glassblowing of Colorado, 14775 East Hinsdale Ave., Centennial, CO, United States 80112, 303-693-7329, Internet: www.precisionglassblowing.com The source-manufacturer and supplier of OEM glass consumables for the ICP/ICP-MS industry offering torches, injectors, spray chambers and the industry's widest array of nebulizers. Additionally, we manufacture custom laboratory glassware from quartz and borosilicate glass. Our state-of-the-art QC-department ensures your parts are made to specification, both prototype and full-scale production. **427**

Proton OnSite, 10 Technology Drive, Wallingford, CT, United States 06492, 203-678-2182, Internet: www.protononsite.com Proton OnSite is the global leader in on-site gas generation for laboratories. We offer safe, affordable and high-performance solutions for hydrogen/nitrogen/zero air generators and air compressors. Proton's units are manufactured in a wide range of space-saving stackable systems. We offer a complete line of advanced equipment for LCMS and GC markets. **414**

PSS USA, Inc., 160 Old Farm Road, Suite A, Amherst, MA, United States 01002, Internet: www.pssgpcshop.com PSS is dedicated to the advancement of macromolecular characterization by providing expertise and tools to perform

EXPOSITION

GPC/SEC analysis. WinGPC software suite is an industry leader and the only platform that provides a validated environment that meets CFR 21 part 11 requirements. We provide a comprehensive array of GPC/SEC columns and standards for organic and aqueous environments for the analysis of synthetic and biopolymers. We provide method development and sample analysis services. GPC/SEC instrumentation for basic, multi-detector, multi-dimensional and hyphenated techniques including FT-IR, NMR and MS. **235**

Pure Chemistry Scientific Inc., 206A Adams Street, Unit 4 Newton, MA 02458 United States 857-928-2050 Fax: 617-206-9595, Internet: www.chemreagents.com. In USA are Stannanes, Vitamin D serious, Boronic Acids/Esters, PEG items. Itemidiates. In addition to the catalog products, we also provides custom synthesis and custom manufacturing services with thousands of chemical reagents. **306**

Quantachrome Corp., 1900 Corporate Drive, Boynton Beach, FL 33426, 5617314999125, fax: 5617329888, Internet: www.quantachrome.com **430**

Quark Glass, P.O. Box 2396, Vineland, NJ 08362-2396, 800-955-0376, fax: 856-455-3373, e-mail:sales@quarkglass.com, Internet: www.quarkglass.com **1008**

Rapp Polymere GMBH, Ernst Simon Strasse 9, Tuebingen, Germany D-72072, 49-7071763157, fax: 49-7071763158, e-mail:rapp-polymere@t-online.de, Internet: www.rapp-polymere.com **Rapp Polymere** is a world leader for high quality polymer supports. TentaGel or polystyrene resins are used in solid phase chemistry, combinatorial chemistry, as polymer supported reagents, library generation, peptide and oligonucleotide synthesis. Our reagents for PEG'ylation comprises hundreds of high sophisticated derivatives from Methoxy PEG's, homofunctional PEG's to hetero-bifunctional PEG's. **1113**

Reaction Analytics Inc., 2711 Centerville Road, Suite 5992, Wilmington, DE 19808, 858-472-2393, Email: administrator@ichemexplorer.com, Internet: www.ichemexplorer.com The iChem-Explorer from Reaction Analytics adds heating and stirring to your HPLC so you can do your chemistry in the sample vial. iChemExplorer helps you automate sampling, temperature control and record keeping using Agilent Chemstation or Waters Empower. Come take a look at booth 1134. Thanks. **1134**

Restek Corp., 110 Benner Circle, Bellefonte, PA, United States 16823, 800-356-1688, fax: 814-353-1309, Internet: www.restek.com Restek is a leading developer and manufacturer of chromatography columns and accessories. We provide analysts around the world with the innovative tools they need to monitor the quality of air, water, soil, foods, medical cannabis, pharmaceuticals, chemical, and petroleum products. **506**

Richman Chemical Inc., 768 North Bethlehem Pike, Lower Gwynedd, PA 19002, 216-628-2946, fax: 215-628-4262, e-mail:clk@richmanchemical.com, Internet: www.richmanchemical.com Richman Chemical specializes in custom chemical synthesis and manufacturing. Our capabilities include full cGMP manufacturing, method development, regulatory assistance, and raw material sourcing. We tailor our production solutions to each client's unique needs, saving them both time and money. **405**


Rieke Metals, LLC, 1001 Kingbird Road, Lincoln, NE, United States 68521, 402-434-2775, fax: 402-434-2777, e-mail:sales@riekemetals.com, Internet: www.RiekeMetals.com Rieke Metals began in 1991 with its foundation in 40+ years of active metal research. Headquartered in Nebraska, the company sells active Rieke Zinc and Magnesium, Grignard and organozinc reagents, fine organic chemicals and organic semi-conducting polymers/monomers including P3HT and water soluble polymers. **336**

Rigaku Americas Corp., 9009 New Trails Drive, The Woodlands, TX 77381, 281-362-2300, fax: 281-364-3628, Internet: www.rigaku.com Rigaku provides the worlds most complete line of X-ray diffraction and X-ray fluorescence instruments and components. Systems include the MiniFlex XRD and Supermini WDXRF benchtop systems, the SmartLab® multi-purpose diffractometer with SAXS and in-plane capabilities, DMAX Rapid II micro-diffraction system, SMAX3000 small angle scattering systems and the ZSX Primus WDXRF spectrometers. **1025**

Roberts and Company Publishers, 4950 S. Yosemite Street, F2 #197, Greenwood Village, CO 80111, 303-221-3325, fax: 303-221-3326, e-mail:info@roberts-publishers.com, Internet: www.roberts-publishers.com **906**

Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, United Kingdom CB4 0WF, 44-1223-432-378, fax: 44-1223-426-017, e-mail:sales@rsc.org, Internet: www.rsc.org The Royal Society of Chemistry is the world's leading chemistry community, advancing excellence in the chemical sciences. Talk to us about our books, peer-reviewed journals, leading databases, and Open Access publishing options on stand - we'd love to meet you. **701**

Rudolph Research Analytical, 55 Newburgh Road, Hackettstown, NJ 07840, 973-584-1558, fax: 973-584-5440, e-mail:info@rudolphresearch.com, Internet: www.rudolphresearch.com **301**

 **Sapling Learning**, 211 East 7th Street, 4th Floor, Austin, TX 78701, (512) 323-6565, e-mail:info@saplinglearning.com, Internet: www.saplinglearning.com Created and supported by educators, Sapling Learning's instructional online homework drives student success and saves educators time. **1200**

Schrödinger, Inc., 101 SW Main Street, Suite 1300, Portland, OR 97204, 503-299-1150, fax: 503-299-4532, e-mail:info@schrödinger.com, Internet: www.schrödinger.com Founded in 1990, Schrödinger is widely recognized as a scientific and technological leader in developing state-of-the-art chemical simulation software for use in pharmaceutical and materials science research. The company's products range from general molecular modeling programs to a full-featured suite of drug design software that uses both ligand- and structure-based methods. **608**

SCIENCE/AAAS, 1200 New York Avenue, NW, Washington, DC 20005, 202-326-6417, fax: (202) 842-1065, e-mail:membership@aaas.org, Internet: www.aaas.org Since 1848, AAAS and its members have worked together to advance science and serve society. As part of these efforts, AAAS publishes Science, a multidisciplinary peer-reviewed journal, and offers programs focused on science policy, international cooperation, science education, diversity, and career development for scientists. **829**

Semichem, 12456 W. 62nd Terrace, Suite D, Shawnee, KS 66216, 913-268-3271, fax: 913-268-3445, e-mail:jana@semichem.com, Internet: www.semichem.com Semichem features AMPACT™ and CODESSA™. AMPACT™ is a semiempirical quantum mechanical program, including an industry leading graphical user interface (GUI) that builds molecules and offers full visualization of results. CODESSA™ is an advanced quantitative structure/activity relationship (QSAR) program that ties information from AMPACT™ and other QM programs with experimental data. **404**

Serena Software, P.O. Box 3076, Blomington, IN 47402, 812-333-0823, e-mail:gilbert@serenasoft.com, Internet: www.serenasoft.com Announcing the release of Pcmol version 10. A complete molecular modeling program with a redesigned user interface, support for multiple force fields (MMX, MM3, MMFF94, OPLSAA), organometallic complexes, conformational searching, normal mode analysis, and interfaces

to many quantum chemistry programs (Gaussian, Mopac2012, Gamess, TurboMole). New features include support for CIF files and crystal structures and display of Molecular Orbitals and Densities and animated Vibrations. You can now take the output of a conformational search and write multiple input files for Gaussian and then read the Gaussian output files and plot the Boltzmann weighted IR, VCD or NMR spectra. Available for Windows, Macintosh and Linux. **342**

Shanghai Running Industrial Engineering Co., Ltd., Room1005, BuildingA3, Greenland Future Center, Fengxian District, Shanghai, China 201400. **1030**

SHELL LAB (Sheldon Manufacturing, Inc.), 300 N. 26th Ave., Cornelius, OR, United States 97113, Internet: www.shellab.com **417**

Shimadzu Scientific Instruments Inc., 7102 Riverwood Drive, Columbia, MD 21046, 800-477-1227, fax: 410-381-1222, Internet: www.shimadzu.com Shimadzu is a leading manufacturer of scientific instrumentation, including chromatography, spectroscopy, FTIR, environmental monitoring, and physical measurement. Markets/industries served include pharmaceuticals, metals, forensics, educational, government, agriculture and petrochemical. **613**

Sichuan Leshan Fuhua Tongda Agro-Chemical Technology Co. Ltd., 1806 Huaxia Bank Tower, No.256 South Pudong Road, Shanghai, China 200120, 0086-21-68865055/58360196, fax: 0086-21-68865055 ex 811, e-mail:info@fuhua-tongda.com **224**

Sigma-Aldrich, 3050 Spruce St., St. Louis, MO 63103, 314-771-5765, fax: 314-286-7817, Internet: www.sigma-aldrich.com Sigma-Aldrich has combined our scientific expertise with our history of working with pharmaceutical companies, resulting in a focus to strengthen and support Translational Research to enable and improve the quality of life. Our comprehensive approach to strengthen and support Translational Research is based on ensuring greater accuracy, reproducibility and confidence in drug discovery research through our products and services. Sigma-Aldrich recognizes that highly-validated products are critical at every stage of the drug discovery workflow and is dedicated to offering the industry's most validated products. **1216**

Snowy Range Instruments, 407 S. 2nd Street, Laramie, WY, United States 82070, Internet: www.wysri.com Snowy Range Instruments® designs and manufactures spectroscopic instrumentation for novel applications. Creative, cost-effective handheld and portable Raman spectroscopy solutions are made possible by SnRI's experience with diverse optical technologies and our experience with complex applications. **810**

SoftA Corporation, 11005 Dover Street, Unit 300, Westminster, CO 80021 United States, 303-465-1106, Fax: 626-608-2784 Internet: www.softacorporation.com. SoftA Corporation is a leading manufacturer of Evaporative Light Scattering Detectors for HPLC. Our innovative detectors help chemists optimize the information obtained from their chromatographic analyses. ELSDs are an ideal substitute, or supplement to, traditional detectors for chromatography concentration detection. SoftA designs and manufactures ELSDs with unmatched performance and affordability. **1404**

Sorbent Technologies, 5955 Peachtree Corners East, Suite A, Norcross, GA 30071, 866-767-2832, ext. 0281, e-mail:dschurer@sorbtech.com, Internet: www.sorbtech.com Sorbent Technologies, the leading chromatography and purification specialist to the scientific community, specializes in premium products and services for laboratory, pilot, and production. Separating small and large molecules, natural products, proteins, peptides, oligos, polymers, and more! Sorbents: Silicas, Bonded Phases, Aluminas,

Polymer Resins, Florisil, Polyamide TLC Plates Purity Flash Cartridges compatible with All Flash Systems EZ Flash Systems HPLC Columns: Analytical & Semi-Prep, & Prep (Grace Vydac, Macherey-Nagel, Jordi) GC columns: Capillary, Glass & Metal FPLC, Prep & Process Columns (Essential Life Solutions) SPE Cartridges Solvent Evaporator Lab Supplies: Pipet Tips, PCR, Tubes, Pipettors, Gloves, Racks, Boxes, Dispensers We are your Separation Solution Source! **914**

Specac, Specac, Ltd., River House, 97 Cray Avenue, ORPINGTON, Kent, United Kingdom BR5 4HE, 44 (0)1689 873134, fax: 44 (0)1689 878527, Internet: www.specac.com Specac is a high quality manufacturer of FTIR accessories and sample preparation products, bringing new and innovative solutions to the market place on a regular basis. Specac's spectroscopic accessory products cover a range of techniques, including ATR, Diffuse Reflectance, Specular Reflectance and Transmission. Providing the right solution for any sample. **1032**

Spectrum Chemical Mfg Corp., 769 Jersey Ave, New Brunswick, NJ 08901, (732) 801-5651, e-mail: sales@spectrumchemical.com, Internet: www.spectrumchemical.com **612**

Springer, 233 Spring Street, New York, NY 10013, 212-460-1600, fax: 201-348-4505, Internet: www.springer.com Come and browse over 10,100 key titles. Get 20% off print books and eBooks – and learn about MyCopy (a printed eBook for \$/€ 24.99). We are proud to be the publisher of choice for books such as *Far-Field Optical Nanoscopy* (co-edited by Prof. Stefan Hell), *Natural Products in the Chemical Industry*, *Polymer Blends Handbook*, and cutting-edge journals such as *Journal of Cheminformatics*, *Catalysis Letters*, *Cellulose*, *ChemTexts* and *Lipids*. Meet our editors, Kenneth Howell, Judith Hinterberg, Charlotte Hollingworth, Samuel Winthrop and Steffen Pauly, to discuss your publishing proposal. Ensure maximum readership for your work, too! Springer, your partner in publishing. Find all offers online: springer.com/acs **801**

StellarNet Inc., 14390 Carlson Circle, Tampa, FL 33626, 813-855-8687, fax: 813-855-0394, e-mail: dpersell@stellarnet.us, Internet: www.StellarNet.us StellarNet provides low cost miniature spectrometer systems and software for product analysis, research, education, and OEM. StellarNet instrumentation is rugged for any environment – lab, process, or field. Applications include absorbance & transmission (190–2300nm), fluorimetry, microscopy, optical metrology, colorimetry, LED/Laser/Solar, LIBS, OES, NIR, & Raman (532, 785, 1064). Come See the SpectraWizard! **1125**

STOE & Cie GmbH, Hilpertstrasse 10, Darmstadt, Germany D 64295, +49 6151 988722, fax: +49 6151 988788, Internet: www.stoe.com STOE, originally founded in 1887, to manufacture equipment for the optical analysis of crystals, has been a pioneer in powder and single crystal X-ray diffraction since the 1960s, e.g. STOE invented and patented the transmission geometry technique for Powder XRD as well as, for single crystals, produced the first pixel detector XRD system with an open Eulerian cradle. STOE is based in Darmstadt, Germany, and keeps the R&D, software programming, electrical and mechanical engineering and production all in house, allowing STOE to provide customers with standard as well as individual solutions. **939**

Strem Chemicals, 7 Mulliken Way, Dexter Industrial Park, Newburyport, MA 01950-3104, 978-499-1600, fax: 978-465-3104, Internet: www.strem.com Strem Chemicals, an employee-owned company, established in 1964 manufactures and markets over 4,500 metals, inorganics and organometallics for research and development, including metal catalysts, ligands and biocatalysts for organic synthesis, MOCVD/ALD precursors, bubblers and nanomaterials, for

use in pharmaceutical, microelectronics, chemical and petrochemical industries. Custom synthesis services are also provided. **813**

Struchem Co., LTD, Bldg. # 6-201, No. 2358 Chang'an Road, Suzhou City, Jiangsu Province, China 215200, +86-512-63009836, fax: +86-512-63006936, Internet: www.struchem.com **931**

Supercritical Fluid Technologies, One Innovation Way, Suite 303, Newark, DE 19711, 302-738-3420, fax: 302-738-4320, e-mail: info@supercriticalfluids.com, Internet: www.supercriticalfluids.com Equipment for supercritical fluid extraction (SFE), reaction (SFR), and high pressure chemistry. Laboratory SFE: 5 ml to 4 L; Pilot scale SFE Systems: Single or dual 10 liters with fraction collectors and automation. HPR-Series™ Chemical Reactors: 50 ml to 4 liter. Customized reactors and extractors to your specifications, including SCWO and larger volume systems. Phase Monitor™ for visual solubility determinations in supercritical fluids. CO₂ and solvent pumps, parts and service. Consultation and contract research services. **908**

Supra Sciences, 3000 B Street, #559, Sacramento, CA, United States 95816, 916-287-3877, e-mail: info@suprasciences.com, Internet: suprasciences.com Simplifying synthesis and purification, we offer supported scavengers, reagents, peptide synthesis, and Solid Phase Extraction (SPE) products. Improve productivity by reducing the complexity of isolation and removal of byproducts or impurities. Chat with our team of experts in the field for personal, cutting edge support. www.suprasciences.com **437**

Symphotic Tii, 880 Calle Plano, Camarillo, CA, United States 93012, 949-955-0258, Internet: www.symphotic.com Symphotic Tii represent ADANI's compact ESR (EPS) instrument CMS8400. The CMS8400 is designed for scientific research, education and application-oriented tasks in material science, environmental and petro-chemistry, pharmaceutical research. It is ideal for users who require affordable device with resolution and sensitivity comparable to large systems **1408**

Synquest Laboratories, Inc., P.O. Box 309, Alachua, FL 32616-0309, 386-462-0788 or 877-4-FLUORO (toll free), fax: 386-462-7097, e-mail: info@synquestlabs.com, Internet: www.synquestlabs.com SynQuest Laboratories specializes in fluorinated organic and inorganic chemicals, providing a creative and innovative range of building blocks, reagents and compressed and liquefied gases. We offer chemical services designed to expedite your research from conception to pilot quantities. Our website currently offers 63,000+ chemicals. **513**

Synthonix, 2713 Connector Drive, Wake Forest, NC 27587, 919-875-9277, fax: 919-875-9601, Internet: www.synthonix.com **328**

TA Instruments, 159 Lukens Drive, New Castle, DE 19720, 302-427-4000, fax: 302-427-4001, e-mail: info@tainstruments.com, Internet: www.tainstruments.com **1011**

Taylor & Francis (Journals), 530 Walnut Street, Suite 850, Philadelphia, PA, United States 19106, 215-625-8900, Internet: www.tandfonline.com Taylor & Francis boasts a growing, wide-ranging and high calibre journals portfolio in Chemistry. Our journals are edited by some of the most prominent academics in the field. Visit us at Booth 713 to browse our portfolio of books and journals and talk to us about publishing your work. www.chemistryarena.com **713**

TCI America, 9211 N. Harborside Street, Portland, OR 97203, 800-423-8616, fax: 888-520-1075, e-mail: sales-us@tcichemicals.com, Internet: www.TCichemicals.com TCI is a leading global manufacturer and supplier of specialty chemicals to the pharmaceutical, electronic, cosmetic, chemical, environmental, and biotech industries. Drawing on over 80 years of synthetic

organic chemistry experience, TCI develops new technology that produces rare and novel compounds. Our current catalog lists over 23,000 organic and biochemical products for use in research and production with 1/3 unique to TCI. Our manufacturing capabilities include multi step synthesis and continuous production from milligram to ton scale for custom and contract research services. Our modern facilities provide cGMP manufacturing with FDA validation. Please visit our website www.TCIchemicals.com/ **1004**

Teledyne Isco - Chromatography, 4700 Superior St, Lincoln, NE 68504, 402-464-0231, fax: 402-465-3064, e-mail: iscoinfo@teledyne.com, Internet: www.isco.com The Teledyne Isco Chromatography product line includes instruments and accessories for purification of organic compounds in normal-phase and reversed phase separations, and for bio-purification of proteins, peptides, and other biopolymers. **716**

ThalesNano Nanotechnology Inc., 7. Zahony u, Budapest, Hungary H-1031, 00 36 1 8808 500, fax: 00 36 1 8808 501, Internet: www.thalesnano.com ThalesNano is dedicated to making dangerous and difficult chemistry safe and easy to perform while assisting advances in the scientific field of chemistry. The company is widely recognized for its expertise in transforming chemical processes to microscale continuous-flow operations and developing manual or robotic continuous microreactors for the chemical industry. **1225**

The Committee for Cannabis Chemistry Division Formation, 531 West J Street, Ontario, CA, United States 91762, 617-429-0983, Internet: <http://www.gopetition.com/petitions/petition-for-a-new-ac-s-professional-division-cannabis-chemists.h> We are giving people the opportunity to show support for the formation of a division of cannabis chemistry within the American Chemical Society. We will be providing educational materials and giving attendees the opportunity to speak to its founding members and sign a petition. **237**

Thermo Scientific, 355 River Oaks Parkway, San Jose, CA, United States 95134, 800-532-4752, Internet: www.thermoscientific.com Visit Thermo Scientific booth 1014-1015 for integrated laboratory workflow solutions utilizing chromatography, mass spectrometry, and molecular spectroscopy. Come see the very latest solutions in LC, LC/MS, GC/MS, UV-Vis, FT-IR, Raman and NMR technologies to help streamline your processes, deliver more confident results, yield higher throughput, and reduce sample preparation. **1014,1015**

Thrupore Technologies LLC, 1118 Cannon Road N, Tuscaloosa, AL, United States 35406, 205-534-2060, Internet: www.ThruPore.Com Superior Fixed Bed Catalysts **542**

Tosoh Bioscience LLC, 3604 Horizon Drive, Suite 100, King of Prussia, PA 19406, 484-805-1219, fax: 610-272-3028, Internet: www.tosohbioscience.com We are a global leader in high quality, innovative pre-packed HPLC columns and bulk resins with the TSKgel® and TOYOPEARL® brand names, as well as our EcoSEC® GPC Systems. Tosoh Bioscience offers a GPC Sample Analysis Program to help your team with extensive analysis of organic and aqueous soluble polymers. **501**

University of Illinois - Nano Plasmonics, 405 N. Mathews Avenue, Urbana, IL 61801, United States 217-244-9481, Internet: <https://nanohub.org/tools/dda> Calculate scattering and absorption of light by targets with arbitrary geometries and complex refractive index. **239**

University Science Books, 20 Edgehill Rd., Mill Valley, CA 94941, 415-332-5390, fax: 415-383-3167, e-mail: univscibks@igc.org, Internet: www.uscibooks.com Displaying a splendid assortment of landmark books and textbooks including our newest physical chemistry text by

EXPOSITION

Chang & Thoman, Girolami's X-RAY CRYSTALLOGRAPHY, and a preview of the forthcoming PRINCIPLES OF NMR SPECTROSCOPY by Goldenberg. We are committed to publishing quality books at affordable prices. Please stop by to say hello! **605**

US EPA Green Chemistry Program, 1200 Pennsylvania Avenue, Mail Code 7406M, Washington, DC 20460, Internet: www.epa.gov/greenchemistry The U.S. EPA Green Chemistry Program is a voluntary, partnership program whose mission is to promote innovative chemical technologies that reduce or eliminate the use or generation of hazardous substances in the design, manufacture, and use of chemical products and processes. The Program accomplishes these goals through multiple activities including: The Presidential Green Chemistry Challenge Awards; designing tools, databases, and educational materials; and supporting research through grants and fellowships. **528**

Vacuubrand, Inc., 11 Bokum Rd., Essex, CT 06426, 860-767-2562, fax: 860-767-2563, e-mail: kpouliot@brandtech.com, Internet: www.vacuubrand.com **915**

Vacuum Atmospheres Co., 4652 West Rosecrans Avenue, Hawthorne, CA 90251, 310-644-0255, fax: 310-970-0980, e-mail: info@vac-atm.com, Internet: www.vac-atm.com VAC has set the standards for gloveboxes and inert gas purification for over 50 years. Once again, our ongoing research and development has produced an exciting new glovebox design, NO REGENERATION required by the user. Please visit us in booth 1100 for a demonstration on our Genesis and NexGen systems. **1100**

Vacuum Technology Inc., 15 Great Republic Drive, Unit #4, Gloucester, MA, United States 01930, 978-879 4302, fax: 978-879 4387, e-mail: sam.cai@vti-glovebox.com, Internet: www.vti-glovebox.com Vacuum Technology Inc. is committed to developing innovative products for clients around the world. With its North American facility located in Gloucester, Massachusetts USA, VTI offers UL certified Super-Purified Glove Boxes and Gas Purification Systems. A variety of Accessories can also be integrated into the glove box: Evaporator, Spin Coaters, Freezers, Cold Wells, and Microscope Units, among others. In addition to standard products, VTI specializes in working with our clients to create custom designs and solutions. **311**

Vapourtec Ltd., Unit 16, Park Farm Business Centre, Fornham St Genevieve, Bury St Edmunds, Suffolk IP28 6TS, United Kingdom, 44 1284 728659 Fax: 44 1284 728352 e-mail: duncan.guthrie@vapourtec.com, Internet: www.vapourtec.com **1307**

Vernier Software & Technology, 13979 SW Millikan Way, Beaverton, OR 97005, 888-837-6437, fax: 503-277-2440, e-mail: info@vernier.com, Internet: www.vernier.com Stop by the Vernier Software & Technology booth to see our exciting products for college chemistry such as our Organic Chemistry with Vernier lab book. We offer several affordable spectroscopy options including our new Vernier UV-VIS Spectrophotometer. Try out the Polarimeter that can graph light intensity versus angle so students don't have to determine optical maximum with their eye. Additional instruments include the Melt Station Melting Temperature Sensor, SpecroVis Plus spectrophotometer with fluorescence

capabilities, and an improved Vernier Mini GC Plus. Use any of these devices on a computer or our stand-alone LabQuest 2 lab interface. **901**

Vigor Gas Purification Technologies, 5100 Westheimer Road, Suite 200, Houston, TX 77056, 716 200 1200, e-mail: info@vigor-glovebox.com, Internet: www.vigor-glovebox.com **900**

ViridisChem, Inc., 4344 Moorpark Ave., Suite 1, San Jose, CA, United States 95129, (408) 250-6905, fax: (408) 351-7900, Internet: www.viridischem.com With comprehensive database of over 30 million substances, ViridisChem offers: "Green Pocketbook" that provisions chemical and toxicological data with visual analysis tools, allows tox.endpoint based quick comparisons, identifies greener alternatives, and points out govt. defined hazardous chemicals "Green Analyzer": Offers drill-down analysis of multi-step synthesis, identifies areas of improvements. **538**

VUV Analytics, Inc., 611 Eagle, Austin, TX, United States 78734, 512-333-0860, fax: 512-261-1011, Internet: www.vuvanalytics.com **432**

W.H. Freeman & Company, 41 Madison Avenue, New York, NY, United States 10010, 212-576-9400, fax: 212-689-2383, e-mail: john.britch@whfreeman.com, Internet: www.whfreeman.com/chemistry Starting in 1946 with Linus Pauling's General Chemistry, W.H. Freeman & Company, a Macmillan Education imprint, has been the premier publisher of chemistry textbooks and media. A new edition of Harris Quantitative Chemical Analysis and additional titles are due this year. Visit Booth 401 and www.macmillanhigher.com/chemistry. **401**

W.W. Norton, 500 Fifth Ave., New York, NY 10110, 212-548-4751, fax: 212-790-4261, Internet: www.wwnorton.com The oldest and largest publishing house owned wholly by its employees, W. W. Norton, Inc. publishes about 400 trade, college, and professional titles each year. **607**

Waters Corp., 34 Maple Street, Milford, MA 01757, 508-482-2000, fax: 508-482-2674, e-mail: info@waters.com, Internet: www.waters.com Waters Corporation, the premium brand in the analytical instruments industry, creates business advantages for laboratory-dependent organizations by delivering practical and sustainable scientific innovation to enable significant advancements in healthcare delivery, environmental management, food safety, and water quality worldwide. Bringing keen understanding and deep experience to those responsible for laboratory infrastructure and performance, Waters helps customers make profound discoveries, optimize laboratory operations, deliver product performance, and ensure regulatory compliance. Pioneering a connected portfolio of separations and analytical science, laboratory informatics, mass spectrometry, as well as thermal analysis, WatersAc?? technology breakthroughs and laboratory solutions provide an enduring platform for customer success. **1117**

Wavefunction, Inc., 18401 Von Karman, Suite 370, Irvine, CA 92612, 949-955-2120, fax: 949-955-2118, e-mail: sales@wavefun.com, Internet: www.wavefun.com Wavefunction offers cutting-edge molecular modeling software for researchers, instructors, and students. Spartan'14 is now available for all chemistry research and teaching needs. Spartan Student Edition applies computational chemistry methods and compelling

graphical models to enrich the study of Organic, Physical, and Inorganic Chemistry. Odyssey provides an interactive molecular environment, rich with content and integrated lab activities for the General Chemistry curriculum. The iSpartan app provides an ideal and inexpensive tool for sketching and exploring at the molecular level. Affordable student pricing, individual faculty and campus-wide site licenses now available. **508**

WebAssign, 1791 Varsity Drive, Suite 200, Raleigh, NC 27606, 919-829-8181, fax: 919-829-1516, e-mail: msantee@webassign.net, Internet: www.webassign.com WebAssign is the only employee-owned and operated online learning chemistry solution to partner with all major textbook publishers, offering content from more than 180 chemistry titles. With easy-to-use tools and customizable pre-coded questions covering every course from preparatory chemistry through physical/analytical chemistry, creating the perfect chemistry course has never been easier. **201**

Weihai CY Dendrimer Technology Co., Ltd., No.369-13, Industrial District, Weihai City, Shandong Province, China 264205, Internet: www.whcyd.com/english/index.asp As the first enterprise in Asia to research, develop & produce dendritic polymers, Weihai CY Dendrimer Technology Co., Ltd has provided many dendritic polymers products to Universities, research centers, etc. for scientific experiments, and now it has already realized the industrialization of dendritic polymers. **243,1319**

WELCH-ILMVAC, 5621 West Howard St., Niles, IL 60714, 847-676-8800, fax: 847-677-8606, Internet: www.welchvacuum.com **300**

Wilmad-LabGlass, 1172 N.W. Boulevard, Vineland, NJ 08360, 856-691-3200, fax: 856-691-6206, e-mail: cs@wilmad-labglass.com, Internet: www.wilmad-labglass.com **431**

Wuxi AppTec (Shanghai) Co., Ltd., 288 Fute Zhong Road, Waigaoqiao Free Trade Zone, Shanghai, China 200131, e-mail: hr@wuxiapptec.com, Internet: www.wuxiapptec.com **933**

Wyatt Technology Corp., 6300 Hollister Avenue, Santa Barbara, CA 93117, 805-681-9009, fax: 805-681-0123, e-mail: info@wyatt.com, Internet: <http://www.wyatt.com> Wyatt Technology is the recognized leader in instrumentation for determining the absolute molar mass, size, charge and interactions of macromolecules and nanoparticles in solution. These tools include: in-line multi-angle static light scattering, high-throughput dynamic light scattering, differential refractometry, electrophoretic mobility, differential viscosity, field flow fractionation and automated composition gradient. **1010**

Xenocs, 19 rue François Blumet, Sassenage, France 38360, +33 (0)4 76 26 98 59, Internet: www.xenocs.com Xenocs provides solutions for nanoscale characterization of materials. Our product portfolio includes innovative high performance instruments that combine Small and Wide Angle X-ray Scattering techniques (SAXS/WAXS) for soft matter, nanomaterials, or polymers characterization. The Xenocs team of experienced scientists and engineers is committed to delivering high quality service to our customers. **941**

Yamazen Science, Inc., 903 Sneath Lane, Suite 125, San Bruno, CA 94066, 650-877-7750, fax: 650-873-6496, e-mail: info@yamazenscience.com, Internet: www.yamazenscience.com **1304**

COMPANIES LISTED BY BROAD CATEGORIES

A more detailed product listing can be found by visiting the Virtual National Exposition at <http://www.acs.org/denver2015>. In addition to Meeting Mail stations in the convention center, product categories, along with companies supplying the products, can be searched using this free service.

Academic & Educational Services

AAPS (Amer Assoc. of Pharm Sci.)	1311
ACS Committee on Chemical Safety	425
ACS Education	624
ACS Green Chemistry Institute	524
Bruker	916,917
CDS Analytical, LLC	302
Cengage Learning, Inc.	1114
Chengdu Aslee Biopharmaceuticals, Inc.	1133
CRC Press	709
De Gruyter	837
Dotmatics Inc.	318
Extrel CMS	717
Frontiers	839
Gaussian	400
Hands-On Learning	304
IIE/Council for International Exchange Of Scholars	902
InfoChem GmbH	809
John Wiley & Sons, Inc.	700
JoVE	207
Kimble Chase LLC	1215
Late Nite Labs, Ltd.	1208
Magritek Inc.	937
Maruzen Co., Ltd.	808
McGraw-Hill Education	1124
MicroLAB, Inc.	317
Nananalysis Corp.	1111
Neaspec GmbH	927
NIST	325
NT-MDT Co.	1000
OpenStax College, Rice University	313
PASCO scientific	219
Pearson	1308
periodictable.co.uk	439
Pine Research Instrumentation	1029
Precision Glassblowing of Colorado	427
Royal Society of Chemistry	701
Sapling Learning	1200
Semichem	404
Serena Software	342
Sigma-Aldrich	1216
Specac, Ltd.	1032
Springer	801
Symphotic Tii	1408
Taylor & Francis (Journals)	713
The Committee for Cannabis Chemistry Division Formation	237
University Science Books	605
University of Illinois - Nano Plasmonics	239
Vernier Software & Technology	901
W.H. Freeman & Company	401
W.W. Norton	607
Waters Corp.	1117
Wavefunction, Inc.	508
WebAssign	201

Accessible Products

AdValue Technology	1325
Anasys Instruments Corp.	540
Chengdu Aslee Biopharmaceuticals, Inc.	1133
Late Nite Labs, Ltd.	1208
Maruzen Co., Ltd.	808
Nananalysis Corp.	1111
NIST	325
NT-MDT Co.	1000
PASCO scientific	219
Pine Research Instrumentation	1029
Symphotic Tii	1408
ViridisChem, Inc.	538

Analytical Research

Advion	1033
AIP Publishing – The Journal of Chemical Physics	831
Anasys Instruments Corp.	540
Biolin Scientific	938
Brookhaven Instruments Corp.	1424
Bruker	916,917
Camag Scientific, Inc.	409
CDS Analytical, LLC	302
Chengdu Aslee Biopharmaceuticals, Inc.	1133
Extrel CMS	717
FEI Company	1400
Gaussian	400
Hidden Analytical Inc.	511
Interchim Inc.	905
John Wiley & Sons, Inc.	700
Knauer	1110
Magritek Inc.	937
Malvern Instruments, Inc.	1107
Maruzen Co., Ltd.	808
Metrohm USA, Inc.	416
MicroLAB, Inc.	317
Nananalysis Corp.	1111
Neaspec GmbH	927
NIST	325
NT-MDT Co.	1000
Parr Instrument Co.	1001
Particle Sizing Systems	1127
Pine Research Instrumentation	1029
PSS USA, Inc.	235
Reaction Analytics Inc.	1134
Rigaku Americas Corp.	1025
Semichem	404
Sigma-Aldrich	1216
Snowy Range Instruments	810
Sorbent Technologies	914
Specac, Ltd.	1032
StellarNet Inc.	1125
STOE & Cie GmbH	939
Symphotic Tii	1408
The Committee for Cannabis Chemistry Division Formation	237
University of Illinois - Nano Plasmonics	239
ViridisChem, Inc.	538
Wavefunction, Inc.	508
Wuxi AppTec (Shanghai) Co., Ltd.	933
Wyatt Technology Corp.	1010

Career Development & Training

AAPS (Amer Assoc. of Pharm Sci.)	1311
Chemistry At Your Fingertips	443
John Wiley & Sons, Inc.	700
Nat'l Res. Council/ Nat'l Academies	504
Royal Society of Chemistry	701
SCIENCE/AAAS	829
The Committee for Cannabis Chemistry Division Formation	237

Chemicals / Reagents / Raw Materials

AK Scientific, Inc.	536
Alfa Aesar-A Johnson Matthey Co.	909
Ark Pharm, Inc.	812
Beantown Chemical Corporation	1131
CDS Analytical, LLC	302
Chemshuttle	1132
Chengdu Aslee Biopharmaceuticals, Inc.	1133
Grace Discovery Sciences	1314
Guizhou Wylton Jinglin Electronic Material Co., Ltd.	929
HE Chemical	1206
Indofine Chemical Co.	1318
Intec, Inc.	326
Interchim Inc.	905
Kimble Chase LLC	1215
Malvern Instruments, Inc.	1107
Matrix Scientific	714
Metrohm USA, Inc.	416

Neaspec GmbH	927
Oakwood Products Inc.	600
Oxchem Corporation	308
Pharmablock USA, Inc.	403
Pine Research Instrumentation	1029
Poly-Med Inc.	904
Pure Chemistry Scientific Inc.	306
Rapp Polymere GMBH	1113
Richman Chemical Inc.	405
Rieke Metals, LLC	336
Rigaku Americas Corp.	1025
Sigma-Aldrich	1216
Sorbent Technologies	914
Strem Chemicals	813
Supra Sciences	437
Synquest Laboratories, Inc.	513
TCI America	1004
Thrupore Technologies LLC	542
Waters Corp.	1117
Weihai CY Dendrimer Technology Co., Ltd.	243,1319
Wuxi AppTec (Shanghai) Co., Ltd.	933

Laboratory Equipment & Services

ACS Committee on Chemical Safety	425
Advion	1033
AGI USA Inc.	1007
Anasazi Instruments Inc.	1027
Anasys Instruments Corp.	540
Biolin Scientific	938
Biotage	1024
Brookhaven Instruments Corp.	1424
Bruker	916,917
Camag Scientific, Inc.	409
CDS Analytical, LLC	302
CEM Corp.	817
Chemglass Life Sciences	514
Chemrus Inc.	334
Edinburgh Instruments	1224
Eicom USA	338
FEI Company	1400
FlackTek, Inc.	1302
Formulation USA	532
FRITTSCH Milling and Sizing	1217
Grace Discovery Sciences	1314
Heidolph North America	1201
Hidden Analytical Inc.	511
Intec, Inc.	326
INTAVIS Bioanalytical Instruments AG	314
Interchim Inc.	905
Japan Analytical Industry Co. Ltd.	241
J-KEM Scientific	424
Kimble Chase LLC	1215
Knauer	1110
KNF Neuberger	225
Krüss America, LLC	331
Late Nite Labs, Ltd.	1208
Magritek Inc.	937
Malvern Instruments, Inc.	1107
Maruzen Co., Ltd.	808
Metrohm USA, Inc.	416
MicroLAB, Inc.	317
Midland Scientific, Inc.	1300
Molymod Models - Spiring Ltd	406
Nananalysis Corp.	1111
NanoMagnetics Instruments	1418
Neaspec GmbH	927
NIST	325
NT-MDT Co.	1000
Parr Instrument Co.	1001
Particle Sizing Systems	1127
PerkinElmer Corp.	1104
Pine Research Instrumentation	1029
Precision Glassblowing of Colorado	427
Proton OnSite	414
PSS USA, Inc.	235
Rigaku Americas Corp.	1025
Rudolph Research Analytical	302
Shimadzu Scientific Instruments Inc.	613
Sigma-Aldrich	1216
SoftA Corporation	1404
Sorbent Technologies	914
Specac, Ltd.	1032
StellarNet Inc.	1125
Supercritical Fluid Technologies	908

EXPOSITION

Teledyne Isco - Chromatography	716
ThalesNano Nanotechnology Inc.	1225
Thermo Scientific	1014,1015
Tosoh Bioscience LLC	501
Vacuum Atmospheres Co.	1100
Vacuum Technology Inc.	311
Vernier Software & Technology	901
Waters Corp.	1117
Wuxi AppTec (Shanghai) Co., Ltd.	933
Wyatt Technology Corp.	1010
Xenocs	941
Yamazen Science, Inc.	1304

Other

AAPS (Amer Assoc. of Pharm Sci.)	1311
ACS Committee on Chemical Safety	425
ACS Meetings & Expositions	624
ACS Member Insurance Program	624
ACS Publications	624
ACS Web Strategy & Operations	624
AIP Publishing - The Journal of Chemical Physics	831
Bentham Sciences Publishers Ltd.	1309
Chemistry At Your Fingertips	443
Elsevier	211
FlacTek, Inc.	1302
Frontiers	839
ICE Publishing	1331f
ISS Incorporated	1406
J-KEM Scientific	424
JEOL USA, Inc.	1101
Metrohm USA, Inc.	416
Nat'l Res. Council/ Nat'l Academies	504
Nature Publishing Group	601
On the Avenue Marketing	215
Paraza Pharma Inc.	1410
periodictable.co.uk	439
Restek Corp.	506
Richman Chemical Inc.	405
Royal Society of Chemistry	701
SCIENCE/AAAS	829
Sigma-Aldrich	1216
Thermo Scientific	1014,1015
US EPA Green Chemistry Program	528

R&D and Manufacturing Services

Ark Pharm, Inc.	812
Beantown Chemical Corporation	1131
Biolin Scientific	938
Boulder Scientific Co.	841
CDS Analytical, LLC	302
Chengdu Aslee Biopharmaceuticals, Inc.	1133
Dotmatics Inc.	318
FlackTek, Inc.	1302
Gaussian	400
Guizhou Wylton Jinglin Electronic Material Co., Ltd.	929
HE Chemical	1206

Indofine Chemical Co.	1318
Interchim Inc.	905
Magritek Inc.	937
NanoMagnetics Instruments	1418
NT-MDT Co.	1000
Oakwood Products Inc.	600
Pharmablock USA, Inc.	403
PharmAgra Labs, Inc.	509
PIKE Technologies	415
Pine Research Instrumentation	1029
Poly-Med Inc.	904
Precision Glassblowing of Colorado	427
PSS USA, Inc.	235
Pure Chemistry Scientific Inc.	306
Reaction Analytics Inc.	1134
Richman Chemical Inc.	405
Rieke Metals, LLC	336
Schrödinger, Inc.	608
Semichem	404
Sigma-Aldrich	1216
SoFTA Corporation	1404
Sorbent Technologies	914
Specac, Ltd.	1032
Supercritical Fluid Technologies	908
Synquest Laboratories, Inc.	513
ThalesNano Nanotechnology Inc.	1225
University of Illinois - Nano Plasmonics	239
ViridisChem, Inc.	538
Wuxi AppTec (Shanghai) Co., Ltd.	933

Scientific Computer & Data Management

Cambridge Crystallographic Data Ctr.	604
CrystalMaker Software Ltd.	233
Dotmatics Inc.	318
InfoChem GmbH	809
J-KEM Scientific	424
NT-MDT Co.	1000
Optibrium Ltd.	1219
PerkinElmer Corp.	1104
Schrödinger, Inc.	608
Semichem	404
Serena Software	342
Thermo Scientific	1014,1015
University of Illinois - Nano Plasmonics	239
Vernier Software & Technology	901
ViridisChem, Inc.	538
Waters Corp.	1117
Wavefunction, Inc.	508

Technical Literature / Websites / Databases

AAPS (Amer Assoc. of Pharm Sci.)	1311
Cambridge Crystallographic Data Ctr.	604
InfoChem GmbH	809
John Wiley & Sons, Inc.	700
Lab Manager/LabX	1331a

NIST	325
NT-MDT Co.	1000
Pine Research Instrumentation	1029
Royal Society of Chemistry	701
Sigma-Aldrich	1216
The Committee for Cannabis Chemistry Division Formation	237
University of Illinois - Nano Plasmonics	239
ViridisChem, Inc.	538
W.H. Freeman & Company	401

Testing & Measurement Instrumentation

Advion	1033
Anasys Instruments Corp.	540
Anton Paar USA	324
Biolin Scientific	938
Brookhaven Instruments Corp.	1424
Bruker	916,917
Camag Scientific, Inc.	409
CDS Analytical, LLC	302
Extrel CMS	717
FEI Company	1400
FRITSCH Milling and Sizing	1217
Gamry Instruments	1009
Hidden Analytical Inc.	511
Instec, Inc.	326
Interchim Inc.	905
J-KEM Scientific	424
JEOL USA, Inc.	1101
Keysight Technologies (formerly Agilent LSCA)	503
Kimble Chase LLC	1215
Knauer	1110
Krüss America, LLC	331
Magritek Inc.	937
Malvern Instruments, Inc.	1107
Metrohm USA, Inc.	416
Midland Scientific, Inc.	1300
NanoMagnetics Instruments	1418
Neaspec GmbH	927
NIST	325
NT-MDT Co.	1000
Parr Instrument Co.	1001
Particle Sizing Systems	1127
Pine Research Instrumentation	1029
Precision Glassblowing of Colorado	427
PSS USA, Inc.	235
Quantachrome Corp.	430
Rigaku Americas Corp.	1025
Rudolph Research Analytical	301
Shimadzu Scientific Instruments Inc.	613
Snowy Range Instruments	810
SoFTA Corporation	1404
Specac, Ltd.	1032
StellarNet Inc.	1125
STOE & Cie GmbH	939
Symphotic Tii	1408
Thermo Scientific	1014,1015
Vernier Software & Technology	901
Waters Corp.	1117
Wyatt Technology Corp.	1010
Xenocs	941

2015 NEW PRODUCT LISTINGS

ACS Member Insurance Program

Booth # 624

Term Life Insurance
International Term Life Insurance
Disability Income
Auto & Homeowners
Professional Liability Income

ACS Publications

Booth # 624

ACS Central Science
ACS Biomaterials Science & Engineering
ACS Infectious Diseases

AGI USA Inc.

Booth # 1007

Thin Film Evaporator
All-in-one Filter Reactor
Short Path Evaporator
Acid Plant
Chemical Engineering Design

Anasys Instruments Corp.

Booth # 540

nanolR2

Anton Paar USA

Booth # 324

Multiwave GO
Monowave EDU

Ark Pharm, Inc.

Booth # 812

2-Amino-4-bromobenzaldehyde, 59278-65-8
5-Fluoro-2-formylpyridine, 31181-88-1
4-Amino-2-methoxybenzotrile, 7251-09-4
7-Chlorothiazolo[5,4-d]pyrimidine, 13316-12-6
4-Iodo-1H-pyrrole-2-carbaldehyde, 33515-62-7

Biolin Scientific

Booth # 938

Q-Sense Omega Auto
Attension Theta
Attension Sigma
KSV NIMA Langmuir and Langmuir-Blodgett
Troughs
Q-Sense E4

Cambridge Crystallographic Data Ctr.

Booth # 604

Cambridge Structural Database System 2015
Release

CDS Analytical, LLC

Booth # 302

CDS 7500 Thermal Desorption Autosampler
CDS 5200 High Pressure Reactor system
CDS 5250T - Trapping Pyrolysis Autosampler
CDS 7400/7000E - Purge & Trap System

Chemistry At Your Fingertips

Booth # 443

Science Does Not Coddle Ideas
Quasicrystals 2011 Nobel Prize
Gorgeous Periodic Table Spanish Stamp Shirt
Sterling Silver Molecular Earrings
Made With Molecules Jewelry

Chemshuttle

Booth # 1132

2,4-dichloronicotinaldehyde
3-amino-2-methoxy-4-pyridinecarboxylic acid
7-bromopyrrolo[2,1-f][1,2,4]triazin-4-amine
2-(tert-butoxycarbonylamino)pyrazolo
[1,5-a]pyrimid
4,6-dichloronicotinaldehyde

Chengdu Aslee Biopharmaceuticals, Inc.

Booth # 1133

Dibromoborane dimethylsulfide complex
organic boronic acids
organic tin
heterocyclic compounds
porphyrins

CrystalMaker Software Ltd.

Booth # 233

CrystalMaker 9
CrystalDiffract 6
SingleCrystal
CrystalViewer

De Gruyter

Booth # 837

books
journals
ebooks
ejournals

Eicom USA

Booth # 338

Smart Evaporator

FEI Company

Booth # 1400

Talos F200X
Titan Themis 300
Titan ETEM
ESEM
Scios/Teneo

Formulation USA

Booth # 532

Micro Rheology Instrument
Film Formation Analyzer

FRITSCH Milling and Sizing

Booth # 1217

Pulverisette 7 premium line Planetary Ball Mill
Analysette 28 Image Analyzer
Pulverisette 1 premium line Jaw Crusher
Pulverisette 14 premium line Rotor Speed Mill

Gamry Instruments

Booth # 1009

Interface 5000 Potentiostat

Gaussian

Booth # 400

Gaussian
GaussView

Hands-On Learning

Booth # 304

LabBridge
Labpaq
STEMpaq

HE Chemical

Booth # 1206

6-Amino-2-fluoronicotinic acid
3-Fluoro-4-(trifluoromethyl)picolinic acid
6-Bromo-2-fluoronicotinic acid
6-Chloro-2-fluoronicotinic acid
3-Bromo-2-mercapto-4-(trifluoromethyl)pyridine

Hide Analytical Inc.

Booth # 511

Compact SIMS
QGA
Catlab
HPR-20

Indofine Chemical Co.

Booth # 1318

Gossypin
Piperlongumine
Ferulic acid
Acetosyringone
Vanillic acid

InfoChem GmbH

Booth # 809

ICsynth
SPRESImobile
Chemisches Zentralblatt
Patent Database
ICcartridge

Instec, Inc.

Booth # 326

Automatic Liquid Crystal Physical Properties
Teste
HCS402 Hot & Cold Microscope Stage

ISS Incorporated

Booth # 1406

Tempo

Japan Analytical Industry Co. Ltd.

Booth # 241

Recycling Preparative HPLC
Portable Curie Point Pyrolyzer
Outgas Collector

J-KEM Scientific

Booth # 424

Automated Reaction Controller and Logger
Precision Vacuum Controller
Precision Temperature Controller
Custom Robotic Systems
Precision Syringe Pumps

JEOL USA, Inc.

Booth # 1101

EDXRF System

Keysight Technologies (formerly Agilent LSCA)

Booth # 503

7500 Atomic Force Microscope
8500B FE-SEM with EDS

Kimble Chase LLC

Booth # 1215

Hydrometer
Raysorb NMR
GL45 Flask

Knauer

Booth # 1110

AZURA Educational System
AZURA Bio LC
AZURA Analytical
Contichrom
Columns

KNF Neuberger

Booth # 225

RC 900 Rotary Evaporator
SIMDOS 10 RC Plus Liquid Dosing Pumps
12V Field Filtration Pump

Nat'l Res. Council/ Nat'l Academies

Booth # 504

Fellowships
Graduate Research
Postdoctoral Research
Senior Research

Neaspec GmbH

Booth # 927

NeasNOM
nano-FTIR

NT-MDT Co.

Booth # 1000

NTEGRA Spectra
Spectrum
Titanium
Next

Oakwood Products Inc.

Booth # 600

(R)-BCNG (1639014-43-9)
(S)-BCNG (1639014-40-6)
N-Nitrosomethylurea
Phosphorous (V) oxybromide solution in Xylene
Tin (IV) Chloride

Parr Instrument Co.

Booth # 1001

6050 Compensated Calorimeter

PASCO scientific

Booth # 219

Spectrometer

PharmAgra Labs, Inc.

Booth # 509

FIGLU

PIKE Technologies

Booth # 415

UV/VIS Peltier Cuvette Accessories
Temperature Controlled Microscope Stage
IR Short Path Gas Cells

PSS USA, Inc.

Booth # 235

Pullulan ReadyCal Kit
HT GPC ReadyCal Kit
Micro-RI detector
Micro-Viscometer
WinGPC 8.2

EXPOSITION

Pure Chemistry Scientific Inc.
Booth # 306
Stannanes
Vitamin D
Boronic Acids/Esters
PEG items
Intermediate

Quantachrome Corp.
Booth # 430
Autosorb iQ Series
New Nova Touch Series
Porometer 3G Series
Quadrasord
Pycnometers

Restek Corp.
Booth # 506
ARC-18
RXI
SKY Liners
Raptor
QuEChERS

Richman Chemical Inc.
Booth # 405
Trimethylene Carbonate

Rieke Metals, LLC
Booth # 336
2-Propylzinc bromide
Cyclobutylzinc bromide
2-Pyridylmagnesium bromide
4-Bromobenzylmagnesium bromide
Poly(3-hexylthiophene-2,5-diyl), regioregular

Schrödinger, Inc.
Booth # 608
Materials Science Suite

SCIENCE/AAAS
Booth # 829
Science
Science Signaling
Science Translational Medicine

Semichem
Booth # 404
Semichem
AMPAC
Codessa

Sigma-Aldrich
Booth # 1216
Phenofluor
TFCS-Na
ESF
COGenerator
Stahl Aerobic Oxidation Kit

SofTA Corporation
Booth # 1404
ELSD Model 2300
ELSD Model 1300
ELSD Model 300S
Evaporative Light Scattering Detector

Sorbent Technologies
Booth # 914
SorbaDex
SorbaRes

StellarNet Inc.
Booth # 1125
Portable and Laboratory Raman Systems
Teaching Lab UV-VIS Specials
NIR Chemical Analyzers

Strem Chemicals
Booth # 813
Buchwald Precatalysts and Ligands
CVD and ALD Precursors
Electropolished Stainless steel CVD bubblers
and A
Metal Nanoparticles
Phosphine Ligands and Metathesis Catalysts

Struchem Co., LTD
Booth # 931
D-Bicuculline
methyl 4-amino-3-methoxy-5-nitrobenzoate
4-AMINO-2-HYDROXYBENZENESULFO
NAMIDE
2-PROPYL-5-THIAZOLECARBOXYLIC ACID
1-(4-(trifluoromethyl)phenyl)propan-2-one

Symphotic Tii
Booth # 1408
CMS 8400

Synquest Laboratories, Inc.
Booth # 513
Triflic acid
Triflic anhydride
Difluoroacetaldehyde ethyl hemiacetal
Hexafluoroisopropanol
1H,1H,5H-Octafluoropentyl methacrylate

Thermo Scientific
Booth # 1014,1015
Vanquish

Tosoh Bioscience LLC
Booth # 501
CaPure-HA(TM) hydroxyapatite resin

University of Illinois - Nano Plasmonics
Booth # 239
Computational Plasmonics
Arbitrary Geometry
Large Scale Computing
Online Simulation
University of Illinois Funded by NSF

University Science Books
Booth # 605
X-Ray Crystallography
Physical Chemistry for the Chemical Sciences
Principles of NMR

Vacuum Technology Inc.
Booth # 311
Glove Box
Gas Purification System
Freezer
Cold Well

ViridisChem, Inc.
Booth # 538
Green Pocketbook
Green Analyzer
GreenSynth
Integrated Planner
ChiroSolve

Wavefunction, Inc.
Booth # 508
Spartan'14 Parallel Suite
Spartan'14
Spartan Student Version 6
Odyssey Version 5
iSpartan

Weihai CY Dendrimer Technology Co.,Ltd.
Booth # 243,1319
Dendritic polymers
PAMAM
Dendrimer
CYD-150A
CYD-160A

Wyatt Technology Corp.
Booth # 1010
DynaPro Plate Reader
DAWN
Mobius
Eclipse
NanoStar

Xenocs
Booth # 941
Xeuss 2.0
Nano-inXider

Yamazen Science, Inc.
Booth # 1304
ELSD
WPrep Dual Channel MPLC
AKROS MPLC
TLC Reader
Premium Columns

249th American Chemical Society National Exposition

Also Featuring the Career Fair Recruiters Row

March 22-24, 2015

Colorado Convention Center - Exhibit Halls A&F
Denver, CO

Entrance to
Career Fair

Entrance to
Posters

CONCESSIONS

142 143 242
140 141 240
138 139 238
136 137 236

243 342
241 340
239 338
237 336

443 542
441 540
439 538
437 536

D&M Exhibits
Recruiters
339

ACS Booth
Society - Tuesday

841 940
839 938
837

1041 1140
1039 1138
1037 1136

1241 1340
1239 1338
1237 1336

1331H 1331h
1331d 1331m
1331e 1331k
1331f 1331g

1131 1232
1131 1230
1129 1228
1127 1226
1125 1224

1327 1426
1325 1424

132 133 232
130 131 230
128 129 228
126 127 226
124 125 224

333 432
331 430
429 528
427 526
425 524

624

932
931 1030
929 1028
927 926
925 1024

1133 1232
1131 1230
1129 1228
1127 1226
1125 1224

1323 1332
1231 1330
1229 1328
1227 1326
1225 1324

1219 1318
1217 1316
1215 1314

1319 1418
1317 1416
1315 1414

1311 1410
1309 1408
1307 1406
1305 1404
1302
1301 1300

1117 1216
1113
1111
1208
1107 1206
1101 1200

1015 1114
1011 1110
1009
1007 1106
1104
1001 1100

915 1014
910 1008
905 1004
901 1000

817 916
814
813
809 908
806
805 904
802
801 900

717
713 812
810
709 808
701

613
612
611
509 608
604
603
601 600

419
417
415 514
411
409 508
407 506
405 504
403
401 500

317 416
315 414
313
311
307 406
305 404
303
301 400

219 318
217 316
215 314
211
207 306
205 304
203 302
201 300

114
1114

100

EXHIBITOR SERVICE CENTER

122

TOWN CENTER

- Lounge
- Breaks
- Poster Sessions
- Meeting Mall
- Networking

1401

MAIN ENTRANCE

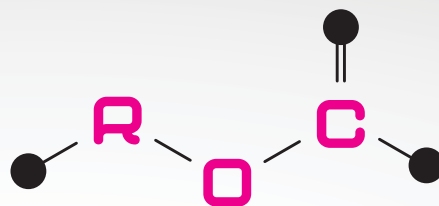
Presidential Candidates
(Monday 3/23, 1:30pm)

Exhibitor
Workshop
#2

Exhibitor
Workshop
#1



Amy (Vocals)



ACS Members are ROCKSTARS OF CHEMISTRY

ACS members who joined in the last 12 months are invited to attend our ROCKSTARS RECEPTION.

ACS looks forward to welcoming you to this very special event, Monday, March 23, from 3:00 p.m. to 4:00 p.m. in the Colorado Convention Center Room 601. New members will network with other Rockstars of Chemistry, such as award winners, published authors, and notable scientists. Light refreshments will be served. Guests will receive reserved seating for the Kavli Lecture Series.

Not a member yet?

Join today for your ticket to the Rockstars Reception. Go to www.acs.org/ROCKSTAR

Been a member for years?

Stop by the ACS Booth and take a commemorative ACS Rockstars photo at the open air photo booth!

Learn about your benefits at the *Membership Rocks* presentation in the ACS Theater on Monday at 10:30 a.m. and 11 a.m. or Tuesday at 11 a.m. and 11:30 a.m.

American Chemical Society

Photo: Peter Cuttis Photography



Diane Grob Schmidt, Ph.D.
ACS President

Saturday, March 21, 2015

10:00 AM-2:00 PM
**Presidential Outreach Event:
Exploring Our World Through
Chemistry**
(Cosponsored by CCA)
Denver Zoo, 2300 Steele Street

Sunday, March 22, 2015

8:00 AM-12:00 PM
**Chemistry Without Borders: The
Transnational Practice of Chemistry
and Allied Sciences and Engineering**
(Cosponsored by IAC, COMSCI, BMGT & SOCED)
Colorado Convention Center,
Mile High Ballroom 3A (Lower Level)

PRESIDENTIAL SYMPOSIA AND EVENTS

Sponsored and Recommended by the ACS President

Sunday, March 22, 2015

1:30-5:30 PM
Monday, March 23, 2015

8:30 AM-4:45 PM
**Nanotechnology: Delivering on
the Promise**

(Cosponsored by the following ACS Divisions and Committees and other scientific societies AGFD, AGRO, ANYL, CARB, CHAS, COLL, ENFL, HIST, I&EC, PMSE, POLY, SCHB, MPPG, CA, CCS, CCPA, COMSCI, DAC, IAC, SOCED; American Institute of Chemical Engineers, Gordon Research Conferences, Materials Research Society & National Academy of Engineering)
Colorado Convention Center,
Mile High Ballroom 3A (Lower Level)

Tuesday, March 24, 2015

8:30-11:30 AM
**DOE Nanoscience Research
Centers: National Resources for the
Nanoscience Community**
(Cosponsored ANYL, ENFL, CCPA, CEI & MPPG)
Colorado Convention Center,
Rooms 506-507 (Street Level)

**OTHER SYMPOSIA
RECOMMENDED BY
THE PRESIDENT**

**Excellence in Graduate Polymer
Research**

(Sponsored by POLY and cosponsored by PRES)

Sheraton Denver Downtown Hotel

**GSSPC: Designed by Nature,
Developed by Science: Inter-
disciplinary Perspectives on
Biocatalysis**

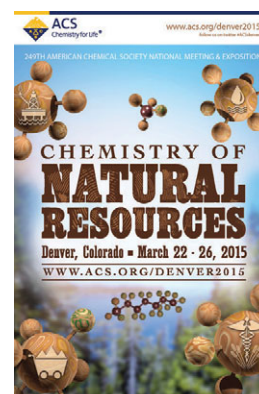
(Sponsored by CHED and cosponsored by PRES, ANYL, BIOL, CATL, ENVR, I&EC, MEDI, & ORGN)

Sheraton Denver Downtown Hotel

**Department, University and National
Models for Faculty Development to
Support Adoption of Evidence-Based
Teaching**

(Sponsored by CHED and cosponsored by PRES, INOR & ORGN)

Sheraton Denver Downtown Hotel



**The Interface of Chemical and
Biological Sciences International
Disarmament Efforts**

(Sponsored by IAC and cosponsored by PRES, ANYL, CHAL & CPRC)

*Hyatt Regency Denver at Colorado
Convention Center*

**Transitioning between Academic
Research into Practical Use: Solar-
Energy and Advanced Materials?**

(Sponsored by COMSCI and cosponsored by PRES & MPPG)

Colorado Convention Center

Chemical Abstracts Service (CAS), ACS Publications, and so much more from the American Chemical Society are in one convenient location —

The ACS Booth in the Colorado Convention Center in Denver.



The ACS Booth is your opportunity to experience the world's largest scientific society all on one carpet!

- Experience SciFinder from CAS, the world's authority for chemical information
- Learn about the newest ACS Journals from ACS Publications, including Editors' Choice
- Discuss how to achieve your career goals with ACS Career Navigator™
- Come to the Membership Benefits kiosk to receive a gift in thanks for your ACS membership
- Enter contests and receive giveaways, including tablets, gift cards, photos and more!

Whether looking for educational resources, powerful research tools, ACS Member Insurance, C&EN, future meeting dates and locations, mole dolls or other ACS merchandise, WE HAVE IT ALL FOR YOU. There is something for every member of the chemistry community at the ACS booth.

Exhibit Hours:

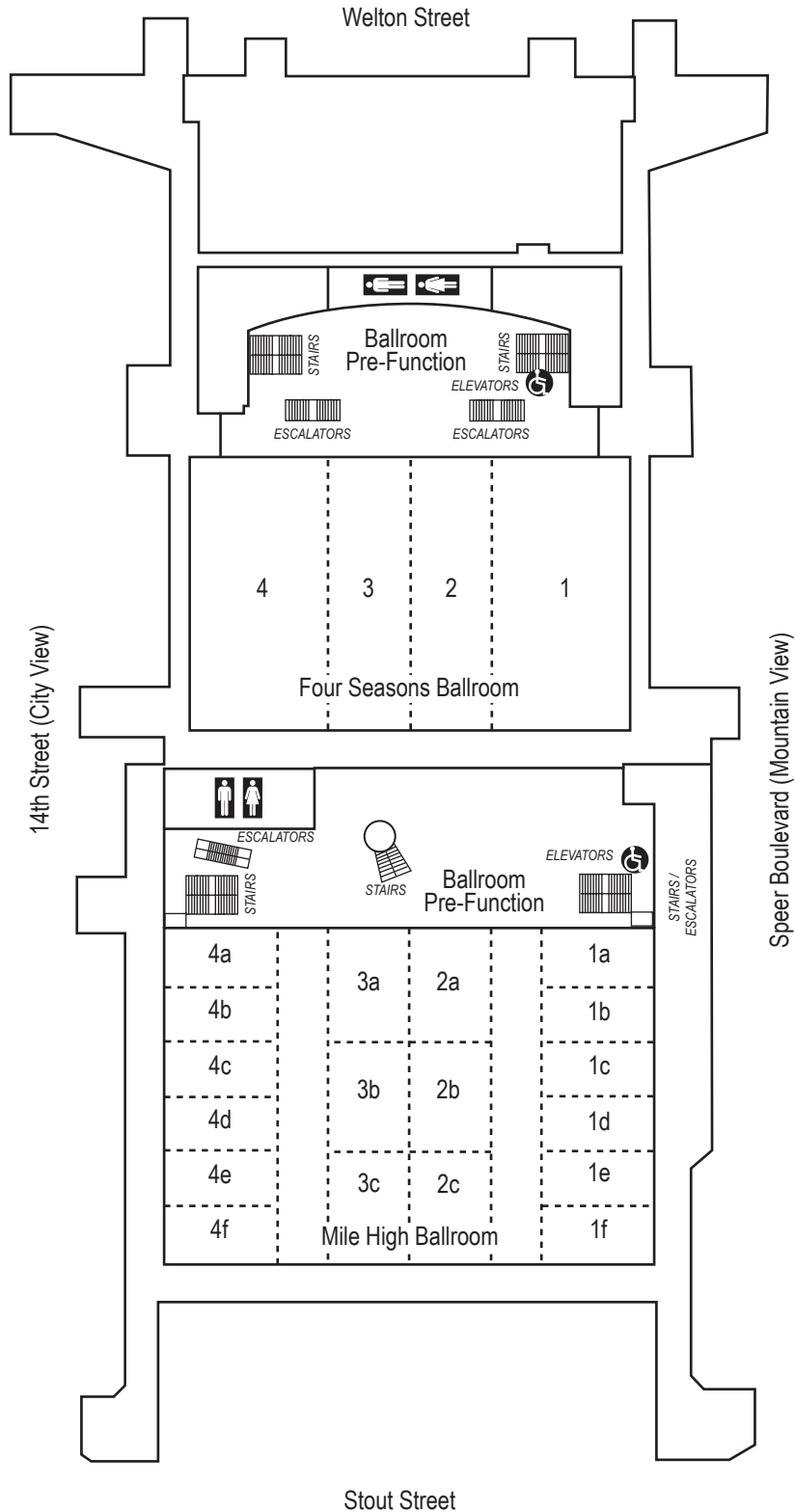
Sunday, March 22
6:00pm - 8:30pm

Monday, March 23
9:00am – 5:00 pm

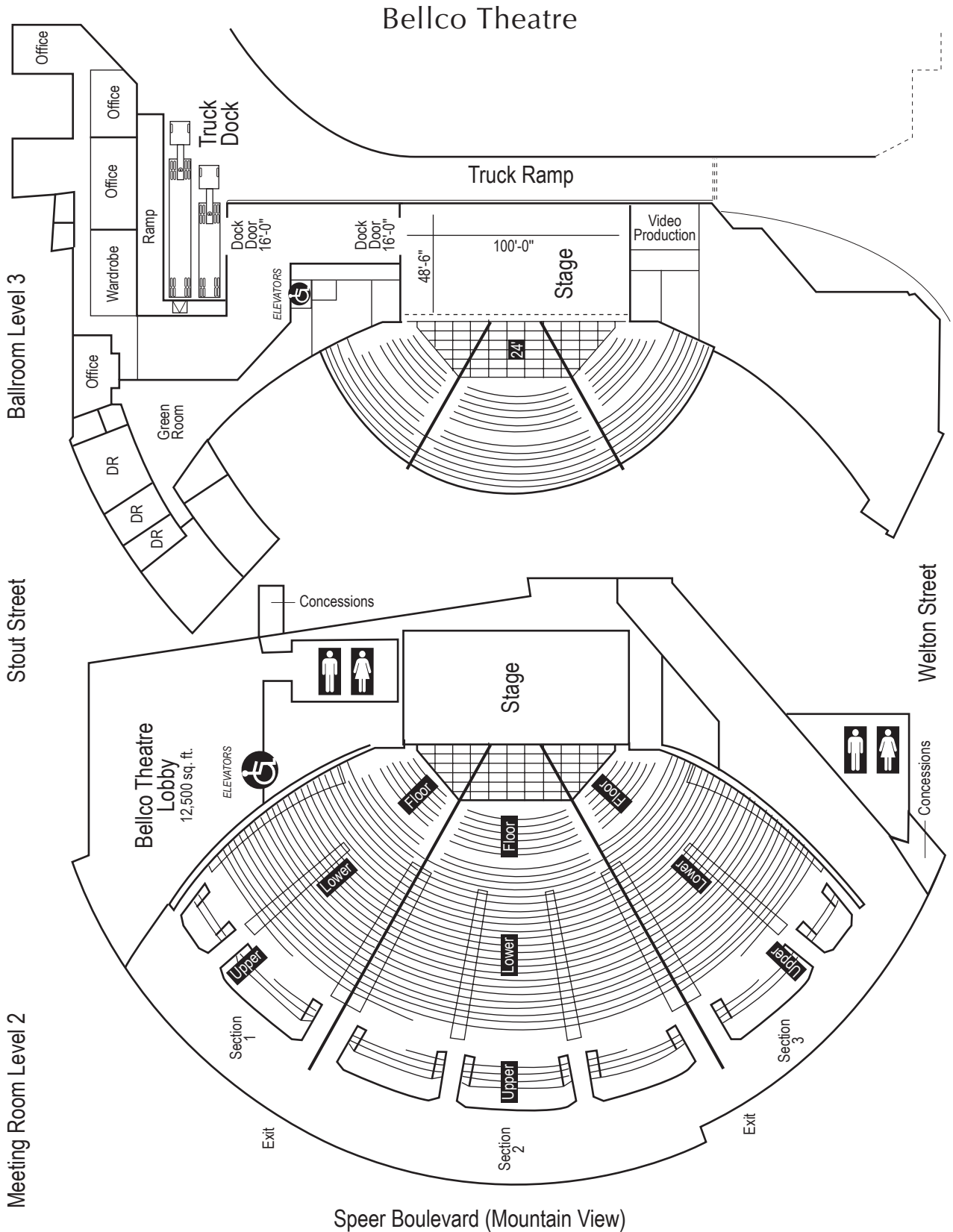
Tuesday, March 24
9:00am – 5:00pm

COLORADO CONVENTION CENTER

Ballroom Level



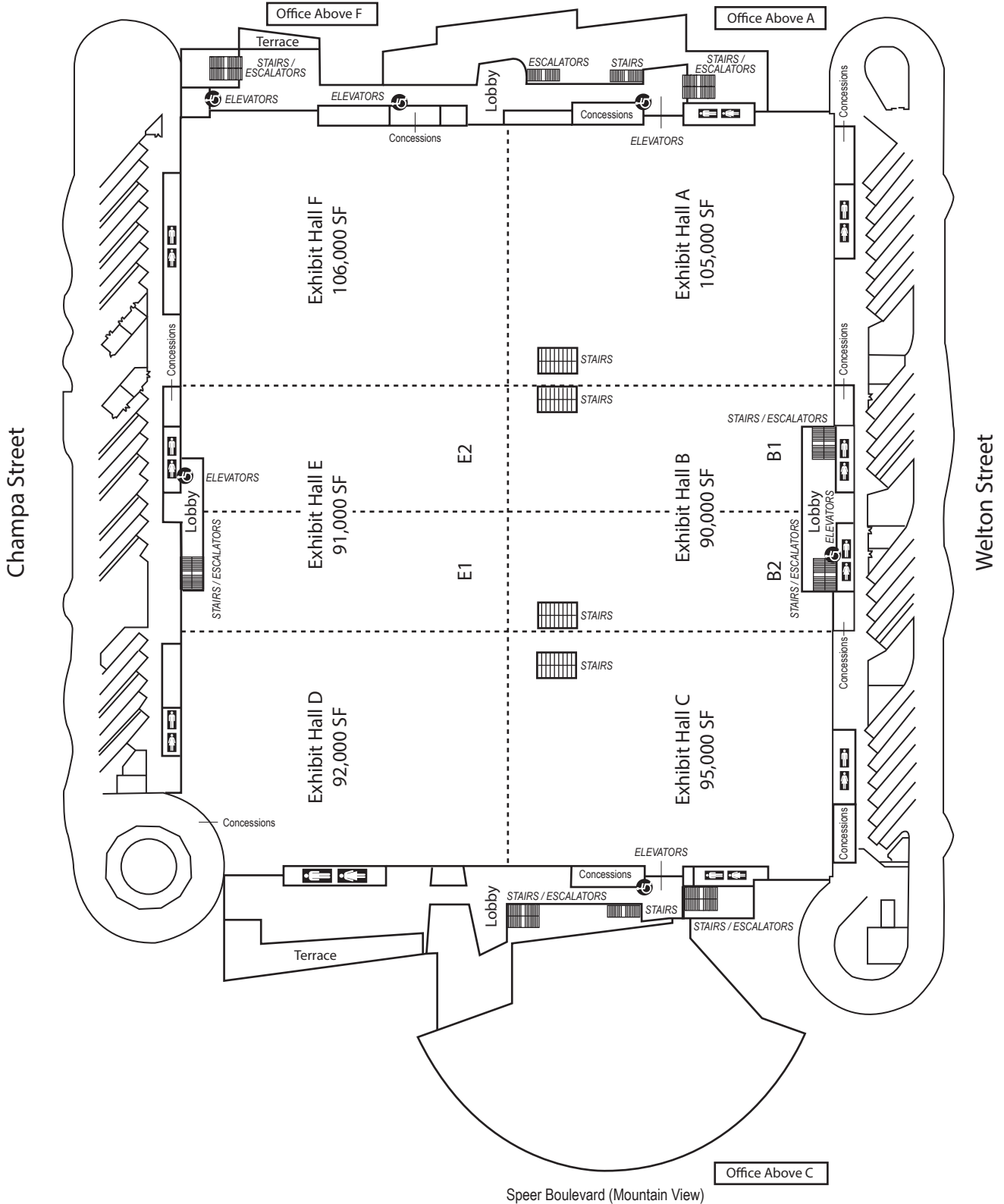
COLORADO CONVENTION CENTER



COLORADO CONVENTION CENTER

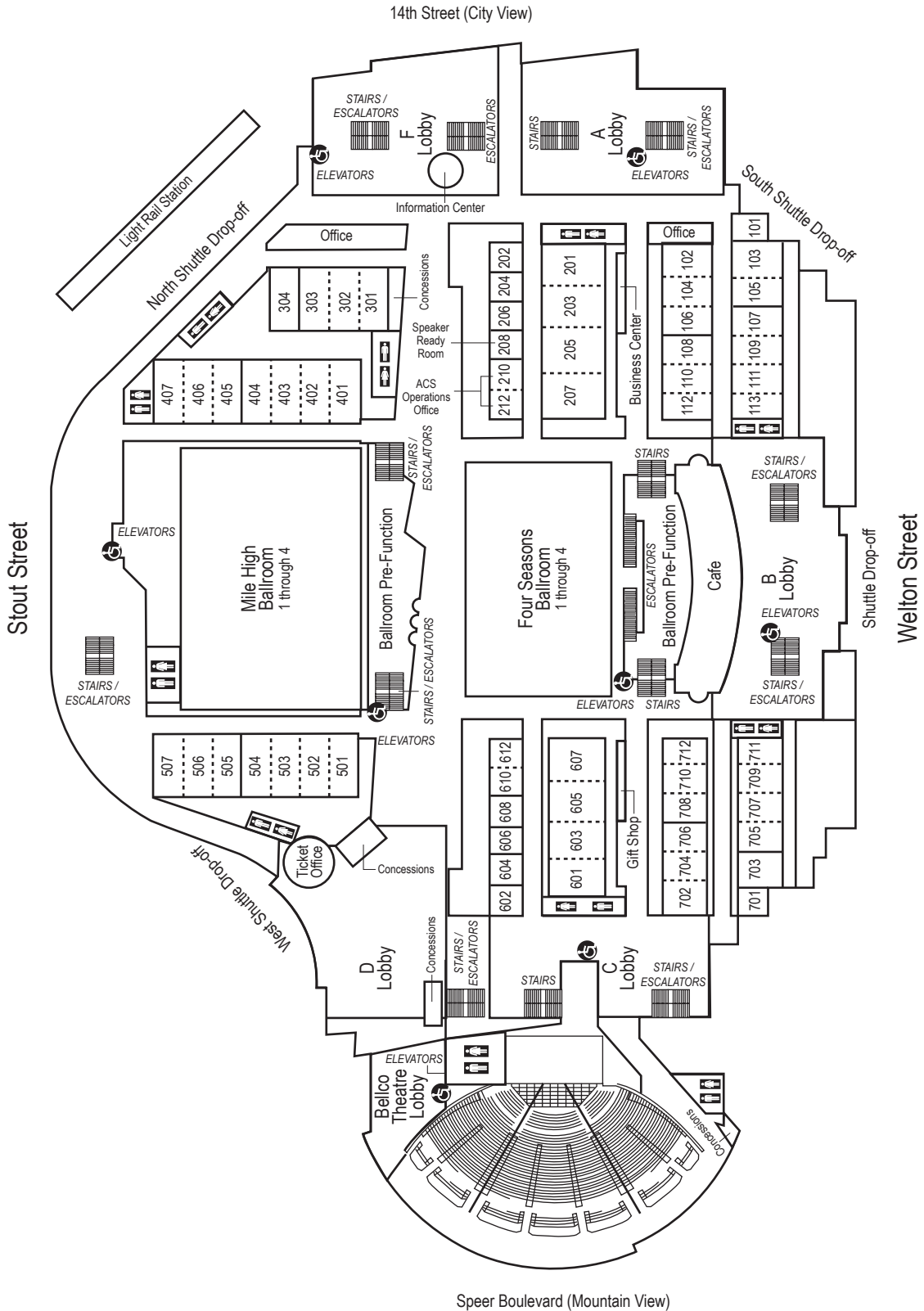
Exhibit Level

14th Street (City View)



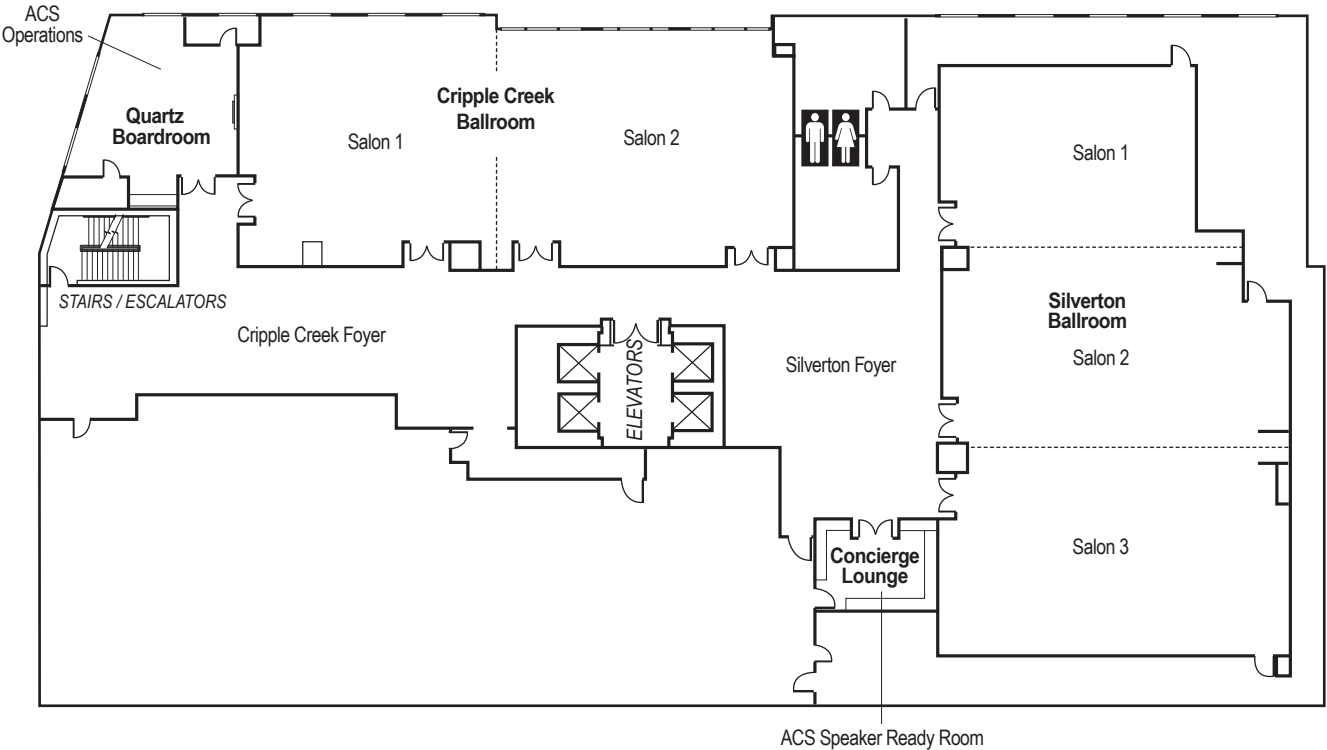
COLORADO CONVENTION CENTER

Meeting Room Level

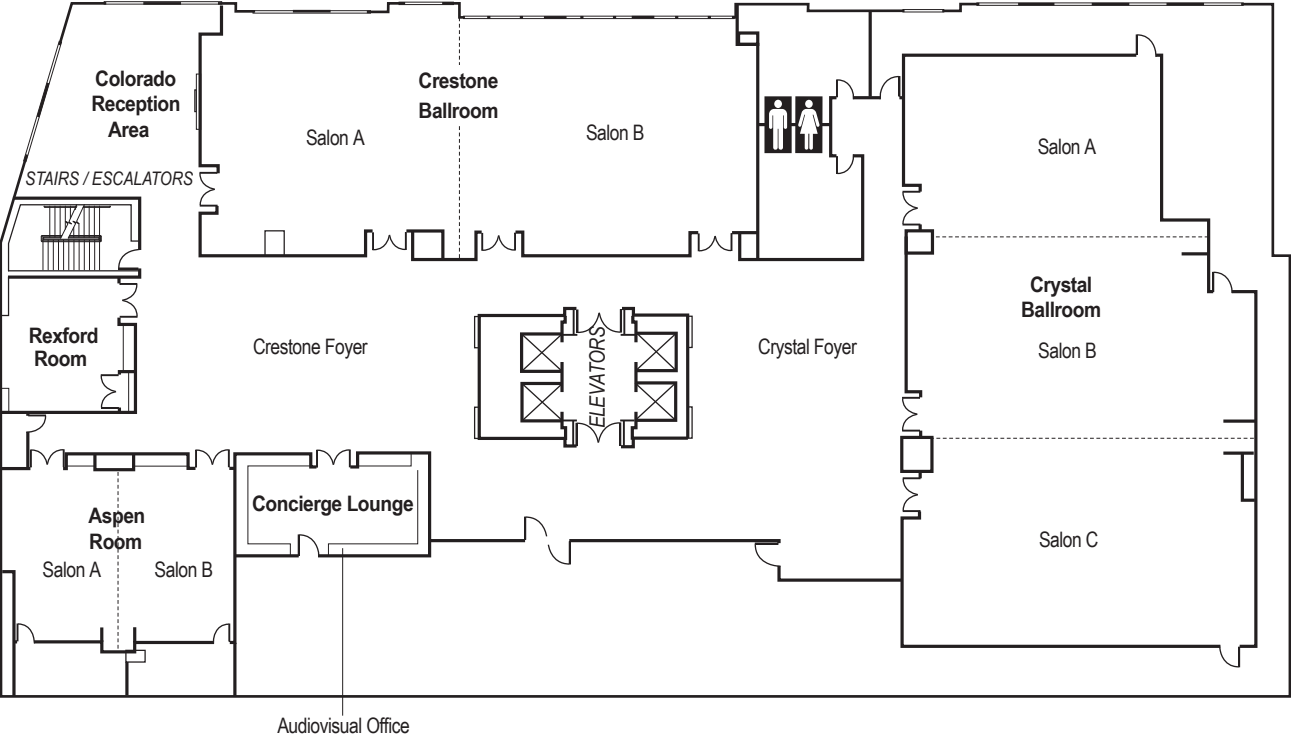


EMBASSY SUITES DENVER DOWNTOWN CONVENTION CENTER

Second Floor



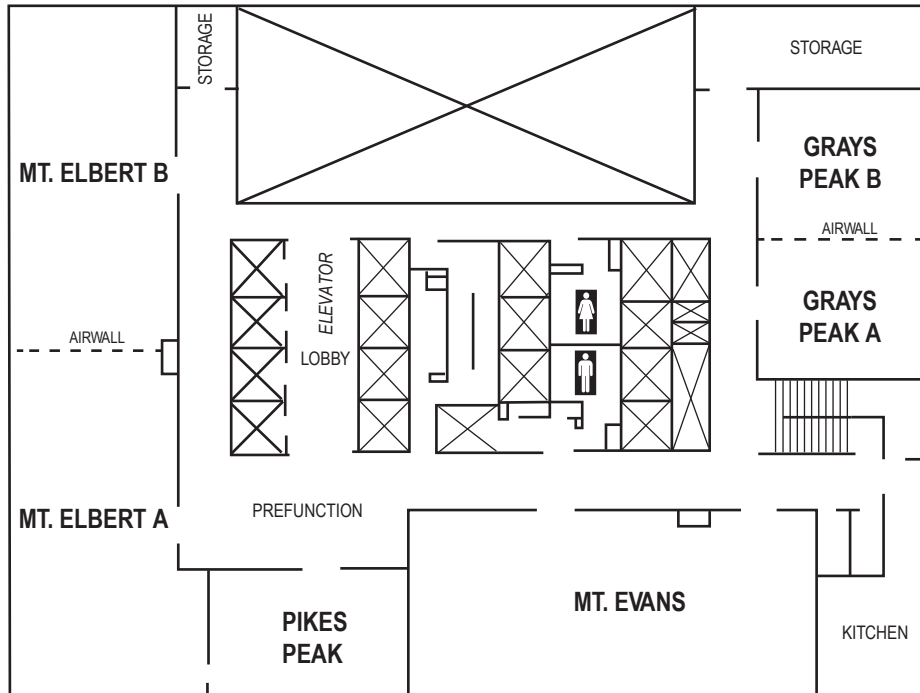
Third Floor



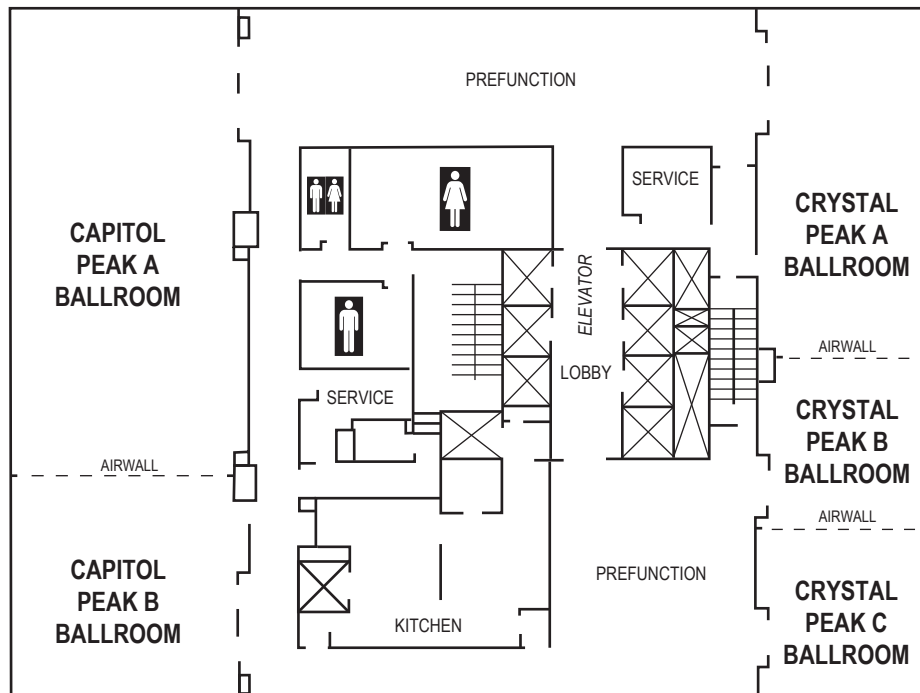
GRAND HYATT CONFERENCE CENTER

Atrium Tower

Second Floor

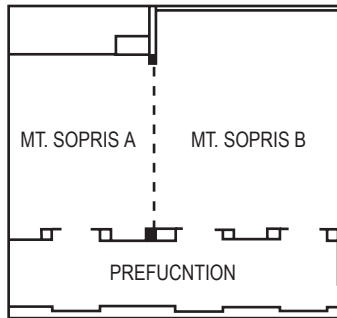


Pinnacle Club—38th Floor

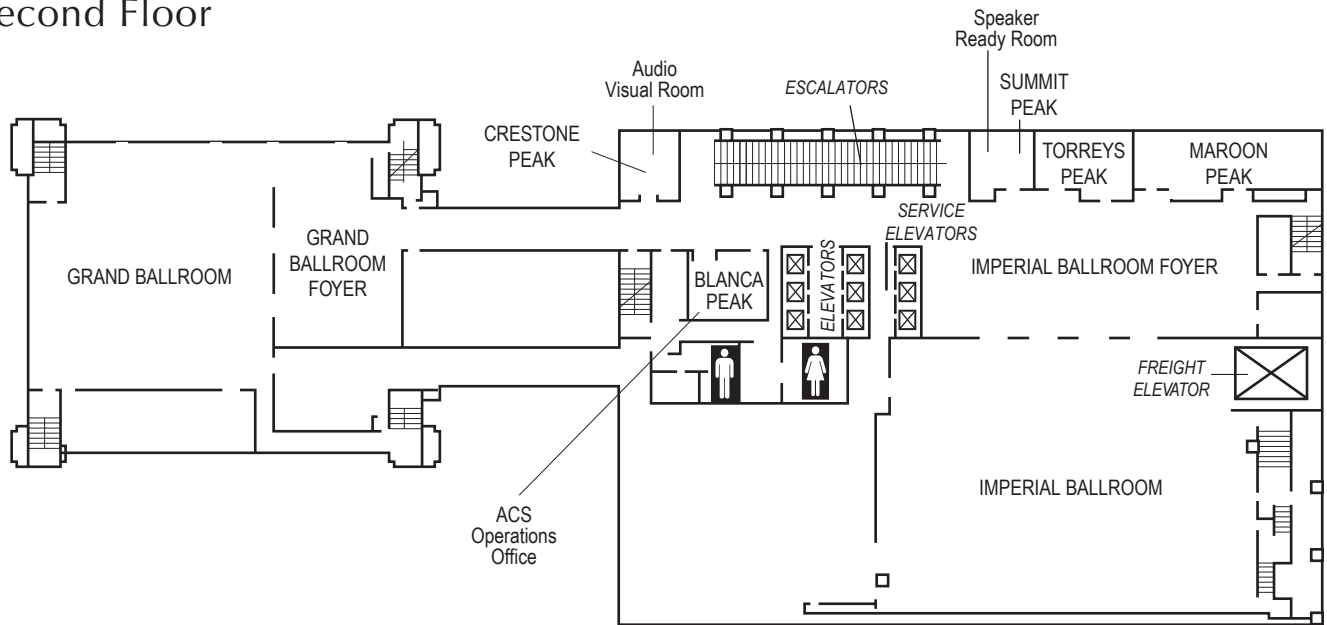


GRAND HYATT DENVER

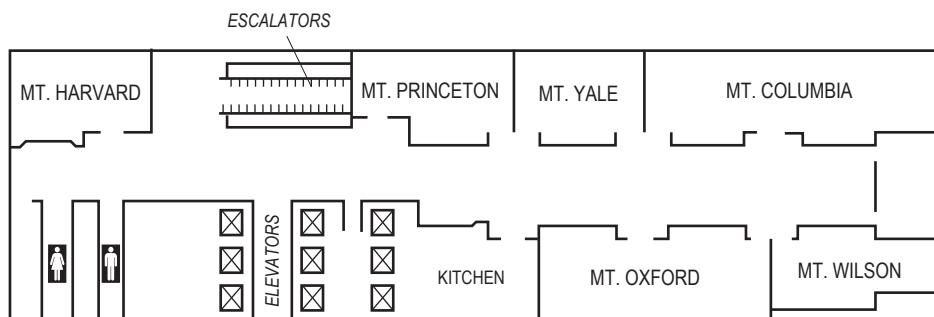
Lobby Level



Second Floor

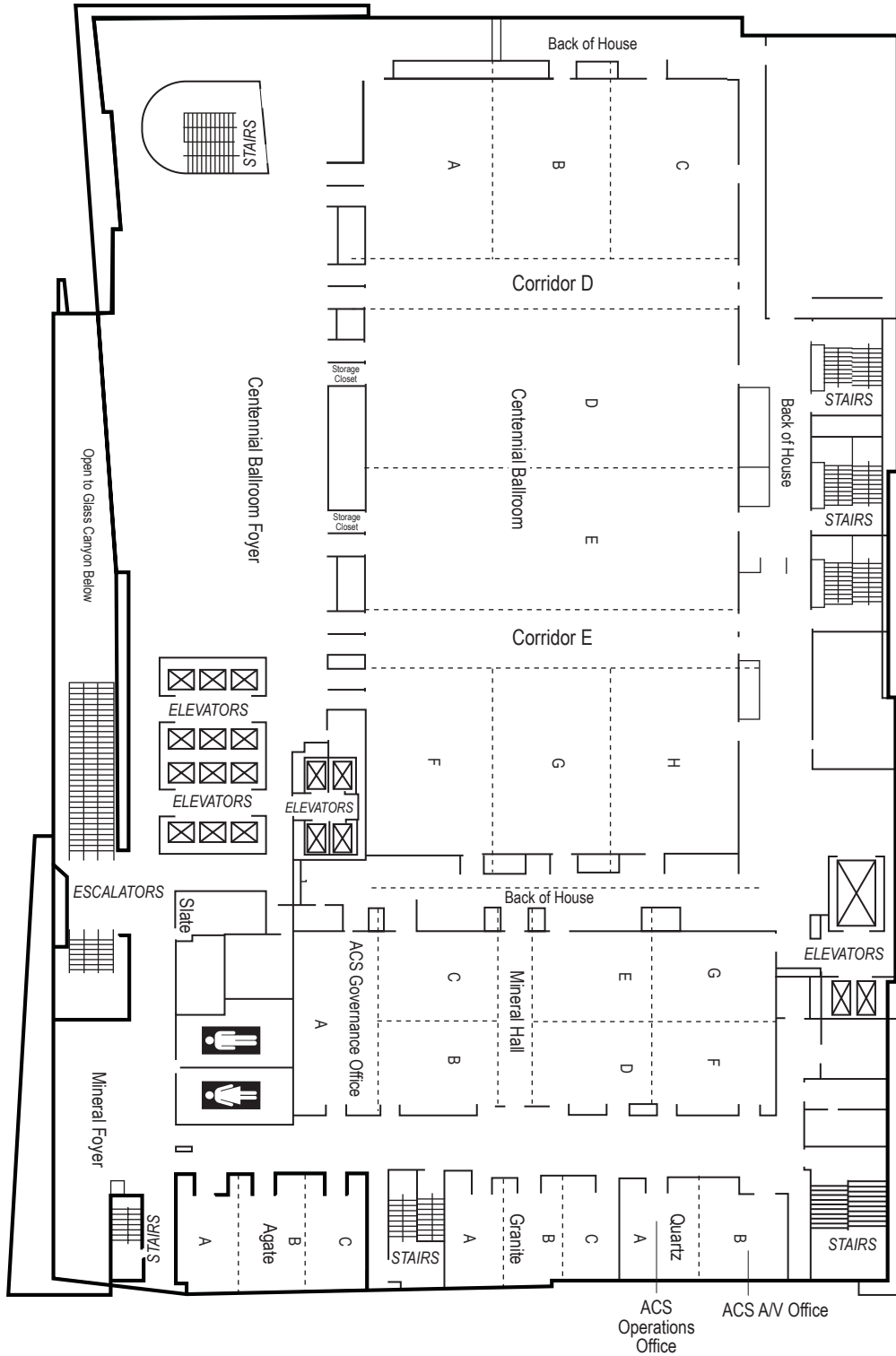


Third Floor



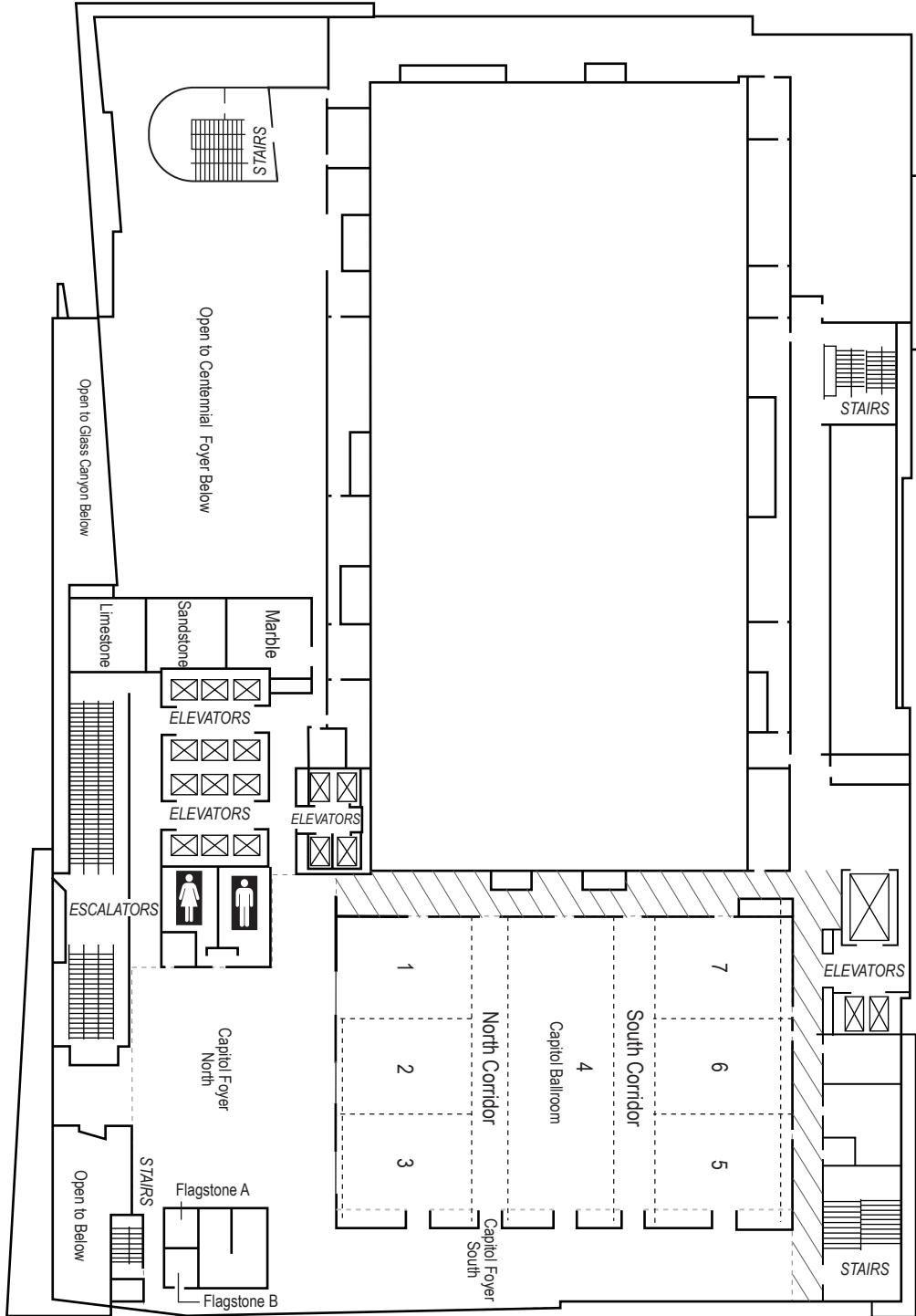
HYATT

Level Three



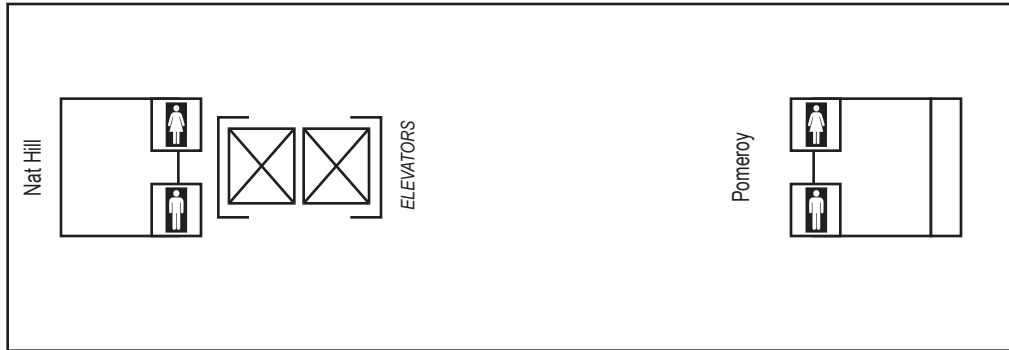
HYATT

Level Four

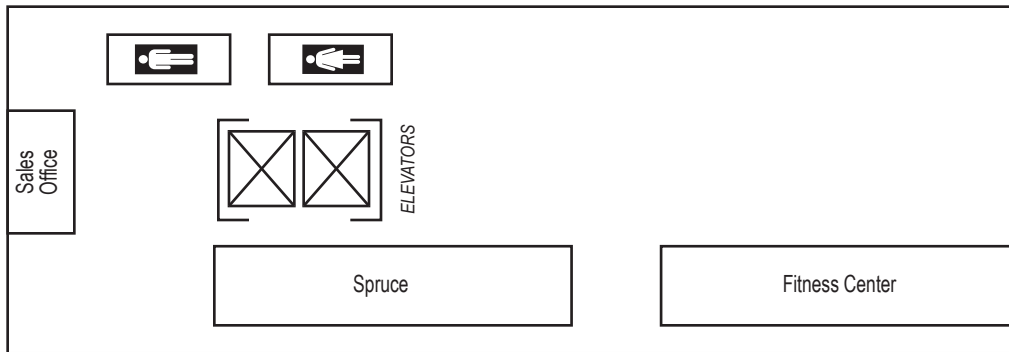


MARRIOTT CITY CENTER

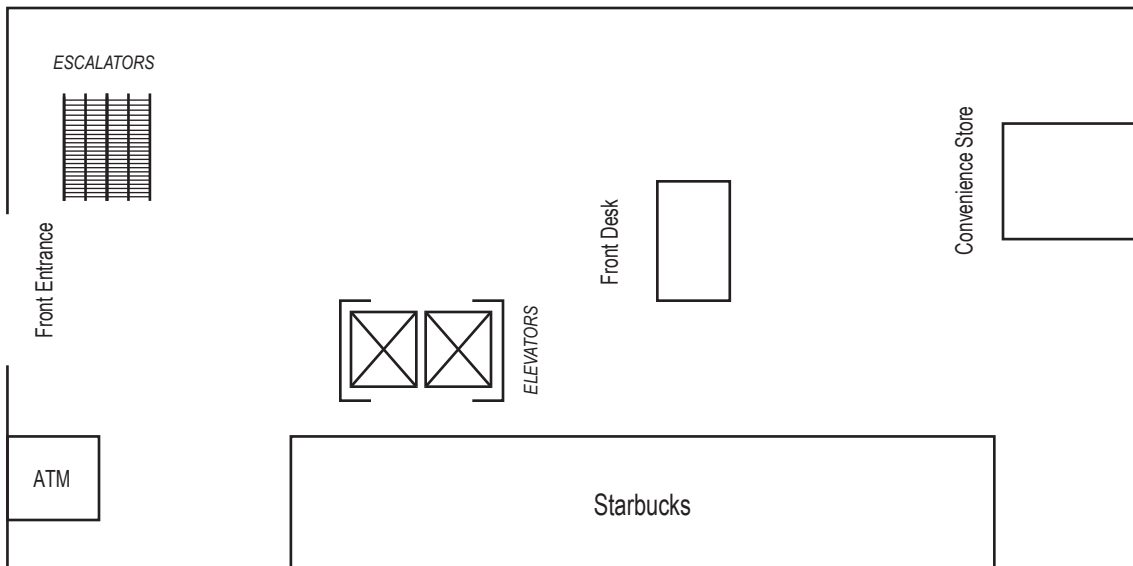
3rd Floor



2nd Floor

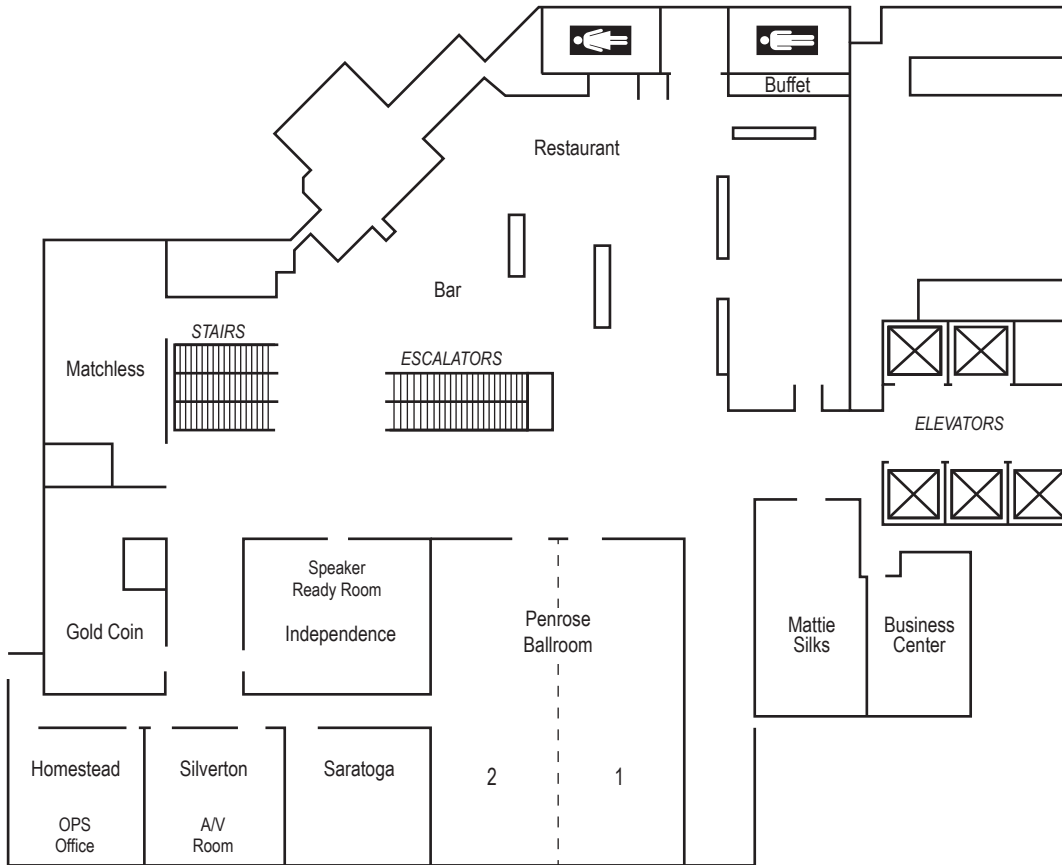


Lobby Level

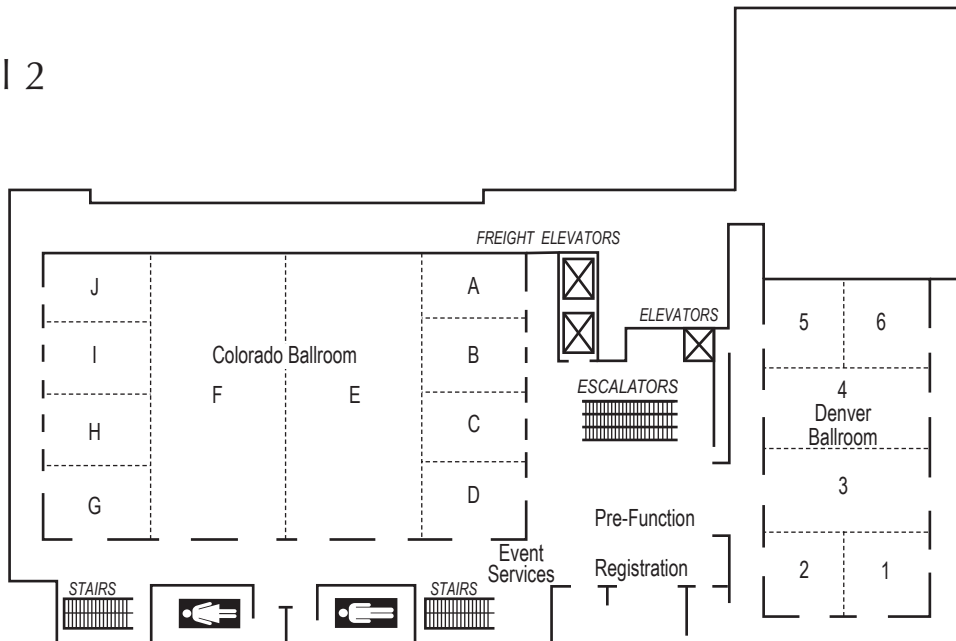


MARRIOTT CITY CENTER

Lower Level 1

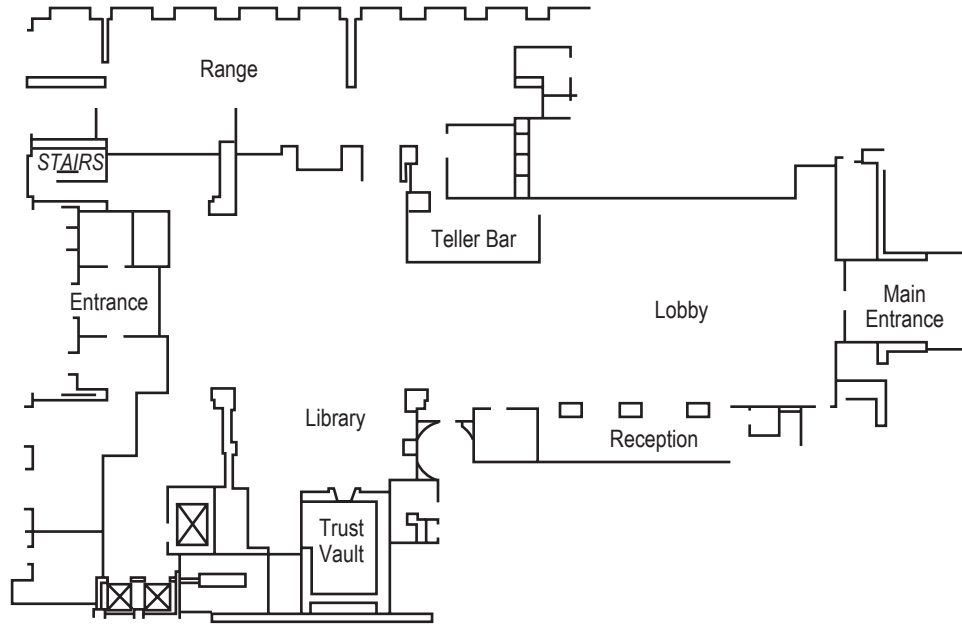


Lower Level 2

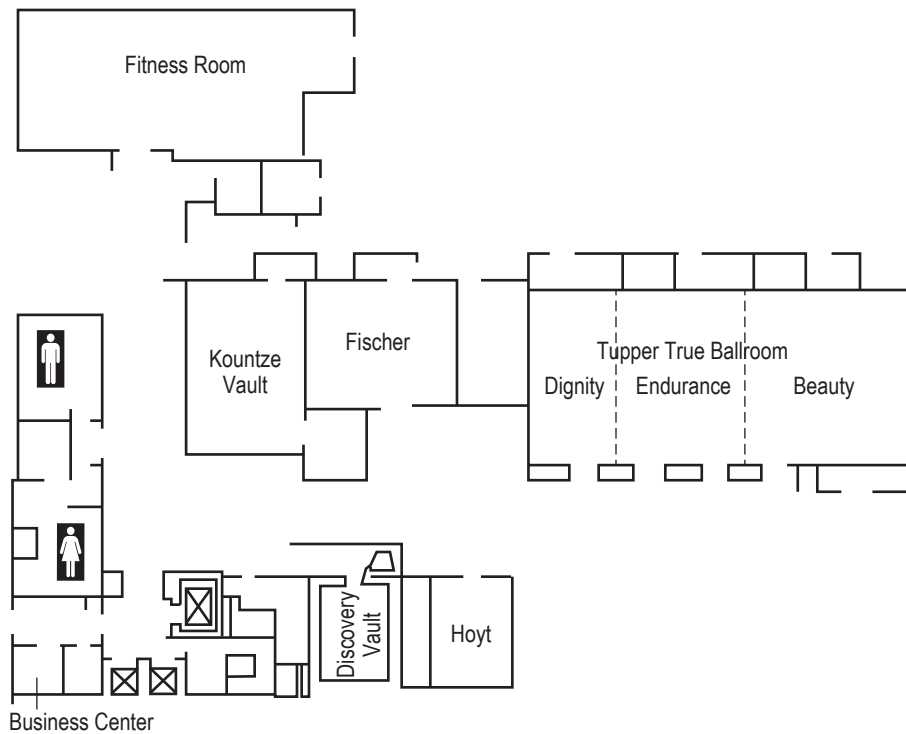


RENAISSANCE DENVER DOWNTOWN

Lobby Level

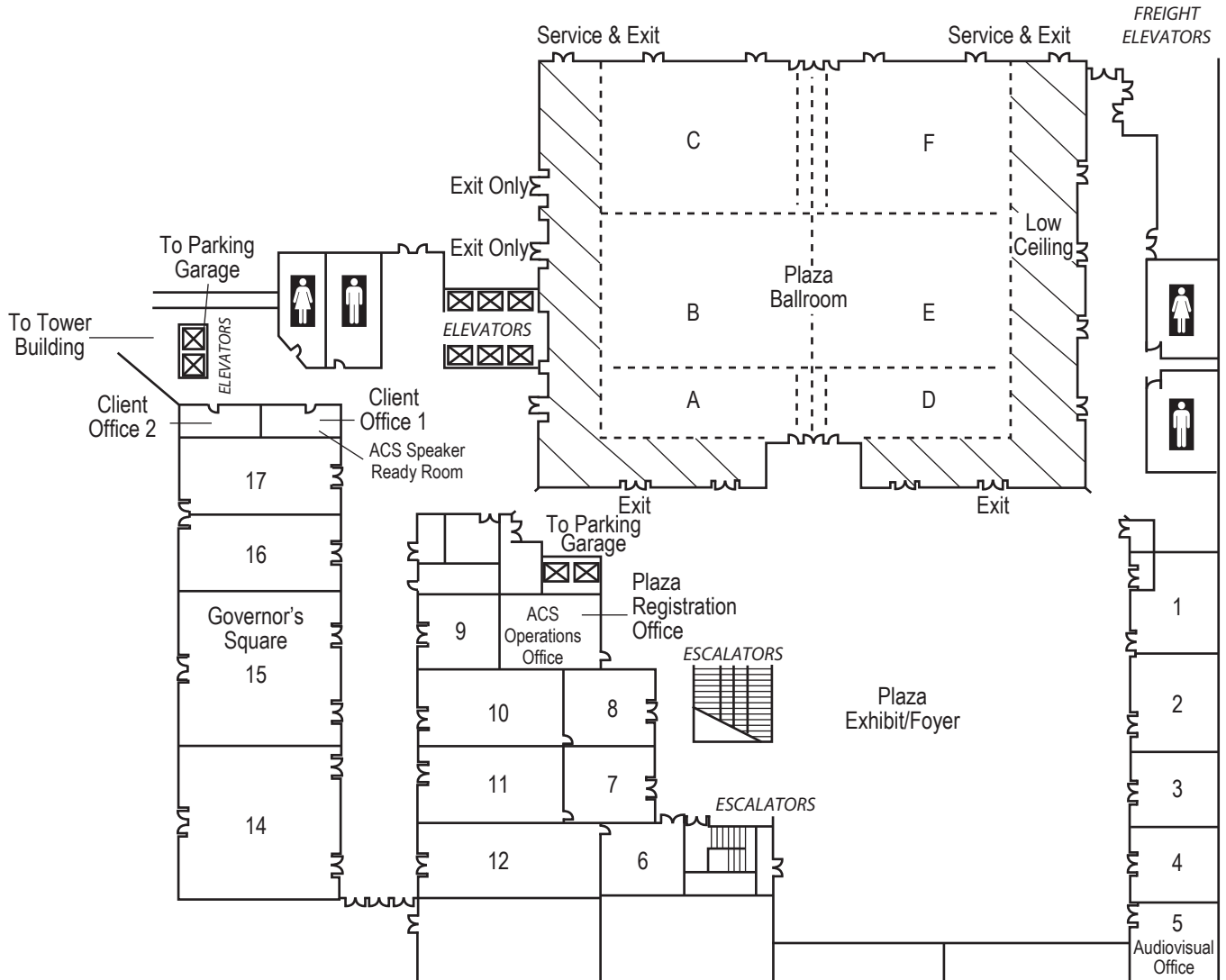


Lower Level



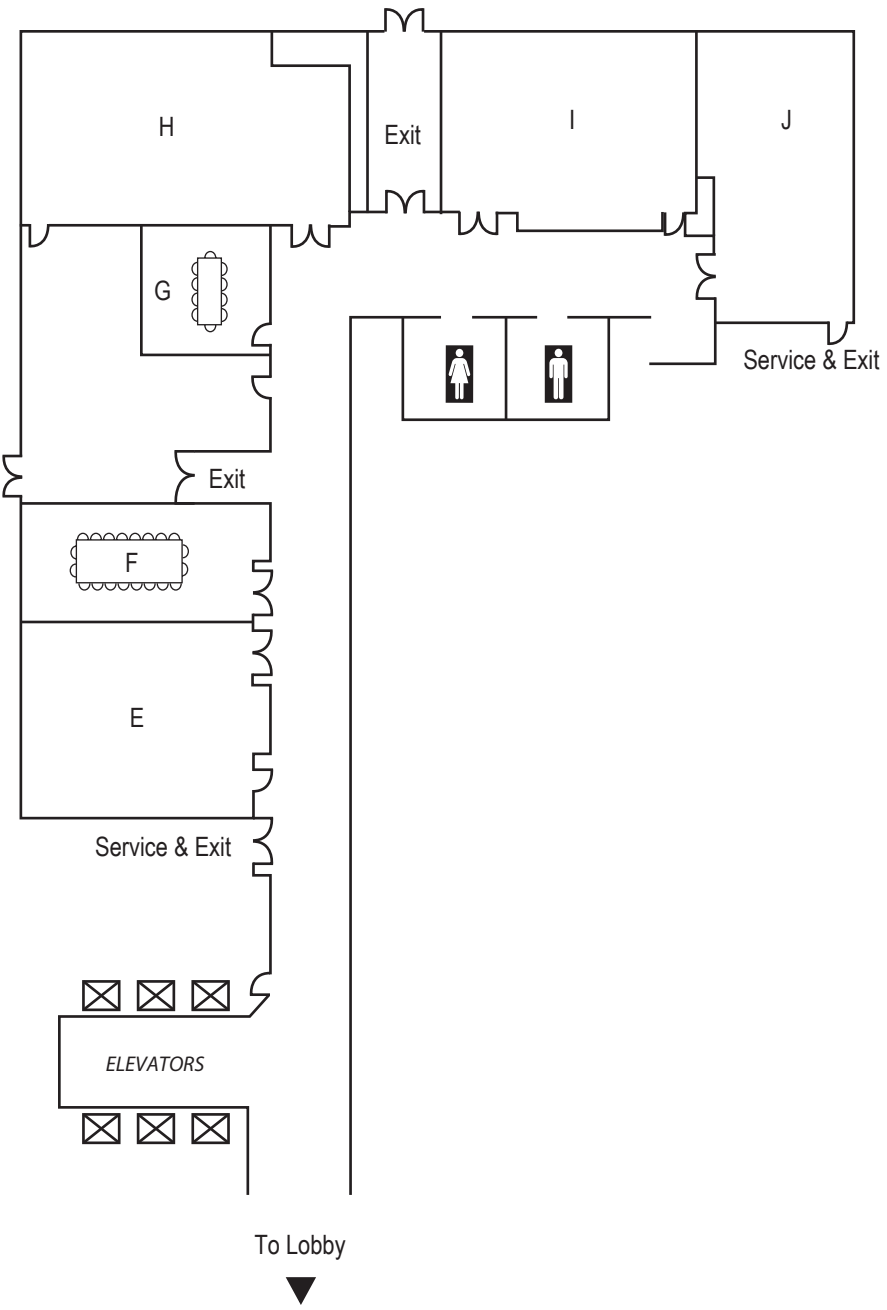
SHERATON DENVER DOWNTOWN

Plaza Building Concourse Level



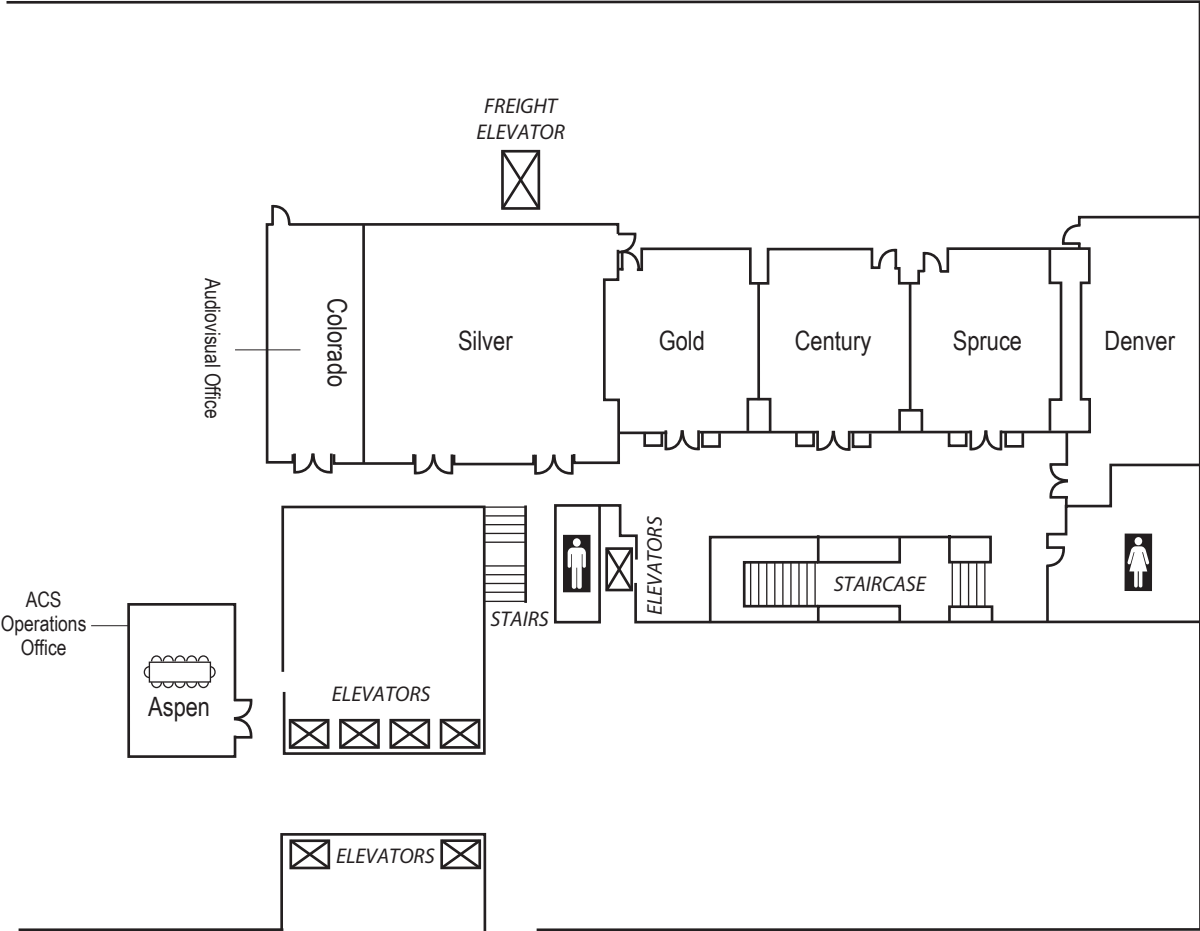
SHERATON DENVER DOWNTOWN

Plaza Building Lobby/Street Level



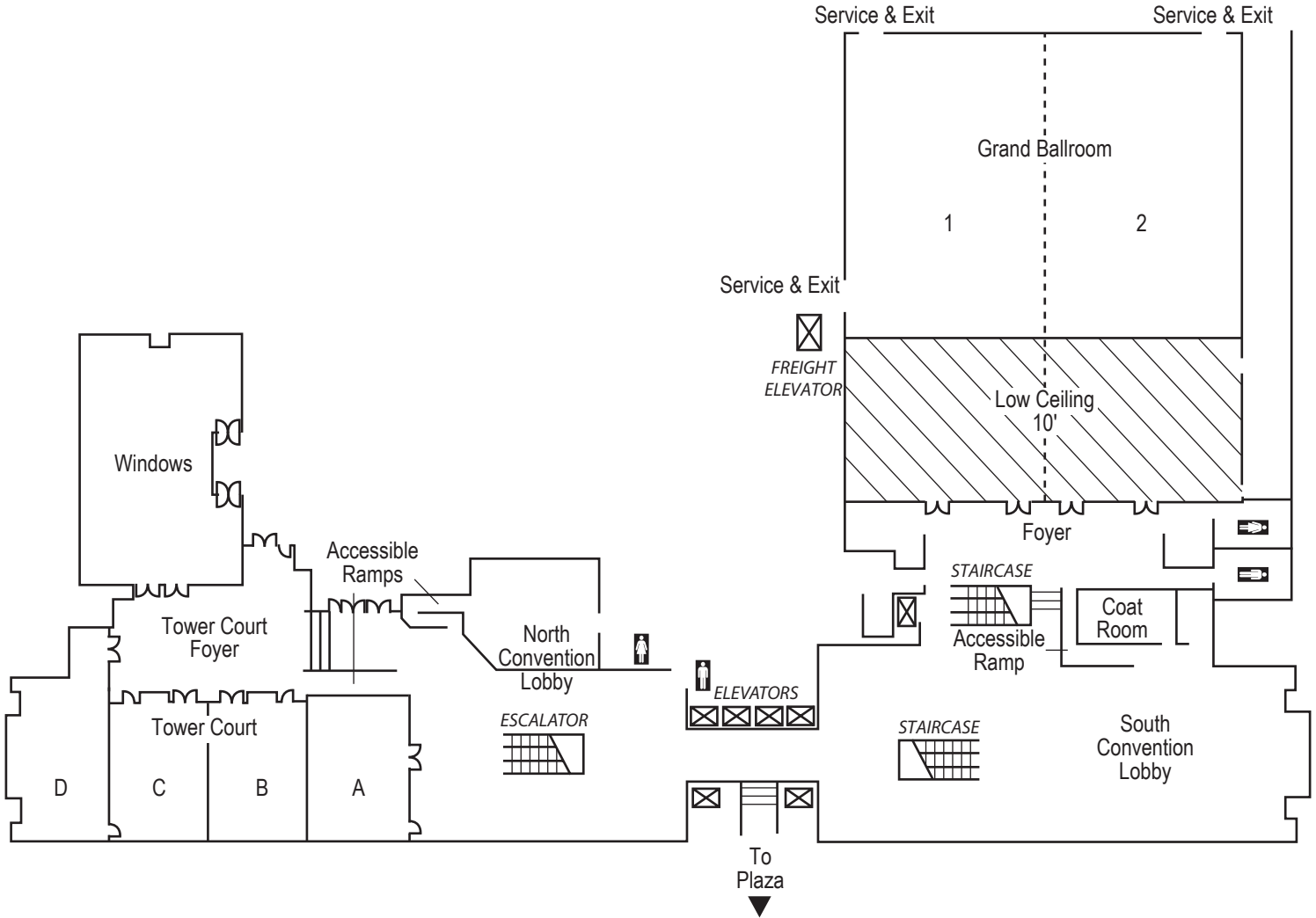
SHERATON DENVER DOWNTOWN

Tower Building Mezzanine Level



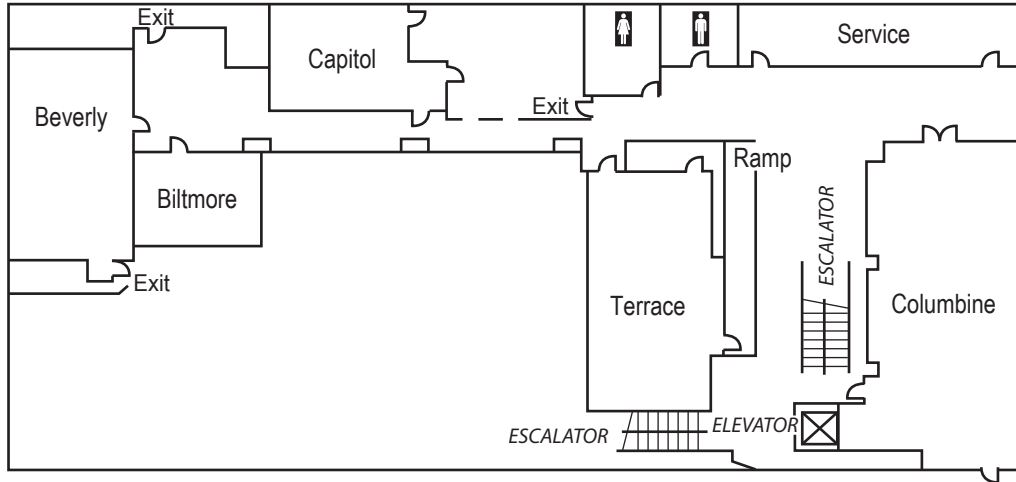
SHERATON DENVER DOWNTOWN

Tower Building Second Level

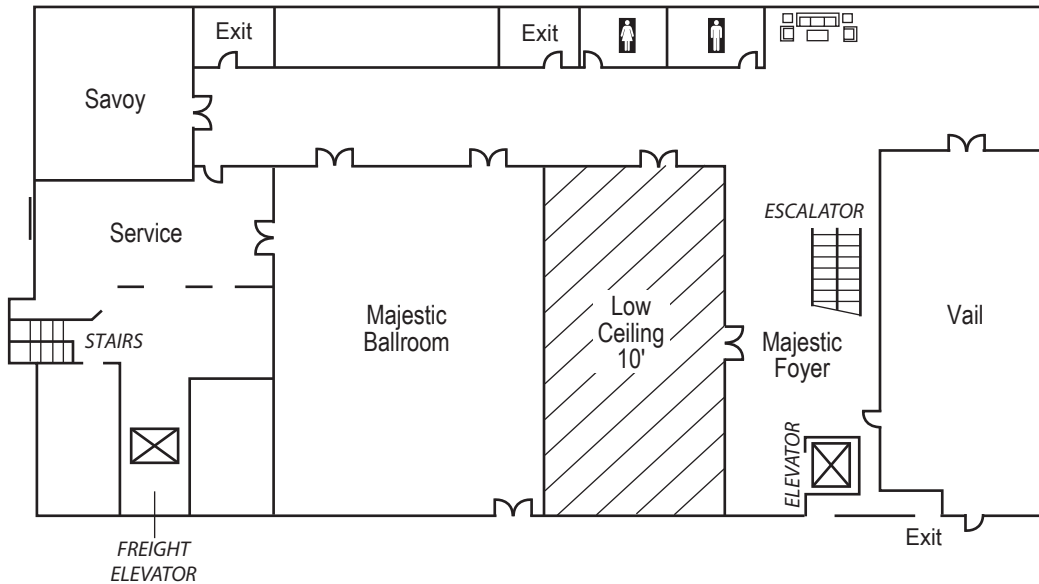


SHERATON DENVER DOWNTOWN

Tower Building Terrace Level

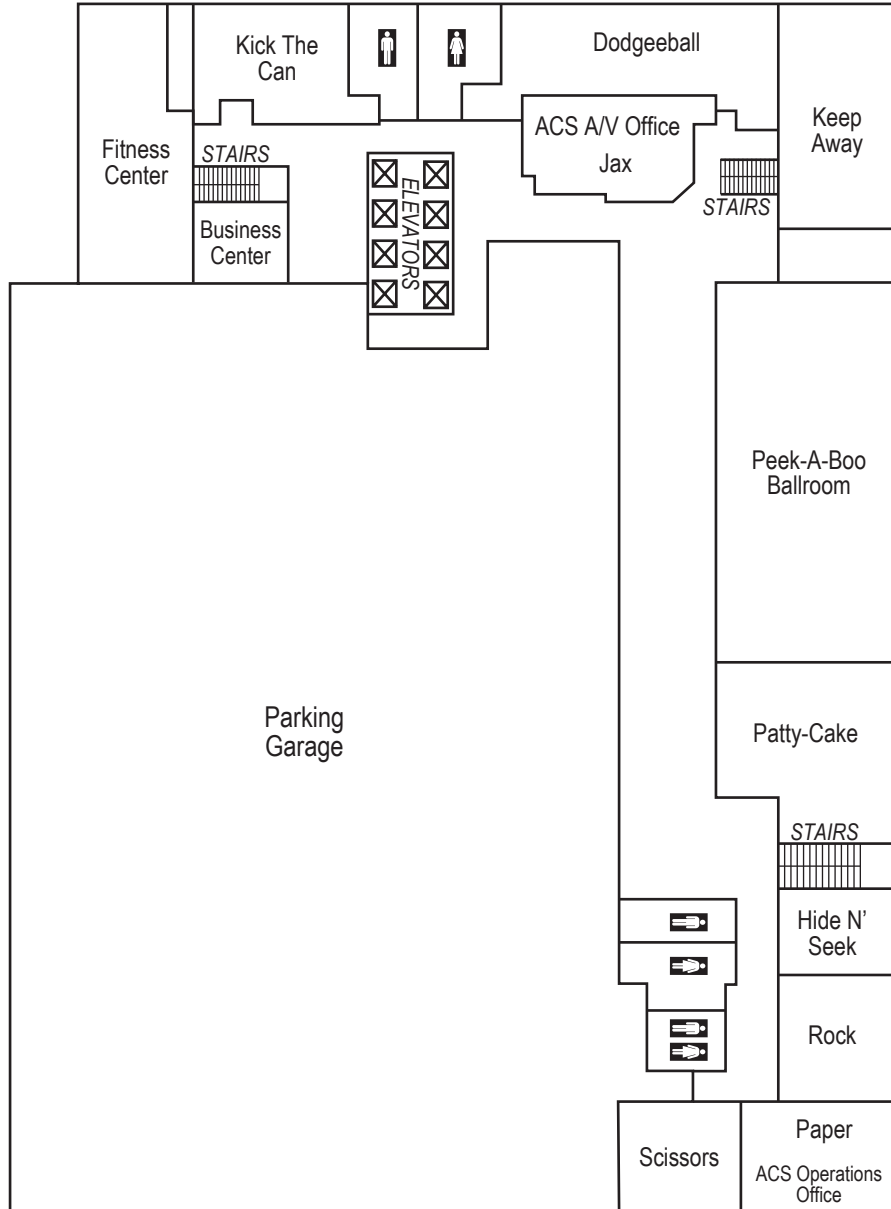


Tower Building Majestic Level



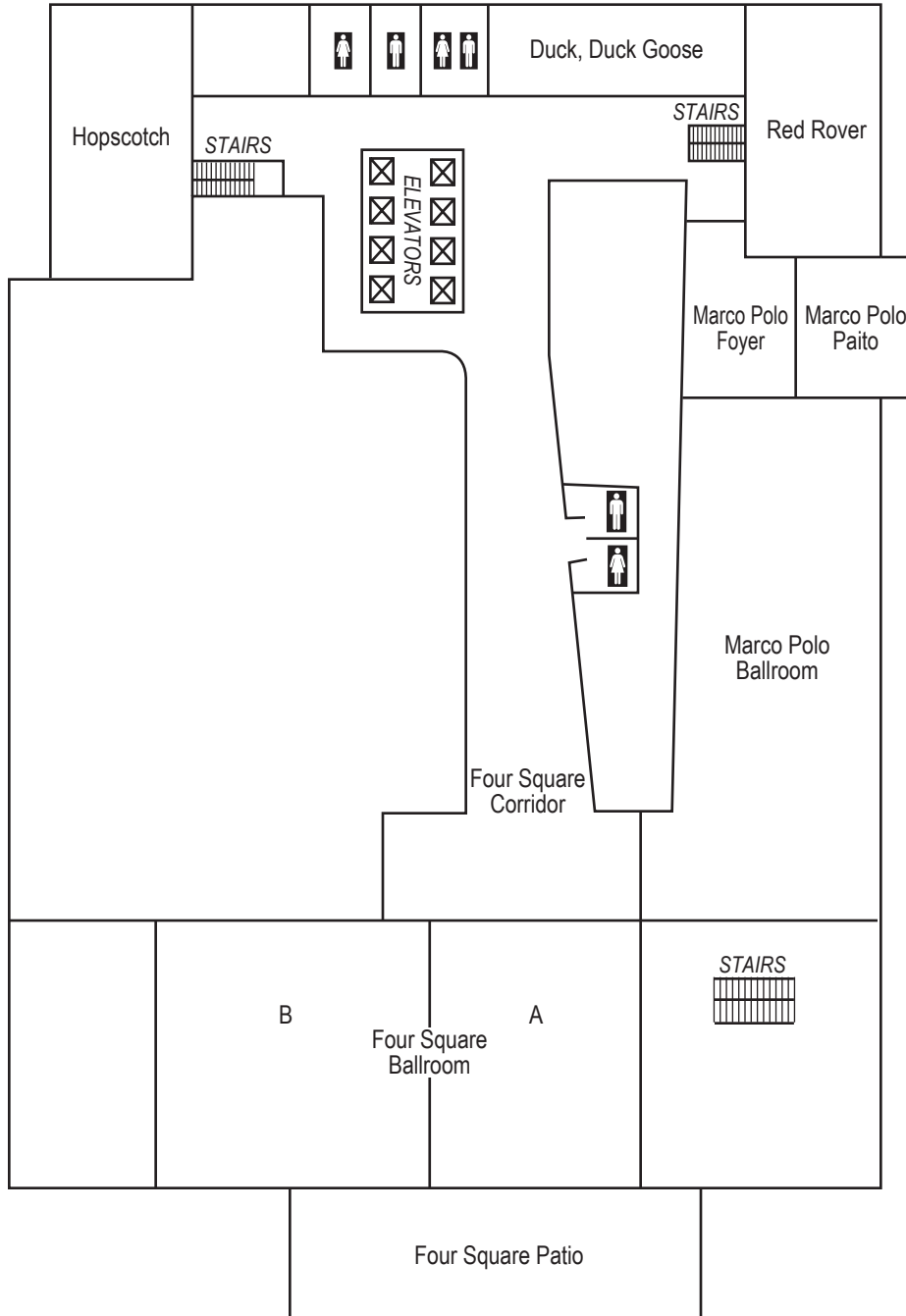
THE CURTIS MEETING SPACE

2nd Floor



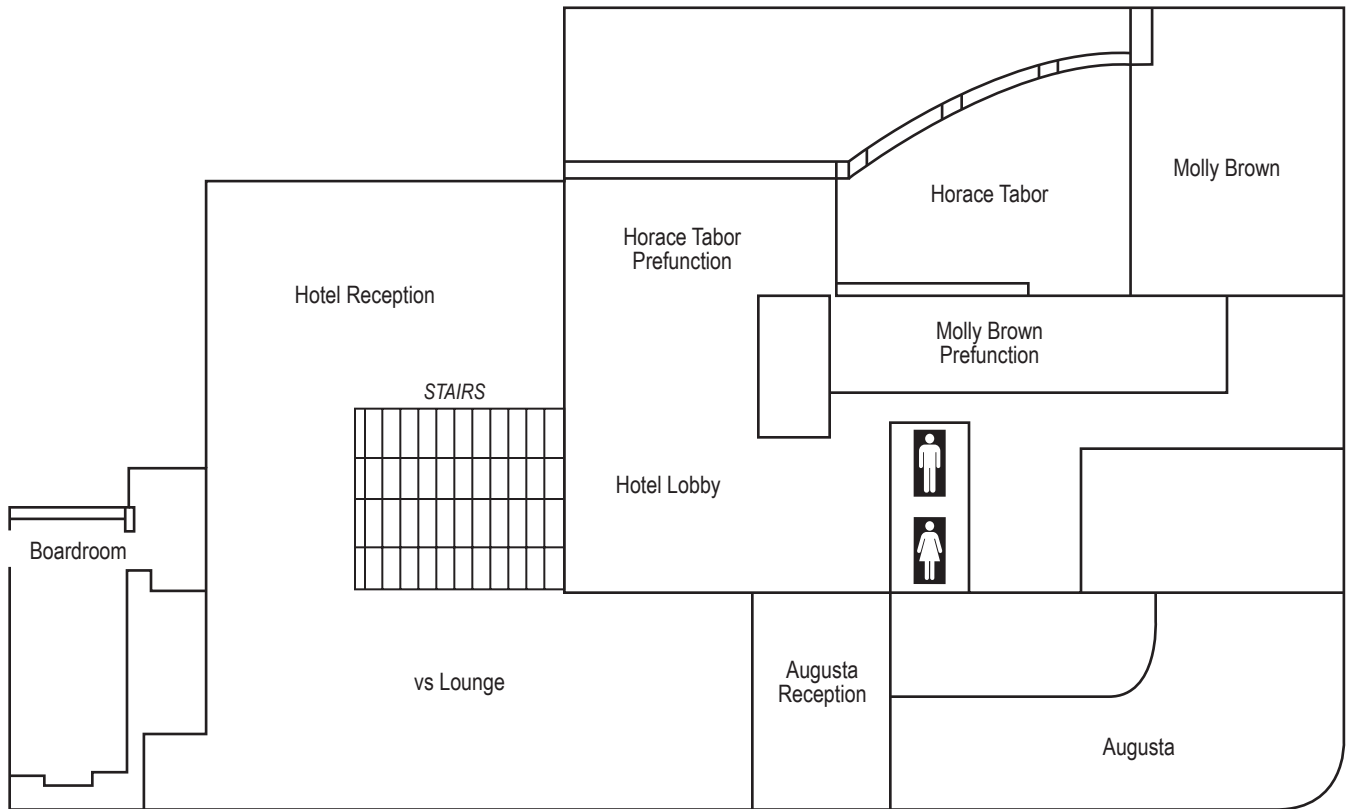
THE CURTIS MEETING SPACE

3rd Floor



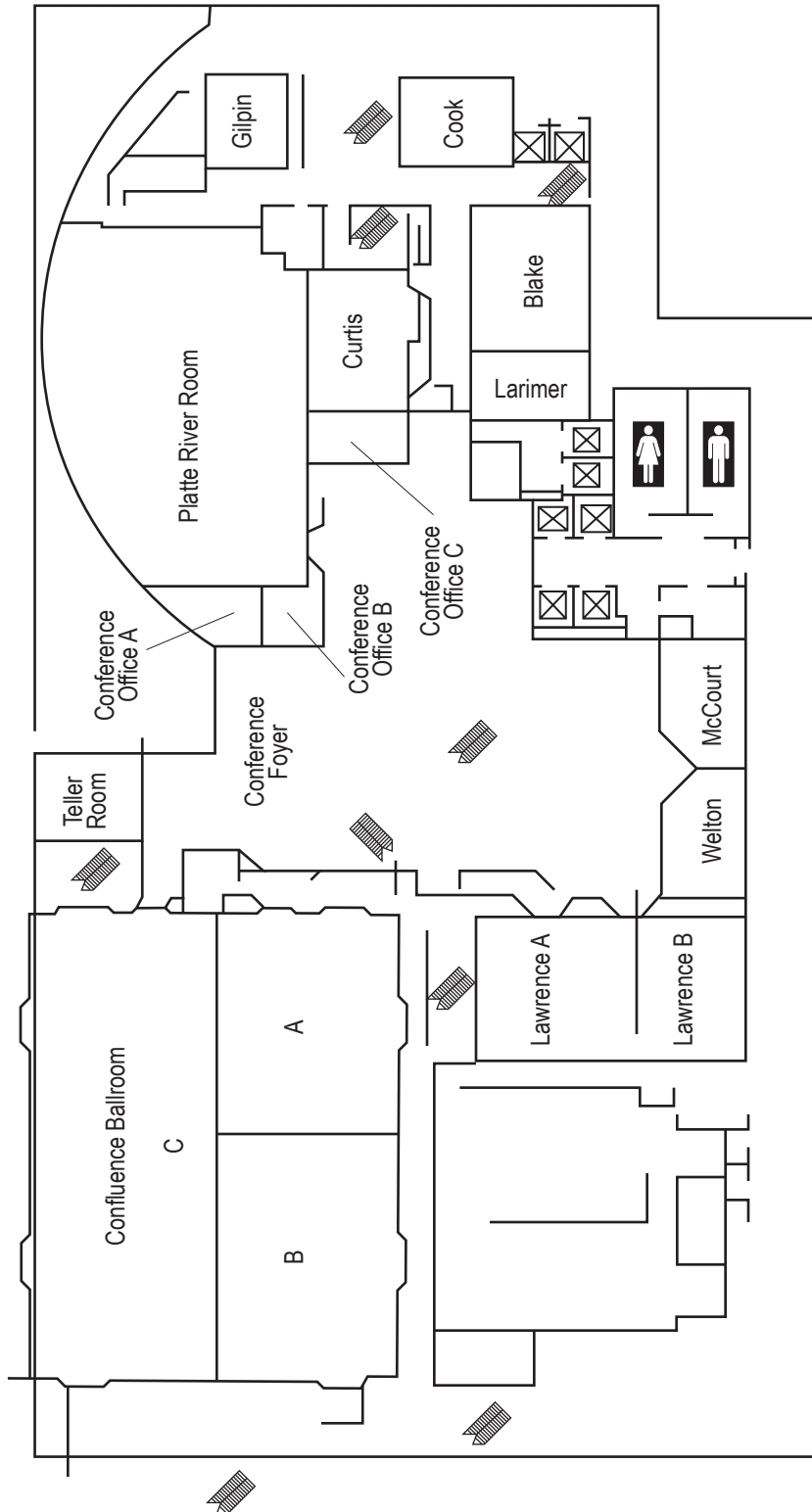
WESTIN DENVER HOTELS

Lobby Level, Second Floor



WESTIN DENVER HOTELS

Lobby Level, Third Floor



EXCEPTIONAL RESEARCH
SHOULD HAVE NO LIMITS.

ACS
central
science

Submit your research to ACS Central Science—
a new, multidisciplinary, open access journal that
presents groundbreaking advances in the world
of chemistry and beyond.

pubs.acs.org/centralscience

PRESIDENTIAL SYMPOSIA

Sponsored and Recommended
by the ACS President

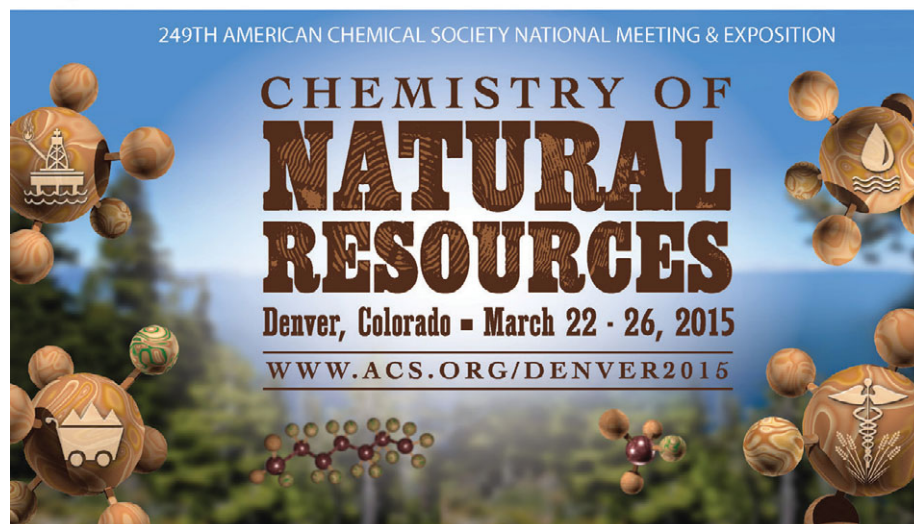
Photo: Peter Curtis Photography



Diane Grob Schmidt, Ph.D.
ACS President



www.acs.org/denver2015
follow us on twitter #ACSdenver



Sunday, March 22, 2015

1:30-5:30 PM

Nanotechnology: Delivering on the Promise

(Cosponsored by the following ACS Divisions and Committees and other scientific societies AGFD, AGRO, ANYL, CARB, CHAS, COLL, ENFL, HIST, I&EC, PMSE, POLY, SCHB, MPPG, CA, CCS, CCPA, COMSCI, DAC, IAC, SOCED; American Institute of Chemical Engineers, Gordon Research Conferences, Materials Research Society & National Academy of Engineering)

Colorado Convention Center, Mile High Ballroom 3A (Lower Level)

Monday, March 23, 2015

8:30 AM-4:45 PM

Nanotechnology: Delivering on the Promise

Tuesday, March 24, 2015

8:30-11:30 AM

DOE Nanoscience Research Centers: National Resources for the Nanoscience Community

(Cosponsored ANYL, ENFL, CCPA, CEI & MPPG)

Colorado Convention Center,
Rooms 506-507 (Street Level)

NANO RELATED SYMPOSIA RECOMMENDED BY THE ACS PRESIDENT

Nanoscience and Nanotechnology of Natural Resources

(Sponsored by MPPG and cosponsored by PRES)

Nanoscience

(Sponsored INOR and cosponsored by PRES)

Applied Nanotechnology for Food and Agriculture

(Sponsored by AGFD and cosponsored by PRES)

Basic Research in Colloids, Surfactants and Nanomaterials

(Sponsored by COLL and cosponsored by PRES)

Functionalization of Complex Nanosurfaces

(Sponsored by COLL and cosponsored by PRES)

Particles at Fluid Interfaces

(Sponsored by COLL and cosponsored by PRES)

Metallic Nanostructures for Optical and Electrochemical Sensing and Alternative Energy Conversion

(Sponsored by COLL and cosponsored by PRES)

Plasmonic Catalysis and Sensing

(Sponsored by COLL and cosponsored by PRES)

Advances in Formulations Science and Technology

(Sponsored by COLL and cosponsored by PRES)

Fundamental Research in Colloids, Surfaces and Nanomaterials

(Sponsored by COLL and cosponsored by PRES)

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

(Sponsored by CHAS and cosponsored by PRES, AGFD & CCS)

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys

(Sponsored by POLY and cosponsored by PRES)

Official ACS Properties in Denver, CO



Visit our website at www.acs.org/denver2015 to view a list of economical hotels.

- 1 Courtyard by Marriott Denver Downtown**
934 16th Street
303-571-1114
www.marriott.com
- 2 Crowne Plaza Denver Downtown**
1450 Glenarm Place
303-573-1450
www.reservations.com/hotel/crowne-plaza-downtown-denver
- 3 Embassy Suites Denver – Downtown Convention Center**
1420 Stout Street
303-592-1000
http://embassysuites3.hilton.com
- 4 Grand Hyatt Denver**
1750 Welton Street
303-295-1234
http://granddenver.hyatt.com
- 5 Hampton Inn & Suites Denver Downtown–Convention Center**
550 15th Street
303-623-5900
www.hamptoninndenver.com
- 6 Hilton Garden Inn Denver Downtown**
1400 Welton Street
303-603-8000
www.hgidenverdowntown.com
- 7 Homewood Suites Denver Downtown—Convention Center**
550 15th Street
303-534-7800
www.thedenverhomewood.com
- 8 Hotel Monaco Denver**
1717 Champa St.
303-296-1717
www.monaco-denver.com
- 9 Hyatt Regency Denver at Colorado Convention Center**
650 15th Street
303-436-1234
http://denverregency.hyatt.com
- 10 Magnolia**
818 17th Street
303-607-9000
www.magnoliahotels.com/denver
- 11 Marriott City Center Denver**
1701 California Street
303-297-1300
marriott.com
- 12 Renaissance Downtown Denver City Center**
918 17th Street
303-867-8100
www.rendendowntown.com
- 13 Residence Inn City Center**
1725 Champa St.
303-296-3444
www.marriott.com
- 14 Sheraton Denver Downtown Hotel**
1550 Court Place
303-893-3333
www.sheratondenverdowntown.com
- 15 The Curtis—a DoubleTree by Hilton**
1405 Curtis Street
303-571-0300
http://thecurtis.com
- 16 The Ritz-Carlton, Denver**
1881 Curtis Street
303-312-3800
www.ritzcarlton.com
- 17 Westin Denver Downtown**
1672 Lawrence Street
303-572-9100
www.westinindenverdowntown.com

Shuttle information

Shuttle Schedule

SUNDAY, MARCH 22

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

MONDAY, MARCH 23

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 24





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 25

7:00 AM – 11:00 PM 30 minute service

THURSDAY, MARCH 26

7:00 AM – 6:00 PM..... 60 minute service

 Route 1
  Route 2
  Walk to Convention Center
X Boarding Location  Pickup/Drop Location at Convention Center



Wheelchair Accessible Transportation is available during hours of operation. Please call 1-866-439-8564 to schedule (please allow 30 minutes).



For all shuttle inquiries, please call: 1-866-439-8564.



Shuttle Services managed and operated by Transportation Management Services.



Carbon Neutral Shuttles.

Scan for copy of shuttle schedule:





ACS
Chemistry for Life®

249th ACS National Meeting & Exposition

March 22 - 26, 2015 | Denver, CO

HOTEL WALKING DIRECTIONS: Scan the corresponding QR code to download walking directions from the hotel to the convention center.



Courtyard by
Marriott Denver
Downtown



Crowne
Plaza Denver
Downtown



Embassy Suites
Denver



Grand Hyatt
Denver



Hampton Inn
and Suites
Denver
Downtown -
Convention
Center



Hilton Garden
Inn Denver
Downtown



Homewood
Suites Denver
Downtown -
Convention
Center



Hotel Monaco
Denver



Hyatt Regency
Denver at
Colorado
Convention
Center



Magnolia



Marriott City
Center Denver



Renaissance
Downtown
Denver City
Center



Residence Inn
City Center



Sheraton
Denver
Downtown
Hotel



The Curtis -
A DoubleTree
Hotel by Hilton



The Ritz Carlton



Westin Denver
Downtown



Scan here to
download
a copy of
the shuttle
schedule.

Take the greener meeting Challenge

Take the Greener Meetings Challenge at www.acs.org/greenermeetings. Tell your story or simply show your support for the ACS Greener Meetings Program. All participants will receive a special thank you (*While supplies last.*). Three participants having the best stories will be awarded prizes on **April 27, 2015**.

To be a catalyst for positive change! Here's what you can do:

1



Take advantage of linen reuse and other initiatives at your hotel, and always turn the lights off when away from your room. If you are staying at the Westin or Sheraton, enroll in their Make A Green Choice program.

2



Responsibly dispose of recyclable materials (paper, plastic, glass, aluminum) at the convention center and hotels.

3



Download the national meeting mobile app or digital program. Limited quantities of the printed Onsite Program are available.

4



Avoid the use of taxis by walking when safe and possible. Stop by the Greener Meetings Booth for your pedometer (*While supplies last*). Burn calories, and enjoy the city.

5



Ride the ACS carbon-neutral shuttle service when walking isn't an option between your hotel and the center. Shuttle service will be provided between many ACS contracted properties.

6



Avoid the use of disposable, plastic water bottles. Stop by the ACS Colorado Host Local Section Booth to pick up a free, reusable water bottle (*While supplies last*). Avoid the cost and waste associated with disposable bottles.

Colorado Convention Center, Lobby A/F

Greener Meetings Booth

Sun., 3 – 6 PM

Mon., 8 – 1PM

Tues., 8 – 1 PM

Colorado Host Local Section Booth

Sat., 3 to 6 PM

Sun., 7:30 AM to 7:30 PM

Mon., 7:30 AM to 9 PM

Tues., 7:30 AM to 5 PM

Wed., 7:30 AM to 4 PM

Thurs., 7:30 AM to 1 PM

ACKNOWLEDGMENTS

Specific ACS Divisions and Committees gratefully acknowledge the financial and other contributions made to their division by the institutions and companies listed below and others who were not known at press time.

Presidential Events

American Institute of
Chemical Engineers
Gordon Research Conferences
Materials Research Society
National Academy
of Engineering

Division of Catalysis Science and Technology

The Dow Chemical Company
Exxonmobil
The Royal Society of Chemistry
Journal of Chemical Science
Strem Chemicals Inc.
University of Florida Center
for Catalysis

Division of Chemical Education

2YC3
ACS Green Chemistry Institute
ACS Education Division
Anasazi Instruments
Bruker
ChemSource, Inc.
The Industrial & Engineering
Chemistry Division's Green
Chemistry Subdivision
Intersociety Polymer
Education Council
JEOL
NSF-CCI Center for Sustainable
Polymers at the University
of Minnesota

Pearson Publishing
Thermo Fisher Scientific

Division of Colloid and Surface Chemistry

Avanti Polar Lipids, Inc.
Institute for Molecular
Engineering – University
of Chicago
Sigma-Aldrich

Division of Computers in Chemistry

Chemical Computing Group
OpenEye Scientific Software

Division of Industrial and Engineering Chemistry

ExxonMobil

Division of Medicinal Chemistry

AbbVie
Actelion Pharmaceuticals Ltd
Amgen
Array BioPharma
Bristol-Myers Squibb
Celgene
ChemPartners
Cubist
EMD Serono
Epizyme
Genentech
Janssen

Lundbeck Research USA
Merck
Paraza Pharma
Pfizer
Pharmaron
Sanofi Aventis
Vertex
Wuxi Aptec

Division of Polymer Chemistry

3M
Avery Dennison
Bayer MaterialScience
The Dow Chemical Company
Green Materials – ICE Science
IAB (POLY)
Kuraray
NIST
POLY
The Royal Society of Chemistry
Sabic Innovative Plastics
Tosoh BioScience
University of Dallas
Waters
Wyatt Technology

Division of Polymeric Materials Science and Engineering

Aldrich
The American Chemical Society
Journal ACS Nano

The American Chemical
Society Journal
Chemistry of Materials
Asylum Research
Bruker
The Dow Chemical Company
ExxonMobil
Genzyme
IBM
Malvern Instruments
Nanosurf
Rigaku
The Royal Society of Chemistry
*Journal of Biomaterials
Science*
The Royal Society of Chemistry
Journal of Chemical Science
The Royal Society of Chemistry
*Journal of Materials
Chemistry A*
The Royal Society of Chemistry
*Journal of Materials
Chemistry B*
The Royal Society of Chemistry
*Journal of Materials
Chemistry C*
The Royal Society of Chemistry
Journal of Soft Matter
SAXSLab MolmeX Scientific Inc.
Solvay
TA Instruments
University of Delaware Materials
Science & Engineering

WE THANK OUR VOLUNTEERS FOR THEIR DEDICATION AND HARD WORK

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 more than 161,000 members with:

- Powerful networks on the local, regional, and national level;

- Specialized technical information and research;
- Expansive career enhancement materials;
- Award-winning publications; and
- 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.

Presenters – Abstract submission varies by division.

Check with your division chair for your deadline.

Housing and Registration Open May 2015

Learn more at www.acs.org/boston2015

CALL FOR PAPERS

250th American Chemical Society National Meeting & Exposition

BOSTON

August 16-20, 2015

INNOVATION
from **D**iscovery
to **A**pplication

Are you a

74

W

Tungsten
183.84

49

In

Indium
114.818

7

N

Nitrogen
14.0067

68

Er?

Erbium
167.259

Visit the ACS Booth,
grab a punch card and complete
interactive tasks for the chance to receive prizes.

All completed punch card holders will receive a prize
and will be entered to win an Apple® iPad Air®.

See you soon in the ACS Booth!

Explore. Discover. Create.



SciFinder®

The choice for chemistry research.™

scifinder.cas.org