

250th American Chemical Society National Meeting & Exposition

Celebration

BOSTON

August 16-20, 2015

BOSTON, MA

www.acs.org/boston2015

#acsBoston

INNOVATION
from **D**iscovery
to **A**pplication

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



*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

EMBRACING SUSTAINABILITY PRACTICES

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

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
- 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.



250th American Chemical Society National Meeting & Exposition

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ACS OPERATIONS OFFICES

- **Boston Convention & Exhibition Center (BCEC) (Room 151A):** 617-954-3970
- **Boston Marriott Copley Place (Falmouth Room):** 617-587-5193
- **Boston Park Plaza Hotel & Towers (Exeter):** 617-457-2443
- **Renaissance Boston Waterfront (Georges):** 617-342-5444
- **Seaport Hotel (Liberty A):** 617-385-4060
- **World Trade Center (South End):** 617-385-4920
- **Sheraton Boston Hotel (Beacon E):** 617-378-6602
- **Westin Boston Waterfront (Hale):** 617-502-2255

INFORMATION CONTACTS

- **Attendee Registration, BCEC, North Lobby:** 617-954-3972
- **Career Fair, BCEC, Hall B2:** 617-954-3976
- **Exhibitor Registration, BCEC, North Lobby:** 617-954-3974
- **Finance Office, Westin Boston Waterfront, Frost Room:** 617-502-2224
- **Hospitality Booth, BCEC, North Lobby:** 617-954-3454
- **Membership Marketing, BCEC, North Lobby:** 617-954-3453
- **Press Center, BCEC, Room 153B:** 617-954-3971
- **Governance's Office, Sheraton Boston Hotel (Gardner Room):** 617-378-6610
- **Shuttle Desk, BCEC, East Side Drive:** 617-954-3455
- **Society Programs, Sheraton Boston Hotel (Beacon A):** 617-378-6604

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

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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 250th National Meeting & Exposition, refer to www.acs.org/boston2015. All Boston photos in this program are courtesy of the Boston 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.

250th American Chemical Society National Meeting & Exposition
Celebration

BOSTON

Where to Find Meeting Information

BOSTON, MA • AUGUST 16 - 20, 2015

WWW.ACS.ORG/BOSTON2015

Official Meeting Website
www.acs.org/boston2015

Announcements & Changes
www.acs.org/meetingupdates

Digital Meeting Program
www.acs.org/boston2015



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

INNOVATION
from **D**iscovery
to **A**pplication



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

Text your question to
754.227.2012 (Standard text rates apply)

Welcome to Boston and the 250th ACS National Meeting

Welcome to Boston and the 250th ACS National Meeting. It is my pleasure to join all of you in the historical and vibrant city of Boston, a favorite location for our meetings.

Twenty-nine technical divisions and nine committees are hosting original programming based on the meeting theme of Innovation From Discovery To Application. More than 9,000 papers will be presented, and nearly 3,000 poster presentations will take place at the meeting. Additionally, 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 chemistry icon Dr. George Whitesides talk about 'Reengineering Chemistry.' Please join your colleagues from noon to 1:00 p.m. in Ballroom West (Level 3) of the Boston Convention & Exhibition Center.

There are five Presidential Symposia that I encourage you to attend as well as several others I am recommending. On Sunday, August 16, "National Science Foundation's Centers for Chemical Innovation" highlights the research at those Centers and features the heads of all eight Centers for Chemical Innovation. A poster session with researchers' work from the various Centers follows the oral presentations. Starting in the afternoon on Sunday and running through Monday morning is the symposium titled "21st Century Education: Formal & Informal." On Monday, August 17, ACS will celebrate the 20-year anniversary of the establishment of the ACS Scholars program with a special symposium of past scholars throughout industry and academia. On Tuesday, August 18, during "Transforming University-Industry Partnerships for an Innovative Future," speakers from both academia and industry will highlight the role better university-corporate partnerships can play in driving more innovation. Finally, the ACS Divisions of HIST, POLY, PROF, and SCHB are all hosting various symposia in honor of



Diane Grob Schmidt
ACS President

the 100th birthday of chemistry pioneer Henry A. Hill. Details of these presidential events and other recommended symposia can be found at www.acs.org/boston2015.

On Monday afternoon, William Dichtel, Associate Professor of Chemistry and Chemical Biology at Cornell University will deliver The Kavli Foundation Emerging Leader in Chemistry Lecture on 'The Spectacular Properties of Porous Polymers.' He is followed by George Whitesides, University Professor of Chemistry at Harvard University with The Fred Kavli Innovations in Chemistry Lecture (Boston Convention & Exhibition Center – Ballroom West, Level 3). Dr. Whitesides will speak on 'Problems, Puzzles, and Inevitabilities in Research.'

Many education-focused programs for high school teachers, undergraduate and graduate students, postdocs, and chemical professionals will be offered. A range of professional development courses will be available. The exposition will feature more than 250 companies showcasing services, instruments, books, and lab equipment in more than 400 booths.

My personal thanks to the members of the Northeastern Local Section; the Committee on Meetings and Expositions; the divisional program chairs and symposium chairs responsible for organizing this meeting's technical sessions; and the ACS staff for making it all happen. Thanks to you for contributing to the success of this meeting, and of course for attending.



Diane Grob Schmidt
ACS President

Welcome Message from Rick Wagner, Boston Thematic Program Chair

The 250th ACS National Meeting will be held in Boston, MA, August 16-20, 2015, and promises to be a very exciting meeting. The theme is Innovation from Discovery to Application. As the birthplace of Benjamin Franklin, Boston is indeed an appropriate venue for this theme! The plenary session, on Sunday afternoon, August 16, will launch the theme with three invited lectures: Dr. Paula Hammond (Massachusetts Institute of Technology) will discuss “Tailored Drug Release Surfaces for Regenerative Medicine and Targeted Nanotherapies;” Dr. Peter Schultz (Scripps Research Institute) will present “A Chemist’s Foray Into Translational Medicine”; and Dr. Karen Wooley (Texas A&M) will present “Targeted Applications as Inspirations to Develop Strategies toward Functionally- Sophisticated Nanoscopic Macromolecules with Diverse Compositions, Structures, and Properties.” The afternoon of Monday, August 17 will see the Kavli Foundation Emerging Leader in Chemistry Lecture by Dr. William Dichtel (Cornell University) “The Spectacular Properties of Porous Polymers” and the Fred Kavli Innovations in Chemistry Lecture by Dr. George Whitesides (Harvard University) “Problems, Puzzles, and Inevitabilities in Research.” Exciting thematic symposia focused on chemical innovation in health and medicine, materials science, chemical synthesis, and the history of innovation have also been organized. In addition, the chemical innovation in design talks or CID talks will be introduced at Sci-Mix.

Twelve divisions and committees contributed 32 symposia to support the thematic program, ‘Innovation from Discovery



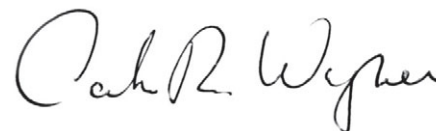
Rick Wagner
Boston Thematic
Program Chair

to Application’. More detail on symposia can be found in the sessions sponsored by AGFD, AGRO, ANYL, CATL, CELL, CINF, CHAL, COLL, ENVR, HIST, I&EC, INOR, MEDI, ORGAN, PHYS, POLY, PMSE, SCHB, CORP, IAC, and YCC. The 2015 ACS Fellows will be inducted on Monday, August 17 and the 17th Annual ChemLuminary Awards is being held on Tuesday, August 18.

Dr. Diane Grob Schmidt will host several presidential symposia and events. The Presidential Outreach Event, “Exploring Our World through Chemistry,” will take place on Saturday, August 15 at the Boston Children’s Museum.

The program for the meeting and other information is available online at the website of the meeting www.acs.org/boston2015.

I am very grateful to the members of the local section, the program chairs of the divisions listed above, the thematic symposia chairs 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 Boston.



Rick Wagner
Thematic Program Chair



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COMMONWEALTH OF MASSACHUSETTS
STATE HOUSE • BOSTON, MA 02133
(617) 725-4000

CHARLES D. BAKER
GOVERNOR

KARYN E. POLITO
LIEUTENANT GOVERNOR

August 2015

Dear Friends:

On behalf of the Commonwealth of Massachusetts, Karyn and I welcome you to The American Chemical Society 250th Annual Fall Meeting.

Since the organization's founding in 1876, The American Chemical Society (ACS) has been at the forefront in the evolution of all fields of sciences, especially chemistry. ACS's programs and workshops enrich our youth with an appreciation for chemistry and promote excellence in the fields of science education and engineering. In addition, ACS's conferences prepare our workforce to stay competitive and thrive in the science industry.

We commend The American Chemical Society's passion for chemistry and excellence in the field. Please accept our best wishes as you gather for another enjoyable meeting.

Sincerely,

A handwritten signature in blue ink that reads "Charles Baker".

CHARLES D. BAKER
GOVERNOR

A handwritten signature in blue ink that reads "Karyn E. Polito".

KARYN E. POLITO
LIEUTENANT GOVERNOR



CITY OF BOSTON • MASSACHUSETTS

OFFICE OF THE MAYOR
MARTIN J. WALSH

August 16, 2015

Dear Friends,

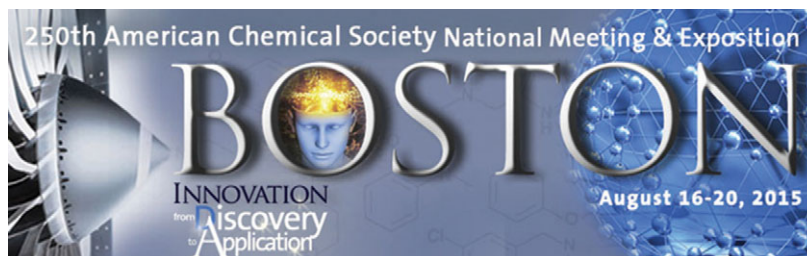
On behalf of the City of Boston, I would like to extend a warm welcome to all members of the American Chemical Society who are visiting our great city to attend the 250th National Meeting and Exposition. For a conference that is focused on promoting groundbreaking discovery, innovative research, and scientific leadership, I believe the City of Boston is a perfect host.

I am thrilled that the American Chemical Society will be convening members from all degree levels and fields of chemistry who are the world's premier leaders in chemical sciences, and invite you all to explore Boston's rich history, dedication to education, and thriving innovation communities. I hope that the City of Boston and all it has to offer will facilitate a productive conference and will help you to achieve even more advanced research, education and innovation.

Again, I appreciate your dedication to the City of Boston and wish you a successful meeting.

Sincerely,

Martin J. Walsh
Mayor of Boston



PRESIDENTIAL SYMPOSIA AND EVENTS

Sponsored by the ACS President

Photo: Peter Cutts Photography



Diane Grob Schmidt, Ph.D.
ACS President

Saturday, August 15, 2015

10:00 AM-1:00 PM

Presidential Outreach Event: Exploring Our World Through Chemistry

(Cosponsored by CCA and ACS Member Communities)

*Boston Children's Museum
308 Congress Street
Boston, MA 02210*

Sunday, August 16, 2015

8:30 AM-2:30 PM

National Science Foundation's Centers for Chemical Innovation

(Cosponsored by AGRO, BMGT, CARB, COLL, ENFL, INOR, PROF, SCHB & WCC)

Westin Boston Waterfront, Burroughs Room (Harborwing, Conference Level)

1:30 PM-3:00 PM

"Mystery of Matter" hosted by PBS

(Cosponsored by CPRC and the ACS Office of Public Affairs)

Boston Convention & Exhibition Center, Room 52A-B (Exhibition Level)

1:30 PM-5:00 PM

21st Century Chemistry Education: Formal and Informal

(Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF, SOCED & WCC)

Boston Convention & Exhibition Center, Room 158 (Level One)

2:00 PM-6:00 PM

Edwin Land and Instant Photography: Massachusetts' First National Historic Chemical Landmark

(Sponsored by HIST and Cosponsored by PRES)

Boston Convention & Exhibition Center, Room 50 (Exhibition Level)

3:00 PM-6:00 PM

National Science Foundation's Centers for Chemical Innovation Poster Session

(Cosponsored by AGRO, BMGT, CARB, COLL, ENFL, INOR, PROF, SCHB & WCC)

Westin Boston Waterfront, Galleria (Harborwing, Conference Level)

Monday, August 17, 2015

8:30 AM-12:00 PM

21st Century Chemistry Education: Formal and Informal

(Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF, SOCED & WCC)

Boston Convention & Exhibition Center, Room 158 (Level One)

8:30 AM-12:00 PM

Memories of Henry Hill: His Legacy in Science and in Professional Service

(Sponsored by HIST & Cosponsored by PRES, AGRO, CARB, COLL, ENFL, POLY, PROF & SCHB)

Boston Convention & Exhibition Center, Room 50 (Exhibition Level)

8:30 AM-4:50 PM

ACS Scholars: Rising Stars in Academe and Industry

(Cosponsored by AGRO, CARB, CMA, COLL, ENFL, ENVR, PROF, SCHB & YCC)

Sheraton Boston Hotel, Back Bay Ballroom A (2nd Floor, Main Building)

Tuesday, August 18, 2015

8:00 AM-5:00 PM

Transforming University-Industry Partnerships for an Innovative Future

(Cosponsored by AGRO, BMGT, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF & SCHB)

Westin Boston Waterfront, Burroughs Room (Harborwing, Conference Level)

5:00 PM-7:00 PM

Henry A. Hill Award and Reception

(Sponsored by PRES)

Seaport Hotel, Plaza Ballroom A-B (Plaza Level)



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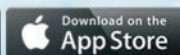
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ACSBOSTON 2015 Mobile App

- Quick Access to the full technical program, maps, and search features.
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- Use your ACS ID to sync your schedule.
- Take notes and share them via email. Connect your meeting experience with social media and more!

American Chemical Society
Mobile Meeting Application

is your free full greener guide to
manage your experience at the 250th
ACS National Meeting in Boston.



Onsite Support – Hours of Operation

Sunday, August 16 from 8AM – 5PM
Monday, August 17 from 8AM – 5PM
Tuesday, August 18 from 8AM – 3PM
Learn more at www.acs.org/meetingapp

Boston Convention & Exhibition Center, North Lobby

The ACS Board of Directors Hosts George M. Whitesides



SUNDAY, AUGUST 16, 2015

Noon – 1:00 PM

Ballroom West (Level 3)

Boston Convention & Exhibition Center

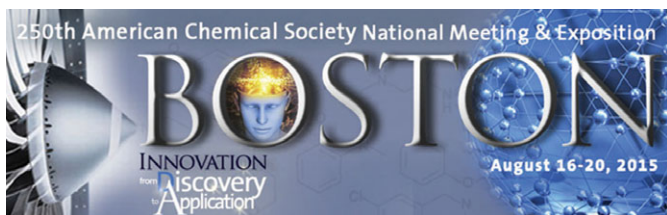
“Reengineering Chemistry”

Chemistry is facing a set of very important challenges, ones very different than those it has addressed in the past. Join Professor George M. Whitesides during the ACS Board of Directors Regular Session for his engaging talk as he discusses how the field is changing, and how chemistry will have to adapt to this change.

Professor Whitesides is the Woodford L. and Ann A. Flowers University Professor in the Department of Chemistry & Chemical Biology at Harvard University. A prolific author and patent holder, he is best known for his work in the areas of NMR spectroscopy, organometallic chemistry, molecular self-assembly, soft lithography, microfabrication, microfluidics, and nanotechnology.

Doors Open at 11:45 a.m.

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



HENRY HILL SYMPOSIA AND EVENTS

Recommended by the ACS President

Sunday, August 16, 2015

1:30 PM-4:30 PM

The Professional Legacy of Henry Hill

(Sponsored by PROF & Cosponsored by PRES)



Henry A. Hill

Monday, August 17, 2015

8:30 AM-12:00 PM

Memories of Henry Hill: His Legacy in Science and in Professional Service

(Sponsored by HIST & Cosponsored by PRES, AGRO, CARB, COLL, ENFL, PROF & SCHB)

1:15 PM-4:45 PM

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector

(Sponsored by SCHB & Cosponsored by PRES)



Diane Grob Schmidt, Ph.D.
ACS President

Tuesday, August 18, 2015

8:00 AM-4:00 PM

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

(Sponsored by POLY and Cosponsored by PRES & PMSE)

5:00 PM-7:00 PM

Henry A. Hill Award and Reception

(Sponsored by PRES)

PRESIDENTIAL SYMPOSIA AND EVENTS

Recommended by the ACS President



Diane Grob Schmidt, Ph.D.
ACS President

Sunday, August 16, 2015

1:00 PM-5:00 PM

True Stories from Entrepreneurs (BRIC Edition)

(Sponsored by SCHB & Cosponsored by PRES)

Monday, August 17, 2015

8:00 AM-12:00 PM

True Stories from Entrepreneurs (BRIC Edition)

(Sponsored by SCHB & Cosponsored by PRES)

8:10 AM-12:10 PM

The Chemistry Enterprise in 2015: Then and Now

(Sponsored by BMGT & Cosponsored by PRES)

1:30 PM-5:00 PM

Leadership Skills as a Strategic Advantage: The Chemist's Competitive Edge

(Sponsored by BMGT & Cosponsored by PRES, CA, CEPA & YCC)

Tuesday, August 18, 2015

8:00 AM-5:00 PM

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

(Sponsored by SCHB & Cosponsored by PRES)

8:30 AM-5:00 PM

International Entrepreneurship: How to Start a Business and Thrive in the Global Marketplace

(Sponsored by IAC and Cosponsored by PRES, AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PROF & SCHB)

Wednesday, August 19, 2015

8:00 AM-10:00 AM

Big Chemistry from Small Businesses

(Sponsored by SCHB & Cosponsored by PRES)

GENERAL MEETING INFORMATION

YOUR MEETING REGISTRATION

entitles you to a wide range of programming, including 1,550 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. U.S. residents who registered by July 13 received their badge credentials by mail before the meeting. International registrants (this includes Canada and Mexico) must pick up their badge credentials at ACS Attendee Registration.

Standard & On-Site Registration. Attendees who registered after July 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/boston2015.

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 contact the ACS National Meeting Registration Center or 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 will receive a confirmation via the original method of registration.

Internet. Register online at www.acs.org/boston2015 until August 20. A valid credit card is required to register online, and online registrations are real-time transactions.

Telephone. Call the ACS National Meeting Registration Center at 800-251-8629 (U.S./Canada only) or 508-743-0192 (international), Monday through Friday, 9:00 AM to 5:00 PM EDT. Mailed registrations will be accepted until August 20.

Fax/Mail. Submit the registration form via fax by August 20: 508-743-9604 or mail: ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532.

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

Registration Payments. Registration fees can be paid by check, money order, credit card (American Express, Discover, MasterCard, or VISA), or bank wire transfer. Make checks payable in U.S. dollars to the American Chemical Society, and include a completed registration form with each payment. Registration fees should not be combined with any other payment (such as membership dues). Purchase orders and training requests are not accepted. For

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	195	235
50-year member	No fee	No fee
Unemployed member (Dues waiver required)	No fee	No fee
Precollege teacher	100	100
Graduate student	195	195
Undergraduate	100	100
One-day registrant	195	235
NONMEMBERS		
Chemical scientist	\$685	\$825
Postdoctoral scientist	685	825
Visitor: Nonchemical scientist or chemical technician	390	470
Precollege teacher	100	100
Graduate student	390	390
Undergraduate	195	195
One-day registrant	390	470
Guest of registrant ^a	40	40
EXPOSITION-ONLY VISITORS		
Adult, exposition only	\$50	\$50
Student, exposition only	25	25

^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

wire transfer payments, contact the ACS Finance Department at bankwires@acs.org. **Registration forms received without payment will not be processed.**

REGISTRATION ASSISTANCE. The ACS National Meeting Registration Center will be available from 9:00 AM to 5:00 PM EDT 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: 508-743-9604; 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 by July 17 to guarantee the registrant a full refund less a \$50 administrative fee. Refund requests made after July 17 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 508-743-9604 (save your fax confirmation sheet).

Social Event Ticket Cancellations/Refunds. Social event cancellations received by July 17 entitle the registrant to a full refund. Refund requests made after July 17 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 discounted 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 who are approved by the ACS Office of Communications (restricted to reporters and editors working full-time for print or broadcast news). Press badges may be picked up with valid media credentials from the Press Room at the BCEC. 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 \$50 or \$25 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 Boston. 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. An on-site housing desk will be available during the meeting in the registration area of the Boston Convention & Exhibition Center to assist with last-minute housing changes or needs.

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

Published ACS rates apply to hotel stays between August 12 and 21. To extend your stay beyond these dates, you must reserve additional nights directly through the hotel.

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 for 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.

Make the greener meetings Pledge

www.acs.org/greenermeetings

Each year, ACS holds two National Meetings, attracting over 30,000 chemistry professionals and students to different regions in the US. Through our ACS Greener Meetings Program, we strive to reduce the environmental impacts of our meetings and expositions while enhancing the positive impacts on communities locally and globally.

To accomplish this, we focus on three key initiatives:



- Calculating and offsetting our event carbon footprint (over 5,700 trees planted in collaboration with American Forests)



- Collaborating with convention centers, hotels and other event partners to raise the bar for sustainable practices (we survey and audit over 90% of our hotels)



- Engage with our attendees—that's YOU! (over 1,300 attendees have made the Greener Meetings Pledge. Join them today!)



Learn more and access the
2014 ACS Sustainability Report
<http://www.acs.org/greenermeetings>

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



ACS
Chemistry for Life®

Make the greener meetings Pledge

www.acs.org/greenermeetings

To be a catalyst for positive change!

Here's how:

Go to <http://acs.org/greenermeetings>

Click the "Greener Meetings Pledge" button (upper right sidebar)

Review and pledge to support these 5 simple "green" practices:

1



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.

2



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

3



Use the meeting mobile app and digital program instead of the printed On-site Program.

4



Enjoy the city, burn calories, and reduce your carbon footprint by walking to and from your hotel or using the ACS carbon-offset shuttle service.

5



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

#ACSGreenerMeetings



Share photos of your sustainable choices with your social networks.



Prizes will be awarded.

GENERAL INFORMATION

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 Grand Award for the "Show with the Most Commendable Green Initiatives." Here are a few reasons why: ACS ...

- Seeks sustainable convention center partners (the past three venues, in Dallas, San Francisco, and Denver, were LEED-certified facilities).
- Offsets staff event emissions in partnership with American Forests (1,347 trees planted in 2014) and shuttle emissions in partnership with Transportation Management Services (TMS) and Carbonfund.org.
- Performs on-site walkthroughs for 98% of our hotel room block properties, surveying hotels on more than 40 sustainability practices.
- Designates Sci-Mix as a "zero waste" event. We achieved nearly 100% diversion for our spring meeting in Denver. Help us keep up the great work in Boston!

Take the ACS Greener Meeting Pledge. Facilities are only as effective as the people who operate and occupy them. Go to www.acs.org/greenermeetings, and take the Greener Meeting Pledge to do your part by doing the following:

- Taking advantage of linen reuse initiatives at your hotel, declining delivery of unread newspapers, and turning off the lights when away from your hotel room.
- Responsibly disposing of recyclable materials (paper, plastic, glass, aluminum) in the convention center and hotels.
- Using the meeting mobile app and digital program instead of the printed On-site Program.
- Enjoying the city, burning calories, and reducing your carbon footprint by walking to and from your hotel.
- When walking isn't an option, using the ACS carbon-offset shuttle service.
- Bringing a reusable water bottle to avoid the cost and waste associated with disposable, petroleum-based plastic water bottles.

Be a catalyst for positive change.

Take the ACS Greener Meetings Pledge at www.acs.org/greenermeetings.

Then share photos of your sustainable choices through social networks!
#ACSGreenerMeetings

For more photo fun, prizes, and educational content, visit the Greener Meetings Lounge inside the Exposition, Town Center located at the BCEC, Halls A & B1.

Suggestions? Contact ACS Greener Meetings Team at greenermeetings@acs.org. See you in Boston!

TRAVEL & TRANSPORTATION

TRANSPORTATION DISCOUNTS. ACS has negotiated special travel discounts with the following partners. 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
Discount codes: NMK2Y, NMJTX (international)

Southwest Airlines

swabiz.com
Discount code: 99331750 (effective July 1, for online reservations only)

United Airlines

united.com; 800-426-1122
Discount code: ZT6F413843

Amtrak

amtrak.com; 800-872-7245
Discount code: X02V-918 (for phone reservations only)

RENTAL CARS:

Advantage Rent A Car

advantage.com; 800-777-5500
Discount code: CD02C826E8

Avis

avis.com; 800-331-1600
Discount code: B923099

Hertz

hertz.com; 800-654-2240
Discount code: CV#02UZ0014

AIRPORT GROUND TRANSPORTATION

Boston's convention centers are close to major transportation systems and feature the fastest airport-to-convention center times in the country.

Round-trip shuttle from Back Bay to Logan Airport.

Shuttle service runs every 20 minutes and picks up passengers from Logan International Airport. The cost is \$5.00 one way, credit or debit card only (or free with valid MBTA pass). See more at <http://goo.gl/cJy1Ht>.

Taxis. Taxi service is available from Logan International Airport to downtown. Approximate fare to a downtown destination is about \$25-\$45. Average time is about 15-20 minutes. Fares are based on current MBTA fare prices. Price and time estimations are based on online quotes for one-way, single-rider fares in taxis. Cost estimations for taxis do not include gratuity or tolls. Travel times are estimated for all modes based on common conditions.

SuperShuttle. ACS has established a 10% discount for attendees of our meeting. Take advantage of these 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. Offer good at all airports except Boston Logan & Back Bay airports.

TRAVELING TO MEETING VENUES

The Boston Convention & Exhibition Center (BCEC) is located at 415 Summer St., Boston, MA 02210.

ACS Shuttle. Complimentary shuttle service will be provided between the Boston Convention & Exhibition Center and official ACS hotels, with the exception of hotels within walking distance.

Parking. Valet parking is available during most events for \$25. From Summer Street, turn onto East Side Drive and the valet area will be immediately on your right. Cash and all major credit cards are accepted.

South Parking Lot. (\$15, \$30 for oversized vehicles) From Summer Street, turn onto East Side Drive, drive past the valet area, and continue straight along the side of the building. At the end of the building, make a right and go down

GENERAL INFORMATION

the ramp. At the bottom of the ramp, turn left and you will see the entrance to the South Parking Lot in front of you.

Alternate Parking. In the event that on-site parking has reached capacity, additional parking may be available at either the Boston Marine Industrial Park (BMIP) or lots on the Waterfront. All alternate parking lots are on a first-come, first-served basis and are within walking distance of the BCEC.

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 the North Lobby, near attendee registration in the Boston Convention & Exhibition Center and is open Saturday, August 15, 3:00 to 6:00 PM; Sunday, August 16, 7:30 AM to 7:30 PM; Monday, August 17, 7:30 AM to 9:00 PM; Tuesday, August 18, 7:30 AM to 5:00 PM; Wednesday, August 19, 7:30 AM to 4:00 PM; and Thursday, August 20, 7:30 AM to 1:00 PM.

ONLINE SOCIAL NETWORKING TOOLS.

Start discussions and connect with other attendees at the ACS Network and the ACS Facebook page. Follow ACS national meetings on Twitter. Read, comment on, and share C&EN's coverage of ACS meetings.

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 FedEx Office Print & Ship Center in the Boston Convention & Exhibition Center offers you nearly everything you need to meet your convention and exhibiting needs, including packing and shipping, signage, copying, and last-minute office supplies. Located on Concourse Level 1 near

Exhibit Hall A, the business center will be open to attendees Monday through Sunday, 9:00 AM to 5:00 PM.

MEMBER INSURANCE PROGRAM. ACS ACS, Booth No. 625. The ACS Member Insurance Program is committed to offering quality comprehensive insurance plans and financial security programs to members and their families. Stop by the Member Insurance Station to learn about Life & Health Insurance, International Term Life, Auto & Homeowners Plus, Disability Income, Long-Term Care, Medicare Supplement, Medical Discount Cards, Pet Insurance, Professional Liability, and more. Also learn about our newest offering: Educators' Legal Liability. Stop by the booth to learn more about this policy designed exclusively for ACS academic chemists. The ACS Member Insurance Program offers coverage and policies for every stage of life, from being a student in college, to raising a family, to enjoying retired life—and everything in between! To learn more about the plans available to you, visit www.acs.org/insurance.

ON-SITE MEETING ARRANGEMENTS

ADA-COMPLIANT MEETING. The Boston Convention & Exhibition Center (BCEC) 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 www.massconvention.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 June 29 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 greeters will be positioned throughout the meeting and can help you navigate the On-site Program, find a particular session or room, and answer questions. Lost-and-found items at the convention center should be directed to the ACS Operations Office located in Room 151A. 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/boston2015. Use the Meeting Mail terminals located in the BCEC. Telephone messages left at the ACS Information Booths will be conveyed to attendees via the electronic message center, but the society 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, August 16, through Thursday, August 20. 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. Visit the ACS Operations Office at the BCEC, room 151A to register your child. For your child's safety, the location

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of Camp ACS will not be communicated until your registration is confirmed. On-site registration will be accepted on a space-available basis.

ELECTRONIC DEVICES. As a courtesy to other meeting attendees, electronic devices must be operated in silent/vibrate mode within 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.

TIPS FOR A SAFE STAY IN BOSTON

- 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.

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 Northeastern 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 BCEC, North Lobby.

INTERNATIONAL REGISTRANTS. Many international visitors are required to hold a visa prior to being admitted to the U.S. because of security measures in place at airports and other border crossings. 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/boston2015.

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 BCEC.

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 opportuni-

THANK YOU

The society thanks the many volunteers of the Northeastern local section who are contributing to the 250th 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.

ties. No one is authorized to place any promotional items in public meeting space except the ACS Operations Office 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.

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

MEETING OFFICES. The following ACS offices will be located in the BCEC:

Attendee Registration: North Lobby

Career Fair: Hall B2

Exhibitor Registration: North Lobby

Exposition: Halls A & B1

Finance Office: Westin Boston Waterfront, Frost Boardroom

Host Local Section Center: North Lobby

Member Services: North Lobby

Press Center: 153B

Shuttle Desk: East Side Drive

The following offices are located at the identified properties:

Operations Offices: BCEC, Boston Marriott Copley Place, Boston Park Plaza Hotel & Towers, Renaissance Boston Waterfront, Seaport Hotel and World Trade Center, Sheraton Boston Hotel, Westin Boston Waterfront, Westin Copley Place.

Governance Office: Sheraton Boston Hotel

Society Programs: Sheraton Boston Hotel

MOTHERS ROOM. For your convenience and privacy, ACS will provide a room for nursing mothers at the BCEC. Please see the Operations Office, Room 151A, for access to the room.

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

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

Introduce new products and services

Highlight innovative applications for existing instrumentation

Build skills with specific tools and techniques

Please visit www.acs.org/boston2015 to register for their workshops.

Highlights

Exposition, BCEC, Halls A & B1

- Sunday, 6 – 8:30 PM
- Monday & Tuesday, 9AM – 5 PM

- Join us on Sunday from 6 – 8:30 PM for our 250th Celebration
- Meet the ACS president-elect candidates inside the exposition on Monday, from 1 – 4 PM
- Visit the Daily Prize Booth 255 Sunday through Tuesday for a chance to win a prize!

Monday, August 17

Cyber Security Awareness: How to Protect Yourself and Your Small Business

Sponsor: ACS Member Insurance Program, 9:30 AM – Noon
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 1

Designing a Distance Learning Lab Curriculum for Chemistry

Sponsor: Carolina Biological Supply Co., 9:30 AM – Noon
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 2

SciFinder Training

Sponsor: CAS, 12:30 PM – 3:00 PM
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 1

Origin 2015 User Group Meeting and Product Demo

Sponsor: OriginLab Corp. 3:30 PM – 6:00 PM
BCEC, Room 101

Tuesday, August 18

SciFinder Training

Sponsor: CAS, 9:30 AM – Noon
BCEC, Room 258B

What's New from Waters

Sponsor: Waters Corporation, 9:30 AM – Noon
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 2

The State-Of-The-Art In Infrared and Raman Analysis

Sponsor: Bruker, 12:30 PM – 3:00 PM
BCEC, Room 258B

CDD Vision Workshop

Sponsor: Collaborative Drug Discovery, 9:30 AM – Noon
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 1

FTIR, Atomic Spectroscopy, HPLC, GC, and Mass Spectrometry

Sponsor: Agilent Technologies, 9:30 AM – 6:00 PM
BCEC, Room 101

Research in Germany Science Lunch

Sponsor: Research In Germany, 12:30 PM – 3:00 PM
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 1

Wednesday, August 19

Nanomaterials Analysis by X-ray Scattering Methods

Sponsor: PANalytical, 12:30 PM – Noon
BCEC, Room 101

Inhibitor Design Using MOE Structure-Based Drug Design Applications

Sponsor: Chemical Computing Group, 3:30 PM – 6:00 PM
BCEC, Room 101

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

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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 Boston. ACS encourages its members to get active in governance at all levels in order to contribute their vision to the direction of the Society. You can share ideas and insights into the Society and the chemical profession, network with peers, and catch up with friends through these volunteer connections. With nearly thirty national governance committees and leadership opportunities in technical divisions and local sections to choose from, there are many opportunities for members to

become actively involved in ACS at the national level. If you are an ACS member interested in volunteering for a governance committee, contact the Office of the Secretary by email at secretary@acs.org 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, August 19, at the Sheraton Boston Hotel. 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.



Boston skyline. SHUTTERSTOCK.COM

GOVERNANCE MEETINGS

For the complete list of committee meetings and agendas, please consult www.acs.org/boston2015 or the on-site program distributed during the meeting.

BOARD & COUNCIL MEETINGS

ACS BOARD OF DIRECTORS. The ACS Board of Directors meeting, open to members who wish to participate, will be held in the Boston Convention & Exhibition Center from noon to 1:00 PM on Sunday, August 16. The guest speaker will be George Whitesides, the Woodford L. & Ann A. Flowers University Professor at Harvard University.

ACS COUNCIL. The ACS Council meeting will begin at 8:00 AM, Wednesday, August 19, at the Sheraton Boston Hotel. 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, August 18, 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/boston2015 or the on-site program distributed during the meeting.

COUNCILOR CAUCUS MEETINGS

District I Councilor Caucus

Sunday, August 16, 6:00 – 7:00 PM
Sheraton Boston
Berkeley A/B

District II Councilor Caucus

Sunday, August 16, 6:00 – 7:00 PM
Sheraton Boston
Fairfax A

Middle Atlantic Councilor Caucus

Sunday, August 16, 6:00 – 7:00 PM
Sheraton Boston
Republic B

District IV Councilor Caucus

Sunday, August 16, 6:00 – 7:00 PM
Sheraton Boston
Fairfax B

District V Councilor Caucus

Sunday, August 16, 6:00 – 7:00 PM
Sheraton Boston
Hampton A/B

District VI Councilor Caucus

Sunday, August 16, 6:00 – 7:00 PM
Sheraton Boston
Republic A

Division Officers/Councilors Caucus

Tuesday, August 18, 4:00 – 6:00 PM
Boston Convention & Exhibition Center
Room 107A

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, August 15, 8:00 to 10:30 AM
Sheraton Boston, Constitution A

1. Report of the Chair
2. Report of the Treasurer & CFO:
 - a. 2015 Probable Financial Performance
3. Reports from the B&F Subcommittees:
 - a. Communications
 - b. Program Funding Requests
 - c. Program Review
 - d. Financial Impacts of Constitution & Bylaw Amendments

CHEMICAL SAFETY

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

Combined Open Meeting and Executive Session

Monday, August 17, 8:30 to 11:30 AM
Sheraton Boston, Back Bay C

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

GOVERNANCE & BUSINESS MEETINGS

CHEMISTRY & PUBLIC AFFAIRS

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

Open Meeting

Saturday, August 15, 3:00 to 4:30 PM

Sheraton Boston, Republic B

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

CHEMISTS WITH DISABILITIES

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

Combined Open Meeting and Executive Session

Sunday, August 16, 8:30 AM to 4:30 PM

Sheraton Boston, Commonwealth

1. Welcome
2. Chair Report
 - a. Update of CWD Activities/Events, and Collaborative Opportunities
 - b. Diversity & Inclusion Advisory Group Report
 - c. Strategic Planning Retreat Report and Follow-Up
 - d. Minutes from (Denver, 2015)
3. CWD 35th Anniversary/ADA 25th Anniversary Celebration
4. Ratification of the UN Human Rights for Persons with Disabilities Treaty
5. Staff Report
6. Future Event and Programming Planning
7. Subcommittee Progress Reports
8. Reports of Liaisons to/from other committees
9. Ongoing Business
10. New Business

COMMITTEES

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

Open Session

Monday, August 17, 1:30 to 2:15 PM

Sheraton Boston, Back Bay D

1. Welcome
2. Minutes of March 23-24, 2015
3. Reports of chair/staff liaison
4. Reports of Subcommittees and Task Forces on:
 - a. Diversity
 - b. Leadership Development
 - c. Streamlining the Committee Performance Review Process
5. Topics from floor

COMMUNITY ACTIVITIES

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

Open Executive Session

Sunday, August 16, 7:45 AM to noon

Boston Marriott Copley Place, Tremont

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

CCA/LSAC Joint Open Meeting

Tuesday, August 18, 2:00 to 3:30 PM

Boston Marrior Copley Place, Salon H-J

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

CONSTITUTION & BYLAWS

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

Open Meeting

Sunday, August 16, 1:15 to 1:45 PM

Sheraton Boston, Berkeley A/B

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

Executive Session

Sunday, August 16, 9:00 AM to noon and 1:45 to 4:30 PM

Sheraton Boston, Berkeley A/B

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, August 17, 8:00 AM to noon

Sheraton Boston, Republic A

1. Welcome
2. Approval of Minutes
3. Chair's Report
4. Reports from Subcommittee Chairs
 - a. Strategic Investment and Awards
 - b. Grants and Awards
 - c. Public Policy
 - d. CA Relations
 - e. Industry Insights
 - f. CA Member benefits
5. Staff liaison report

COUNCIL POLICY

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

Open Meeting

Tuesday, August 18, 9:30 AM to noon

Sheraton Boston, Back Bay C

1. Committee and Officer Reports
2. Report of CPC vice chair
3. Reports of Subcommittees on:
 - a. Petitions, Constitution & Bylaws
 - b. Long Range Planning
4. Reports of Task Force on Councilor and member duties and conduct
5. Schedule of business sessions, spring 2016
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, August 16, 8:00 AM to noon

Boston Marriott Copley Place, Simmons

1. Welcome
2. Review Boston Agenda
3. Minutes from 249th ACS National Meeting in Denver, CO
4. DAC Chair Report
5. Subcommittee Reports

ECONOMIC & PROFESSIONAL AFFAIRS

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

Executive Session

Saturday, August 15, 8:00 AM to 3:30 PM

Boston Marriott Copley Place, Salon A/B

1. Opening Remarks/Introductions
2. Subcommittee Meetings
3. Staff Reports

Open Executive Session

Saturday, August 15, 3:30 to 5:30 PM

Boston Marriott Copley Place, Salon A/B

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

EDUCATION

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

Open Meeting

Monday, August 17, 3:00 to 4:00 PM

Sheraton Boston, Berkeley A/B

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

Executive Session

Friday, August 14, 1:00 to 5:30 PM

Sheraton Boston

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

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

ENVIRONMENTAL IMPROVEMENT

Laura Pence, chair; lpence@hartford.edu

Open Executive Session

Saturday, August 15, 4:00 to 6:00 PM

Sheraton Boston, Back Bay A

1. Chair's report and review of interim actions
2. Subcommittee on Public Policy
3. Subcommittee on Sustainability
4. Staff reports from OPA and GCI
5. Reports of other working groups and liaisons
6. Committee business
7. Open discussion

ETHICS

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

Open Executive Session

Sunday, August 16, 9:00 AM to 4:30 PM

Sheraton Boston, Liberty A/B

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

GOVERNANCE & BUSINESS MEETINGS

- 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, August 15, 1:00 to 3:00 PM
Sheraton Boston, Independence West

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; Univ. of Wisconsin-Fox Valley, Chemistry/Dean's Office, 1478 Midway Rd, Menasha, WI 54952-1224; martin.rudd@uwv.edu

LSAC/CCA Joint Open Meeting

Tuesday, August 18, 2:00 to 3:30 PM
Boston Marriott Copley Place, Salon H-J

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

Open Executive Session

Sunday, August 16, 8:00 AM to noon

Boston Marriott Copley Place

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, August 16, 7:00 AM to noon

Boston Marriott Copley Place, Salon B-D

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

MEMBERSHIP AFFAIRS

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

Executive Session

Sunday, August 16, 8:00 AM to 4:00 PM

Sheraton Boston, Back Bay A/B

1. Welcome
2. Minutes of March 21-22, 2015 meeting
3. Reports of Chair and Staff Liaison
4. Reports of Subcommittees:
 - a. Categories & Dues
 - b. Recruitment & Admissions
 - c. Retention, Benefits & Services

Open Meeting

Monday, August 17, 1:00 to 2:00 PM

Sheraton Boston, Liberty A/B

1. Update of MAC activities
2. Topics, questions and concerns from the floor

MINORITY AFFAIRS

Madeleine Jacobs, chair; madeleine.s.jacobs@gmail.com

Closed Executive Session

Sunday, August 16, 8:00 AM to 12:30 PM

Sheraton Boston, Republic B

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

Open Session

Sunday, August 16, 12:30 to 2:00 PM

Sheraton Boston, Republic B

1. Subcommittee Reports
2. Old Business
3. New Business
4. Open Discussion
5. Wrap-Up and Process Check

NOMENCLATURE, TERMINOLOGY & SYMBOLS

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

Open Meeting

Monday, August 17, 2:00 to 5:00 PM

Sheraton Boston, Dalton A

1. Review Denver minutes, March national meeting
2. Chair/Staff Liaison reports
3. Subcommittee Reports
 - a. Communication/Outreach
 - b. Education
 - c. Liaison
 - d. Long Range Planning
4. IUPAC Reports
5. Update to Kilogram, Amount of Substance and Mole issues
6. Task Force on new SI definitions
7. New Business

NOMINATIONS & ELECTIONS

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

Open Executive Session

Monday, August 17, 11:00 AM to noon

Sheraton Boston, Independence East

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

PATENTS & RELATED MATTERS

Sadiq Shah, chair; sadiq@utpa.edu

Open Meeting

Saturday, August 15, 9:00 AM to 5:00 PM

Sheraton Boston, Back Bay D

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, August 16, 4:00 to 5:00 PM

Boston Convention & Exhibition Center, Room 211

1. Implementation of 2015 ACS Guidelines
2. Macromolecules/Materials Requirement
3. Supplements to the ACS Guidelines
4. Planning for Graduate Work in the Chemical Sciences
5. PhD Recipient Survey Results

6. Topics from floor

PROJECT SEED

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

Open Meeting

Sunday, August 16, 8:00 to 9:00 AM

Sheraton Boston, Fairfax B

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

Closed Executive Session

Saturday, August 15, 10:30 AM to 5:00 PM

Sheraton Boston, Berkeley A/B

1. Subcommittee meetings 10:30 AM - 12:00 Noon
2. Minutes of March 21, 2015
3. Reports of Chair/Staff Liaison
4. Report of Subcommittees:
5. Old and new business

PUBLIC RELATIONS & COMMUNICATIONS

David S. Gottfried, chair; Institute for Electronics & Nanotechnology, Georgia Tech, dsgett@gatech.edu

Open Executive Session

Tuesday, August 18, 8:00 AM to 1:00 PM

Sheraton Boston, Constitution B

1. Welcome and Chair's Remarks
2. Approval of Minutes of March 1-2, 2015 Meeting
3. Subcommittee Reports:
 - a. Chemistry Ambassadors
 - b. Awards
 - c. Technology
4. Liaison Reports—CCPA, LSAC, CCA, IAC
5. Old Business
6. New Business
7. Helen Free Award Address

PUBLICATIONS

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

Open Meeting

Friday, August 14, 4:30 to 5:00 PM

Sheraton Boston, Republic A/B

1. Updates from ACS Publications Division
2. Open Discussion

Executive Session

Friday, August 14, 1:00 to 5:00 PM (Closed Executive Session until 4:30 PM)

Sheraton Boston, Republic A/B

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

SCIENCE

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

Open Meeting

Saturday, August 15, 8:30 AM to 4:30 PM

Sheraton Boston, Back Bay B

1. Welcome
2. Approval of Minutes

GOVERNANCE & BUSINESS MEETINGS

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, August 17, 8:00 AM to noon

Sheraton Boston, Back Bay B

1. Welcome & Introductions
2. Discussion and approval of Denver Meeting Minutes
3. Reports of Chair & Staff Liaison
4. Subcommittee Reports
 - a. Newsletter – June 2015
 - b. National Meeting Programming
 1. Boston
 2. San Diego
 - c. Senior Activities in Local Sections
 1. Mini Grant Awards
 2. ChemLuminary Awards
 - d. Consulting & Mentoring
 1. Undergraduate Speed Networking Event
 - e. Planning and Priorities
 1. SCC Fall Strategic Planning Retreat
5. Old Business
 - a. Senior Chemists Breakfast
6. New Business
7. Adjournment

TECHNICIAN AFFAIRS

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

Closed Executive Session

Sunday, August 16, 8:30 AM to 2:00 PM

Sheraton Boston, Independence West

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

Open Session

Sunday, August 16, 2:00 to 2:30 PM

Sheraton Boston, Independence West

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

WOMEN CHEMISTS

Amber Charlebois, chair; Fairleigh Dickinson University, Madison, NJ 07940, afcharleb@gmail.com

Executive Session

Saturday, August 15, 8:00 AM to 5:00 PM

Sheraton Boston, Fairfax A/B

1. Welcome
2. Review of Action Items and Minutes
3. Reports of Chair and Staff Liaison

4. Subcommittee Meetings and Reports
5. Committee Liaison Reports
6. New Business & Special Discussion Topics

WCC Open Meeting & Just Cocktails Reception

Tuesday, August 18, 4:00 to 5:00 PM

Sheraton Boston Hotel

YOUNGER CHEMISTS

Douglas B. Hausner, chair; doug.hausner@gmail.com

Open Session

Sunday, August 16, 8:00 AM to noon

Sheraton Boston Hotel, Back Bay 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
8. Adjourn

DIVISION MEETINGS & SOCIAL EVENTS

Division of Agricultural & Food Chemistry — AGFD

Special Committee Meeting - Awards	Sunday, August 16	12:00 PM - 1:00 PM	Room 102A, BCEC
Executive Committee Meeting	Sunday, August 16	5:00 PM - 8:00 PM	Room 158, BCEC
Future Programs Planning Meeting	Monday, August 17	12:00 PM - 1:00 PM	Room 211, BCEC
Business Meeting	Tuesday, August 18	12:00 PM - 1:00 PM	Room 211, BCEC

Division of Agrochemicals — AGRO

Social/ Posters (AM Sessions)	Sunday, August 16	10:00 AM - 10:45 AM	Terrace Room, Boston Park Plaza
Social/Posters (PM Sessions)	Sunday, August 16	3:00 PM - 3:45 PM	Terrace Room, Boston Park Plaza
General Posters	Sunday, August 16	1:00 PM - 5:00 PM	Terrace Room, Boston Park Plaza
Business Meeting	Sunday, August 16	5:00 PM - 9:00 PM	Imperial Blrm, Boston Park Plaza
Social/Posters (AM Sessions)	Monday, August 17	10:00 AM - 10:45 AM	Terrace Room, Boston Park Plaza
General Posters	Monday, August 17	8:00 AM - 10:00 AM	Terrace Room, Boston Park Plaza
Graduate Student Luncheon	Monday, August 17	12:00 PM - 1:20 PM	Boylston Room, Boston Park Plaza
General Posters	Monday, August 17	1:00 PM - 5:00 PM	Terrace Room, Boston Park Plaza
Social/Posters (PM Sessions)	Monday, August 17	3:00 PM - 3:45 PM	Terrace Room, Boston Park Plaza
General Posters	Tuesday, August 18	8:00 AM - 10:00 AM	Terrace Room, Boston Park Plaza
Social/Posters (AM Sessions)	Tuesday, August 18	8:00 AM - 10:00 AM	Terrace Room, Boston Park Plaza
USDA-ARS Sterling B. Hendricks Reception	Tuesday, August 18	1:00 PM - 1:30 PM	Boylston Room, Boston Park Plaza
General Posters	Wednesday, August 19	8:00 AM - 10:00 AM	Terrace Room, Boston Park Plaza
Blues-N-Brews	Wednesday, August 19	5:15 PM - 7:00 PM	Boylston Room, Boston Park Plaza
Social/Posters (AM Sessions)	Wednesday, August 19	10:00 AM - 10:45 AM	Terrace Room, Boston Park Plaza
Social/Posters (PM Sessions)	Wednesday, August 19	3:00 PM - 3:45 PM	Terrace Room, Boston Park Plaza
Awards Social	Wednesday, August 19	6:00 PM - 8:00 PM	Boylston Room, Boston Park Plaza

Division of Analytic Chemistry — ANYL

Long Range Planning Meeting (Closed Meeting)	Friday, August 14	6:00 PM - 10:00 PM	Atlantic Blrm 3, Renaissance Boston Waterfront
Long Range Planning Meeting (Closed Meeting)	Saturday, August 15	9:00 AM - 5:00 PM	Atlantic Blrm 3, Renaissance Boston Waterfront
General Analytical Posters	Sunday, August 16	6:00 PM - 8:00 PM	Room 52 A/B, BCEC
Executive Committee Meeting	Monday, August 17	4:00 PM - 7:00 PM	Spectacle Room, Renaissance Boston Waterfront
Analytical Division Dinner (Ticketed Event)	Tuesday, August 18	6:00 PM - 9:00 PM	Joe's American - Waterfront

Division of Biological Chemistry — BIOL

Poster Session	Sunday, August 16	5:30 PM - 7:30 PM	Cityview Blrm, Seaport Hotel & World Trade Center
Poster Session	Tuesday, August 18	6:00 PM - 8:00 PM	Galleria, Westin Boston Waterfront

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

GOVERNANCE & BUSINESS MEETINGS

Division of Business Development & Management — BMGT

Annual Open Meeting	Tuesday, August 18	10:00 AM - 11:00 AM	Pacific Blrm C, Renaissance Boston Waterfront
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Division of Catalysis and Surface Science — CATL

Business Meeting	Monday, August 17	5:00 PM - 7:00 PM	Pacific Blrm A, Renaissance Boston Waterfront
Catalysis Poster Session	Monday, August 17	6:00 PM - 8:00 PM	Galleria, Westin Boston Waterfront

Division of Chemistry and Law — CHAL

Drug & Power Luncheon (Ticketed Event)	Monday, August 17	12:00 PM - 1:30 PM	Room 52B, BCEC
CHAL Reception	Monday, August 17	5:00 PM - 8:00 PM	Room 152, BCEC

Division of Chemical Health & Safety — CHAS

Laboratory Safety Workshop A N	Friday, August 14	8:00 AM - 5:00 PM	Room 157A, BCEC E D
Laboratory Waste Management Workshop	Friday, August 14	8:00 AM - 5:00 PM	Room 157B, BCEC
Reactive Chemical Management N	Saturday, August 15	8:00 AM - 5:00 PM	Room 157B, BCEC E D
Hazard Analysis Workshop	Saturday, August 15	8:00 AM - 5:00 PM	Room 157A, BCEC
How to be a More Effective Chemical Hygiene Officer Workshop	Saturday, August 15	8:00 AM - 5:00 PM	Room 157C, BCEC
Executive Committee Meeting	Sunday, August 16	7:15 AM - 11:30 AM	Seaport Blrm A, Seaport Hotel & World Trade Center

Division of Chemical Education — CHED

Exams Institute Board of Trustees Meeting	Saturday, August 15	7:30 AM - 12:00 PM	Room 160B, BCEC
JCE Board of Publication Meeting	Saturday, August 15	8:00 AM - 12:30 PM	Room 160A, BCEC
High School Chemistry Committee Meeting	Saturday, August 15	8:00 AM - 10:00 AM	Room 159, BCEC
Program Committee Meeting	Saturday, August 15	10:30 AM - 12:00 PM	Room 159, BCEC
Executive Committee Meeting	Saturday, August 15	1:00 PM - 5:30 PM	Room 160C, BCEC
Biennial Conference on Chemical Education Committee Meeting	Saturday, August 15	4:00 PM - 6:00 PM	Room 160B, BCEC
Chemical Education Research Committee Meeting	Sunday, August 16	7:00 AM - 9:00 AM	Cambridge 2 Room, Seaport Hotel & World Trade Center
International Activities Committee Meeting	Sunday, August 16	8:00 AM - 9:30 AM	Cambridge 1 Room, Seaport Hotel & World Trade Center
Finance Committee Meeting	Sunday, August 16	9:30 AM - 11:30 PM	Beacon Hill 1, Seaport Hotel & World Trade Center
High School/College Interface Luncheon (Ticketed Event)	Sunday, August 16	12:00 PM - 1:00 PM	Room 253C, BCEC
Regional Meeting Committee Meeting	Sunday, August 16	12:00 PM - 2:00 PM	Cambridge 2 Room, Seaport Hotel & World Trade Center
Long Range Planning Committee Meeting	Sunday, August 16	2:30 PM - 4:30 PM	Beacon Hill 1, Seaport Hotel & World Trade Center
Younger Chemists Education Scholars Committee Meeting	Sunday, August, 16	3:30 PM - 5:00 PM	Cambridge 2 Room, Seaport Hotel & World Trade Center
Safety Committee	Sunday, August 16	4:00 PM - 5:50 PM	Cambridge 1 Room, Seaport Hotel & World Trade Center
Social Reception	Sunday, August 16	5:30 PM - 7:00 PM	Room 51, BCEC
Green Chemistry Commitment Luncheon	Monday, August 17	12:00 PM - 1:30 PM	Room 258A, BCEC
New Member Committee Meeting	Monday, August 17	12:30 PM - 1:00 PM	Cambridge 1 Room, Seaport Hotel & World Trade Center
General Posters	Monday, August 17	2:00 PM - 4:00 PM	Hall C, BCEC

GOVERNANCE & BUSINESS MEETINGS

Division of Chemical Information— CINF

Education Committee Meeting (Closed Meeting)	Saturday, August 15	1:00 PM - 3:00 PM	Room 107C, BCEC
Program Committee Meeting (Closed Meeting)	Saturday, August 15	1:00 PM - 3:00 PM	Room 108, BCEC
Awards Committee Meeting (Closed Meeting)	Saturday, August 15	1:00 PM - 3:00 PM	Room 109A, BCEC
Executive Meeting (Closed Meeting)	Saturday, August 15	3:00 PM - 6:00 PM	Room 107B, BCEC
Chemical Structure Association Trust (CSAT) Meeting	Sunday, August 16	12:00 PM - 2:00 PM	Adams Room, Westin Boston Waterfront
Welcoming Reception & Poster Session	Sunday, August 16	6:30 PM - 8:30 PM	Lighthouse 1, Seaport Hotel & World Trade Center
Division Luncheon (Ticketed Event)	Tuesday, August 18	12:00 PM - 1:30 PM	Room 52A, BCEC
Herman Skolnik Award Reception Honoring Dr. Jurgen Bajorath	Tuesday, August 18	6:30 PM - 8:30 PM	Room 254A, BCEC

Division of Colloid & Surface Chemistry— COLL

Program/Executive Committee Meeting	Saturday, August 15	5:00 PM - 7:00 PM	Room 151B, BCEC
Social Hour/Open Business/Poster Session	Sunday, August 16	5:30 PM - 8:00 PM	Galleria, Westin Boston Waterfront
Luncheon (Ticketed Event)	Tuesday, August 18	12:00 PM - 1:30 PM	Stone Room, Westin Boston Waterfront

Division of Computers in Chemistry— COMP

Executive & Program Meeting	Saturday, August 15	3:00 PM - 6:00 PM	Commonwealth A Room, Westin Boston Waterfront
Poster Session	Tuesday, August 18	6:00 PM - 8:00 PM	Galleria, Westin Boston Waterfront

Division of Energy & Fuel— ENFL

Program Meeting	Sunday, August 16	12:00 PM - 2:00 PM	Room 102B, BCEC
Business Meeting	Monday, August 17	5:00 PM - 8:00 PM	Room 158, BCEC
Division Dinner (Ticketed Event)	Tuesday, August 18	6:30 PM - 9:30 PM	Morton's Steak House

Division of Environmental Chemistry— ENVR

Program Planning Committee Meeting	Sunday, August 16	2:00 PM - 3:00 PM	Brookline Room, Boston Park Plaza
Long Range Planning Committee Meeting	Sunday, August 16	3:00 PM - 5:00 PM	Brookline Room, Boston Park Plaza
Business Meeting	Sunday, August 16	7:00 PM - 7:30 PM	Boylston Room, Boston Park Plaza
Executive Committee Meeting	Sunday, August 16	7:30 PM - 10:00 PM	Boylston Room, Boston Park Plaza
Social & Reception (Ticketed Event)	Tuesday, August 18	6:00 PM - 7:30 PM	Back Bay Harry's
Division Dinner (Ticketed Event)	Tuesday, August 18	8:00 PM - 10:00 PM	Back Bay Harry's
General Posters	Wednesday, August 19	6:00 PM - 8:00 PM	Hall C, BCEC

Division of Geochemistry— GEOC

Executive Committee Meeting (Closed Meeting)	Sunday, August 16	6:00 PM - 8:00 PM	Beacon Hill 1, Seaport Hotel & World Trade Center
Division Reception	Tuesday, August 18	5:30 PM - 7:30 PM	Flagship A, Seaport Hotel & World Trade Center

GOVERNANCE & BUSINESS MEETINGS

Division of Industrial & Engineering Chemistry— I&EC

Executive Committee Meeting (Closed Meeting)	Sunday, August 16	2:30 PM - 6:00 PM	Pacific Blrm E, Renaissance Boston Waterfront
I&EC Graduate Symposia Luncheon (Ticketed Event)	Tuesday, August 18	11:45 AM - 12:45 PM	Mediterranean, Renaissance Boston Waterfront
General Posters Session	Tuesday, August 18	6:00 PM - 8:00 PM	Hall C, BCEC

Division of Medicinal Chemistry— MEDI

Executive Meeting (Closed Meeting)	Sunday, August 16	8:30 AM - 1:00 PM	Room 151B, BCEC
LRPC Meeting (Closed Meeting)	Monday, August 17	5:30 PM - 9:30 PM	Room 253A, BCEC
Hall of Fame Ceremony	Tuesday, August 18	5:30 PM - 7:30 PM	Room 52A/B, BCEC
General Poster Session	Sunday, August 16	7:00 PM - 9:00 PM	Galleria, Westin Boston Waterfront
Joint MEDI/ORGN Poster Session	Wednesday, August 19	7:00 PM - 9:00 PM	Ballroom, BCEC

Division of Nuclear Chemistry & Technology— NUCL

Executive Committee Meeting	Sunday, August 16	5:00 PM - 7:00 PM	Constitution, Seaport Hotel & World Trade Center
Business Meeting	Tuesday, August 18	5:00 PM - 6:00 PM	Waterfront 2, Seaport Hotel & World Trade Center
Social Hour	Tuesday, August 18	6:00 PM - 8:00 PM	Cityview 1, Seaport Hotel & World Trade Center

Division of Organic Chemistry— ORGN

Executive Committee Meeting (Closed Meeting)	Sunday, August 16	1:00 PM - 5:00 PM	Seaport Blrm A, Seaport Hotel & World Trade Center
Poster Session	Sunday, August 16	8:00 PM - 10:00 PM	Hall C, BCEC
Poster Session	Tuesday, August 18	8:00 PM - 10:00 PM	Hall C, BCEC
Joint MEDI/ORGN Poster Session	Wednesday, August 19	7:00 PM - 9:00 PM	Ballroom, BCEC

Division of Physical Science— PHYS

Workshop for Undergraduates	Sunday, August 16	8:00 AM - 12:30 PM	Room 254A, BCEC
Poster Session	Wednesday, August 19	6:00 PM - 8:00 PM	Hall C, BCEC

Division of Polymeric Materials Science & Engineering— PMSE

Membership Desk	Sunday, August 16	8:00 AM - 5:00 PM	Mezz Foyer, Westin Boston Waterfront
Membership Desk	Monday, August 17	8:00 AM - 5:00 PM	Mezz Foyer, Westin Boston Waterfront
Membership Desk	Tuesday, August 18	8:00 AM - 5:00 PM	Mezz Foyer, Westin Boston Waterfront
Business Meeting & PMSE/POLY Coordinatiuon Meeting	Tuesday, August 18	5:00 PM - 6:00 PM	Douglas Room, Westin Boston Waterfront
PMSE/POLY Poster Session	Tuesday, August 18	6:00 PM - 8:00 PM	Ballroom West, BCEC
Membership Desk	Wednesday, August 19	8:00 AM - 5:00 PM	Mezz Foyer, Westin Boston Waterfront
PMSE/POLY Award Lecture Reception	Wednesday, August 19	6:00 PM - 9:00 PM	Grand Blrm A/B, Westin Boston Waterfront
Membership Desk	Thursday, August 20	8:00 AM - 5:00 PM	Mezz Foyer, Westin Boston Waterfront

GOVERNANCE & BUSINESS MEETINGS

Division of Polymer Chemistry— POLY

Board Meeting	Sunday, August 16	12:00 PM - 2:00 PM	Harbor Blrm 1, Westing Boston Waterfront
Membership Desk	Sunday, August 16	9:00 AM - 5:00 PM	Elm 1, Westin Boston Waterfront
Membership Desk	Monday, August 17	9:00 AM - 5:00 PM	Elm 1, Westin Boston Waterfront
Membership Desk	Tuesday, August 18	9:00 AM - 5:00 PM	Elm 1, Westin Boston Waterfront
Programming Meeting	Tuesday, August 18	12:00 PM - 2:00 PM	Harbor Blrm 1, Westing Boston Waterfront
POLY/PMSE Poster Session	Tuesday, August 18	6:00 PM - 8:00 PM	Ballroom West, BCEC
Membership Desk	Wednesday, August 19	9:00 AM - 5:00 PM	Elm 1, Westin Boston Waterfront
POLY/PMSE Award Lecture Reception	Wednesday, August 19	6:00 PM - 9:00 PM	Grand Blrm A/B, Westin Boston Waterfront
Membership Desk	Thursday, August 20	9:00 AM - 5:00 PM	Elm 1, Westin Boston Waterfront

Division of Professional Relations— PROF

Professional Relations - Executive Committee & Open Meeting	Tuesday, August 18	2:00 PM - 4:00 PM	Room 157C, BCEC
Henry Hill's 100th Anniversary Reception & Award Program	Tuesday, August 18	5:00 PM - 7:00 PM	Plaza Blrm AB, Seaport Hotel & World Trade Center

Division of Small Chemical Business— SCHB

Member Breakfast	Sunday, August 16	7:00 AM - 8:00 AM	Griffin Room, Westin Boston Waterfront
Executive Committee Meeting	Sunday, August 16	8:00 AM - 11:30 AM	Griffin Room, Westin Boston Waterfront
SCHB Luncheon	Sunday, August 16	11:45 AM - 1:00 PM	Commonwealth A, Westin Boston Waterfront
SCHB Luncheon	Monday, August 17	11:45 AM - 1:15 PM	Griffin Room, Westin Boston Waterfront
SCHB Luncheon	Tuesday, August 18	11:45 AM - 1:15 PM	Griffin Room, Westin Boston Waterfront

Division of Toxicology— TOXI

Keynote Address	Tuesday, August 18	5:00 PM - 6:00 PM	Harbor Blrm III, Westin Boston Waterfront
Keynote Reception	Tuesday, August 18	5:00 PM - 6:30 PM	Harbor Blrm III, Westin Boston Waterfront
General Poster Session Dinner	Tuesday, August 18	6:30 PM - 10:30 PM	Grand Blrm A/B, Westin Boston Waterfront

250th
Celebration

American Chemical Society National Meeting & Exposition



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August 16-20, 2015
BOSTON, MA
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networking lounge



Networking Lounge Access
Exposition, Town Center
Boston Convention & Exhibition Center
Halls A & B1
Sunday evening 6:00 • 8:30 PM
Monday and Tuesday 9:00 AM • 5:00 PM

AUGUST 16-18, 2015 BOSTON, MA

SOCIAL & EDUCATIONAL EVENTS

PRESIDENTIAL EVENTS

DIANE GROB SCHMIDT, 2015 ACS president, kicks off the national meeting with a National Historic Chemical Landmark designation of “Edwin Land & Instant Photography” at the MIT Museum on Thursday, August 13, at 3:30 PM. Come join the American Chemical Society and Massachusetts Institute of Technology as they recognize the work of Land and the development of instant photography (Polaroid). On Saturday, August 15, Diane will also host the ACS Public Outreach Event at the Boston Children’s Museum, from 10:00 AM to 1:00 PM for children and their families. There, attendees can experience hands-on, age-appropriate activities showcased under the theme “Exploring Our World through Chemistry.”

Diane’s first presidential symposium, “National Science Foundation’s Centers for Chemical Innovation,” spans all day on Sunday, August 16. Speakers include the heads of all eight Chemical Innovation Centers followed by a poster session and reception. Starting in the afternoon on Sunday and running through Monday morning is the symposium titled “21st Century Education: Formal & Informal.” Also on Sunday, join your colleagues at the symposium honoring “Edwin Land & Instant Photography” sponsored by the HIST Division. This symposium is a follow-on event to the National Historic Chemical Landmark event preceding it on Thursday.

Want to catch a sneak peek of the new show on PBS about chemistry? Please make time on Sunday afternoon to catch a special preview of the upcoming “Mystery of Matter” program exclusive to national meeting attendees.

On Monday, August 17, ACS will celebrate the 20-year anniversary of the establishment of the ACS Scholars Program with a special symposium of past scholars throughout both industry and academia. On Tuesday, an all-day symposium will cover “Transforming University-

Industry Partnerships for an Innovative Future.” Speakers from both academia and corporations will highlight the role of better university-industry partnerships in driving innovation that will lead to a more competitive nation. Finally, the ACS Divisions of HIST, POLY, PROF, and SCHB are all hosting various symposia in honor of the 100th birthday of chemistry pioneer Henry A. Hill. Details of these presidential events and other recommended symposia can be found at www.acs.org/boston2015 and in the on-site program.

SOCIAL & EDUCATIONAL EVENTS

Friday, August 14

CHAS Workshop: Laboratory Waste Management Workshop
8:00 AM to 5:00 PM, BCEC, Room 157B

Saturday, August 15

CHAS Workshop: Hazard Analysis
8:00 AM to 5:00 PM, BCEC, Room 157A

CHAS Workshop: How to be a More Effective CHO
8:00 AM to 5:00 PM, BCEC, Room 157C

COACH Workshop: COACH the COACH Training
8:30 AM to 5:00 PM, Renaissance Boston Waterfront, Pacific Blrm F&G

COACH Workshop: COACHing Powerful Postdocs: Career Launch & Acceleration
8:30 AM to 5:00 PM, Renaissance Boston Waterfront, Pacific Blrm F&G

COACH Workshop: Basics of Entrepreneurship and Commercialization of Research
8:30 AM to 5:00 PM, Renaissance Boston Waterfront, Mediterranean

COACH Reception
5:00 to 7:00 PM, Renaissance Boston Waterfront, Caspian

Sunday, August 16

Undergraduate Hospitality Center
8:00 AM to 5:00 PM, BCEC, Room 205A

ACS Career Fair Workshop: Career Pathways II
8:00 AM to 6:00 PM, BCEC, Room 105

ACS Career Fair Workshop: Career Pathways III
8:00 AM to 6:00 PM, BCEC, Room 106

Careers in Chemical Information and Cheminformatics Panel Discussion & Brunch
9:00 to 11:00 AM, BCEC, Room 52AB

ACS Career Fair
9:00 AM to 4:30 PM, BCEC, Hall B2

ACS Career Fair Workshop Room
9:00 AM to 6:00 PM, BCEC, Room 103

ACS Career Fair Workshop: Career Pathways I
9:00 AM to 6:00 PM, BCEC, Room 104C

Graduate School Reality Check: Getting in! Part 1
11:00 AM to 12:15 PM, BCEC, Room 50

ACS Board Luncheon & Meeting
11:45 AM to 1:00 PM, BCEC, Ballroom West

CHED High School-College Interface Luncheon/SE-05/\$45 (Included at no charge with high school teacher registration.)
Noon to 1:00 PM, BCEC, Room 253C

Graduate School Reality Check: You’re in Now What! Part 2
12:15 to 1:30 PM, BCEC, Room 50

SCHB Poster Session
1:00 to 2:00 PM, Westin Boston Waterfront, Webster

Mystery of Matter PBS Preview
1:30 to 3:00 PM, BCEC, Room 52AB

Networking Social with Graduate School and Research Opportunity Representatives
2:00 to 5:00 PM, BCEC, East Registration

PRES Poster Session
3:00 to 6:00 PM, Westin Boston Waterfront, Galleria

International and Domestic Chapters Panel Discussions
4:00 to 5:30 PM, BCEC, Room 205A

Regional Networking Event: Asia Pacific
4:00 to 5:00 PM, Sheraton Boston Hotel, Liberty A

SOCIAL & EDUCATIONAL EVENTS

Director-at-Large Town Hall Meeting

4:30 to 5:30 PM, Sheraton Boston Hotel, Grand Ballroom

ACS Diversity Reception

5:00 to 7:00 PM, Sheraton Boston Hotel, Independence

University of Wisconsin-Madison Reception

5:00 to 7:00 PM, Westin Boston Waterfront, Adams Room

University of Illinois at Urbana-Champaign Department of Chemistry Reception

5:00 to 8:00 PM, Renaissance Boston Waterfront, Mediterranean

CHED Social Reception

5:30 to 7:00 PM, BCEC, Room 51

ACS PRF/Research Corp. Reception

5:30 to 7:30 PM, Seaport Hotel and World Trade Center, Plaza Blrm C

International Welcome Reception/SE-08/no charge

5:30 to 7:30 PM, Sheraton Boston Hotel, Back Bay C/D

COLL Social Hour/Open Business Meeting/Poster Session

5:30 to 8:00 PM, Westin Boston Waterfront, Galleria

BIOL Poster Session

5:30 to 8:00 PM, Seaport Hotel & World Trade Center, Cityview Ballroom

District I Councilor Caucus

6:00 to 7:00 PM, Sheraton Boston Hotel, Berkeley A/B

District II Councilor Caucus

6:00 to 7:00 PM, Sheraton Boston Hotel, Fairfax A

District IV Councilor Caucus

6:00 to 7:00 PM, Sheraton Boston Hotel, Fairfax B

District V Councilor Caucus

6:00 to 7:00 PM, Sheraton Boston Hotel, Hampton A/B

District VI Councilor Caucus

6:00 to 7:00 PM, Sheraton Boston Hotel, Republic A

Mid Atlantic Councilor Caucus

6:00 to 7:00 PM, Sheraton Boston Hotel, Republic B

INOR Poster Session

6:00 to 8:00 PM, BCEC, Hall C

Expo Attendee Reception

6:00 to 8:30 PM, BCEC, Halls A/B1

CINF Division Welcoming Reception and Poster Session

6:30 to 8:30 PM, Seaport Hotel and World Trade Center, Lighthouse Blrm 1

CHED Poster Session

7:00 to 9:00 PM, BCEC, Hall C

MEDI Poster Session

7:00 to 9:00 PM

ORGN Poster Session

8:00 to 10:00 PM, BCEC, Hall C

Monday, August 17

WCC Women in Chemical Enterprise Breakfast/SE-09/\$40 (Regular)/SE-10/\$20 (student)

7:00 to 9:00 AM, Sheraton Boston Hotel, Commonwealth

YCC/Member Insurance Fun Run

7:00 AM to 9:00 AM
BCEC, East Side Drive

Undergraduate Hospitality Center

8:00 AM to 5:00 PM, BCEC, Room 205A

ACS Career Fair Workshop: Career Pathways II

8:00 AM to 6:00 PM, BCEC, Room 105

ACS Career Fair Workshop: Career Pathways III

8:00 AM to 6:00 PM, BCEC, Room 106

ACS Career Fair

9:00 AM to 5:00 PM, BCEC, Hall B2

ACS Career Fair Workshop: Career Pathways I

9:00 AM to 6:00 PM, BCEC, Room 104C

ACS Exposition

9:00 AM to 5:00 PM, BCEC, Halls A/B1

Cyber Security Trends: How To Protect Yourself and Your Small Business, Sponsor: ACS Member Insurance Program,

9:30 AM to 12:00 PM, BCEC, Exhibit Halls A & B1, Exhibitor Workshop Room 1.

Designing a Distance Learning Lab Curriculum for Chemistry, Sponsor: Carolina Biological Supply Co.

9:30 AM to 12:00 PM, BCEC, Exhibit Halls A & B1
Exhibitor Workshop Room 2

Networking Basics for Students

9:45 to 11:15 AM, BCEC, Room 52A

Wiley Introduction to Publishing – For Early Career Researchers, Sponsor: Wiley

9:45 AM to 12:00 PM, BCEC, Room 101

Women Chemists of Color Social

10:00 to 11:30 AM, Sheraton Boston Hotel, Commonwealth

Committee on Minority Affairs Luncheon/SE-11/\$50

11:30 AM to 1:30 PM, Sheraton Boston Hotel, Independence West

Pinpoint Local Chemistry and Function – New AFM Capabilities for Photovoltaics, Batteries, Fuel cells, Sponsor: Bruker

12:30 PM to 3:00 PM, BCEC, Exhibit Hall A & B1
Exhibitor Workshop Room 2

From Discovery to Practical Applications – Solving Real World Challenges in Spectroscopy, Sponsor: Thermo Scientific

12:30 PM to 3:00 PM, BCEC, Room 101

AGRO Graduate Student Luncheon

Noon to 1:20 PM, Boston Park Plaza, Boylston Room

SciFinder® Skill Builder: Reference Searching, Sponsor: CAS

1:30 PM to 2:30 PM, BCEC, Exhibit Halls A & B1
Exhibitor Workshop Room 1

Undergraduate Eminent Scientist Luncheon & Lecture/SE-12/\$50

Noon to 1:30 PM, BCEC, Room 205A

CHED Green Chemistry Commitment Luncheon

Noon to 1:30 PM, BCEC, Room 258A

CHAL Drug & Power Luncheon/SE-13/\$40

Noon to 1:30 PM, BCEC, Room 52B

Regional Networking Event: Americas and Africa

2:00 to 3:00 PM, Renaissance Boston Waterfront, Pacific Blrm C

Undergraduate Research Poster Session

2:00 to 4:00 PM, BCEC, Hall C

ACS Fellows Ceremony and Reception

2:00 PM to 4:00 PM, Sheraton Boston Hotel, Constitution A/B

University of Rochester Alumni Social Hour

3:00 to 4:00 PM, Westin Boston Waterfront, Revere

SOCIAL & EDUCATIONAL EVENTS

Graphing and Analysis using Origin 2015, Sponsor: OriginLab Corp.

3:30 PM to 6:00 PM, BCEC, Room 101

The Kavli Foundation Emerging Leader in Chemistry Lecture

4:00 to 5:00 PM, BCEC, Ballroom West

Student Speed Networking with Chemistry Professionals

4:00 to 5:30 PM, Westin Boston Waterfront, Galleria

The Fred Kavli Innovations in Chemistry Lecture

5:30 to 6:30 PM, BCEC, Ballroom West

Chinese-American Chemical Society Dinner Banquet/SE-15/\$35

5:30 to 9:30 PM, Hei La Moon Restaurant, 88 Beach St.

CHAL Reception

5:00 to 8:00 PM, BCEC, Room 152

University of Pennsylvania Alumni Reception

6:30 to 8:00 PM, Bastille Kitchen, 49 Melcher St.

CATL Poster Session

6:30 to 8:30 PM, Westin Boston Waterfront, Galleria

ACS Publications Editor/Author/Reviewer Reception In Honor of Kavli Lecture Series Speakers

6:30 to 7:30 PM, BCEC, Ballroom Foyer

ACS Graduate and Postdoctoral Scholars Reception

7:00 to 8:30 PM, BCEC, Room 52AB

Purdue University Department of Chemistry Alumni Reception/SE-16/\$10

7:00 to 8:30 PM, Renaissance Boston Waterfront, Mediterranean

Sci-Mix Interdivisional Poster Session & Mixer (Drink Ticket with registration)

8:00 to 10:00 PM, BCEC, Hall C

Tuesday, August 18

University of Minnesota Alumni & Friends Breakfast/SE-19/\$5

7:30 to 9:00 AM, BCEC, Room 103

Senior Chemists Committee Breakfast/SE-18/\$20

7:30 to 9:30 AM, Sheraton Boston Hotel, Republic A/B

ACS Career Fair Workshop: Career Pathways II

8:00 AM to 6:00 PM, BCEC, Room 105

ACS Career Fair Workshop: Career Pathways III

8:00 AM to 6:00 PM, BCEC, Room 106

ACS Career Fair

9:00 AM to 5:00 PM, BCEC, Hall B2

ACS Exposition

9:00 AM to 5:00 PM, BCEC, Halls A/B1

ACS Career Fair Workshop: Career Pathways I

9:00 AM to 6:00 PM, BCEC, Room 104C

Elsevier — How to Successfully Publish Scientific Articles

9:30 AM to 12:00 PM, BCEC, Room 52AB

CDD Vision Workshop, Sponsor: Collaborative Drug Discovery

9:30 AM- 12:00 PM, BCEC, Exhibit Halls A & B1
Exhibitor Workshop Room 1

What's New from Waters, Sponsor: Waters,

9:30 AM to 12:00 PM, BCEC, Exhibit Halls A & B1
Exhibitor Workshop Room 2

FTIR, atomic spectroscopy, HPLC, GC, and Mass Spectrometry, Sponsor: Agilent Technologies

9:30 AM to 6:00 PM, BCEC, Room 101

SciFinder® Skill Builder: Substance Searching, Sponsor: CAS

10:00 AM to 11:00 AM, BCEC, Room 258B

WCC/Eli Lilly Poster Session

11:00 AM to 12:00 PM, Sheraton Boston Hotel, Republic A/B

Alpha Chi Sigma Luncheon/\$20 (RSVP to gpa@alphachisigma.org)

11:30 AM to 1:30 PM, Atlantic Beer Garden

I&EC Graduate Symposia Luncheon/SE-20/\$40

11:45 AM to 12:45 PM, Renaissance Boston Waterfront, Mediterranean

The State-Of-The-Art in Infrared and Raman Analysis, Sponsor: Bruker

12:30 PM to 3:00 PM, BCEC, Room 258B

Research in Germany Science Lunch, Sponsor: Research in Germany

12:30 PM to 3:00 PM, BCEC, Exhibit Halls A & B1
Exhibitor Workshop Room 1

New Applications in High Resolution Accurate Mass (HR/AM) Mass Spectrometry, Sponsor: Thermo Scientific

12:30 PM to 3:00 PM, BCEC, Exhibit Halls A & B1
Exhibitor Workshop Room 2

CINF Luncheon/SE-21/\$20 (Member Regular)/SE-22/\$15 (Member Student)/SE-23/\$25 (Nonmember)

Noon to 1:30 PM, BCEC, Room 52A

COLL Luncheon/SE-24/\$40

Noon to 1:30 PM, Westin Boston Waterfront, Stone

WCC Lunch/SE-25/\$50 (Regular)/SE-26/\$25 (Student)

Noon to 1:30 PM, Sheraton Boston Hotel, Republic A/B

Flow Chemistry Seminar, Sponsor: ThalesNano Nanotechnology Inc.

3:30 PM to 6:00 PM, BCEC, Room 258B

Meet the Federal Grant Funders and Speed Coaching with Program Officers

1:00 to 5:00 PM, BCEC, Room 102AB

ENFL Poster Session

2:00 to 4:00 PM, BCEC, Halls A/B1

AGFD Poster Session

3:00 to 5:00 PM, BCEC, Halls A/B1

WCC 'Just Cocktails' Open Meeting

4:00 to 5:00 PM, Westin Boston Waterfront, Stone

Division Councilors & Officers Caucus

4:00 to 5:30 PM, BCEC, Room 107A

Committee on Science Networking Session & Panel

4:00 to 6:30 PM, Sheraton Boston Hotel, Liberty A/B

I&EC Poster Session

5:00 to 6:30 PM, BCEC, Hall C

Henry Hill's 100th Anniversary Reception and Award Program

5:00 to 7:00 PM, Seaport Hotel and World Trade Center, Plaza B1rm A/B

University of New Hampshire Chemistry Reception

5:00 to 7:30 PM, Westin Boston Waterfront, Revere

AGRO Blues-N-Brew

5:30 to 6:30 PM, Boston Park Plaza, Boylston Room

SOCIAL & EDUCATIONAL EVENTS

Joint POLY/PMSE Poster Session

5:30 to 7:30 PM, BCEC, Ballroom West

MEDI Hall of Fame Ceremony

5:30 to 7:30 PM, BCEC, Room 52AB

Boston University Department of Chemistry Alumni Reception

5:30 to 7:30 PM, Seaport Hotel and World Trade Center, Cityview 2

Geochemistry Division Reception

5:30 to 7:30 PM, Seaport Hotel and World Trade Center, Flagship Room A

BIOL Poster Session

5:30 to 7:30 PM, Westin Boston Waterfront, Galleria

Regional Networking Event: Europe and the Middle East

6:00 to 7:00 PM, Renaissance Boston Waterfront, Pacific Blrm C

ENVR Social & Reception/SE-28/\$20

6:00 to 7:30 PM, Back Bay Harry's, 142 Berkeley St.

NUCL Social Hour

6:00 to 8:00 PM, Seaport Hotel and World Trade Center, Cityview 1

Presidential LGBT Reception

6:00 to 8:00 PM, Seaport Hotel and World Trade Center, Plaza Ballroom C

COMP Poster Session

6:00 to 8:00 PM, Westin Boston Waterfront, Galleria

INOR Poster Session

6:00 to 8:00 PM, BCEC, Hall C

CARB Poster Session

6:00 to 8:00 PM, BCEC, Hall C

ANYL Dinner/SE-29/\$40 (Regular)/SE-30/\$20 (Student)

6:00 to 9:00 PM, Joe's American-Waterfront, 100 Atlantic Ave.

Herman Skolnik Award Reception Honoring Dr. Jurgen Bajorath

6:30 to 8:30 PM, BCEC, Room 254A

ENFL Dinner/SE-31/\$65

6:30 to 9:30 PM, Morton's The Steakhouse, 2 Seaport Ln.

TOXI General Poster Session

6:30 to 10:30 PM, Westin Boston Waterfront, Grand Blrm A/B

ANYL Poster Session

7:00 to 9:00 PM, BCEC, Hall C

ChemLuminary Poster Session

7:30 to 9:00 PM, Westin Copley Place, Essex Ballroom

ENVR Dinner/SE-32/\$60

8:00 to 10:00 PM, Back Bay Harry's, 142 Berkeley St.

ORGN Poster Session

8:00 to 10:00 PM, BCEC, Hall C

ChemLuminary Awards

9:00 PM to 12:00 AM, Westin Copley Place, America Ballroom

Wednesday, August 19

ACS Career Fair Workshop: Career Pathways II

8:00 AM to 6:00 PM, BCEC, Room 105

ACS Career Fair Workshop: Career Pathways III

8:00 AM to 6:00 PM, BCEC, Room 106

ACS Career Fair Workshop: Career Pathways I

9:00 AM to 6:00 PM, BCEC, Room 104C

Nanomaterials analysis by X-ray scattering methods, Sponsor: PANalytical

9:30 AM to 12:00 PM, BCEC, Room 101

How to Get Your Book Published with Elsevier

12:30 to 3:00 PM, BCEC, Room 102A

Wikipedia Edit-a-thon

1:30 to 5:30 PM, BCEC, Room 102B

Inhibitor Design Using MOE Structure-Based Drug Design Applications, Sponsor: Chemical Computing Group

3:30 PM to 6:00 PM, BCEC, Room 101

PHYS Poster Session

6:00 to 8:00 PM, BCEC, Hall C

ENVR Poster Session

6:00 to 8:00 PM, BCEC, Hall C

INOR Poster Session

6:00 to 8:00 PM, BCEC, Hall C

AGRO Social

6:00 to 9:00 PM, Boston Park Plaza, Boylston Room

Joint MEDI & ORGN Poster Session

7:00 to 10:00 PM, BCEC, 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/boston2015.

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 John C. Warner, president and chief technology officer, Warner Babcock Institute for Green Chemistry, will present "What's in Your Chemical Toolbox?"

SUNDAY, August 16

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

Undergraduate Research Oral Session, 8:30 AM to 5:00 PM

Careers in Chemical Information & Cheminformatics Panel Discussion & Brunch (cosponsored by CINF), 9:00 to 11:00 AM

Graduate School Reality Check, Step I: Getting In (cosponsored by YCC), 11:00 AM to 12:15 PM

Graduate School Reality Check, Step II: You're In—Now What? (cosponsored by YCC), 12:15 to 1:30 PM

Networking Social with Graduate School Recruiters, 2:00 to 5:00 PM

International & Domestic Chapters Panel Discussions, 4:00 to 5:30 PM

MONDAY, August 17

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

Undergraduate Research Oral Session, 8:30 AM to 5:00 PM

Networking Basics for Students (cosponsored by CEPA), 9:45 to 11:15 AM

Eminent Scientist Lecture & Luncheon with John C. Warner, president & CTO, Warner Babcock Institute for Green Chemistry (cosponsored by ENVR and ENFL), noon to 1:30 PM

Undergraduate Research Poster Session (cosponsored by CHED, AGFD, ENVR, INOR, MEDI, PHYS, POLY, GEOC, and BIOT), 2:00 to 4:00 PM

Student Speed Networking with Chemistry Professionals (cosponsored by the ACS Senior Chemists Committee and ACS Corporation Associates), 4 to 5:30 PM

GRADUATE & POSTDOCTORAL SCHOLARS OFFICE. The Graduate & Postdoctoral Scholars Office with support from the Graduate Education Advisory Board provides and promotes programs and resources for graduate students and postdoctoral scholars.

MONDAY, August 17

Student Speed Networking with Chemistry Professionals, (cosponsored by the ACS Senior Chemists Committee and ACS Corporation Associates), 4:00 to 5:30 PM

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

Academic Employment Initiative (AEI), 8:00 to 10:00 PM

For more information about these events and other ACS programs offered to graduate students and postdocs, visit www.acs.org/grad or contact the ACS Graduate & Postdoctoral Scholars Office at 800-227-5558 ext. 4588.

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 on current pedagogies, resources, and activities that align with the meeting's theme, "Innovation from Discovery to Application." 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, August 16

High School Teachers Program, 8:30 AM to 6:00 PM

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: full registration \$375/early registration \$300; non-CHAS member: full registration \$425/early registration \$350. Early registration ends June 26. K-12 science teachers who are American Association of Chemistry Teacher members: \$99. Need-based scholarships are available for K-12 science teachers; contact scholarships@labsafetyinstitute.org. Registration is required for all CHAS workshops. Register online at <https://goo.gl/W5vg7Y>.

Laboratory Safety. Friday, August 14, 8:00 AM to 4:30 PM. BCEC, 157A. 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 laboratory. 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 will provide a forum to speak openly about safety in your workplace.

Laboratory Waste Management. Friday, August 14, 8:00 AM to 4:30 PM. BCEC, 157B. Sponsored by CHAS. Presenter: Russ Phifer. This comprehensive course will identify the various regulatory requirements that apply to laboratories that generate hazardous waste, as well as provide insight to the options for on-site management and off-site disposal. The instructor will include discussion of recycling/reclamation techniques, economical handling of waste, and liability issues.

Chemical Reactivity Hazards:

Laboratory-Scale Recognition & Control.

Saturday, August 15, 8:00 AM to 4:30 PM. BCEC, 157B. Sponsored by CHAS. Presenter: Neal Langerman. The Process Safety Alliance, in cooperation with the Occupational Safety & Health Administration, is presenting this workshop. The objective is to provide participants with the knowledge and skill 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.

How To Be a More Effective Chemical Hygiene Officer,

Saturday, August 15, 8:00 AM to 4:30 PM. BCEC, 157C. 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, August 16, through the National Registry of Certified Chemists. The instructors provide a different slant to safety issues in the laboratory, focusing on what you do and how you can do it better. The course covers all of the content areas of the certification exam, including a sample test in the same format as the real one.

Job Hazard Analysis. Saturday, August 15, 8:00 AM to 4:30 PM. BCEC, 157C. Sponsored by CHAS. Presenter: Samuela Sigmann. The Job Hazard Analysis (JHA) is one method to consider hazards associated with lab research and guide the control of those hazards. A JHA can assist the researcher in uncov-

ering 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. Each participant will create a ready-to-use JHA based on a task specifically applicable to their laboratory. Attendees should come with a specific idea of a chemical or process they would like to investigate.

Career Launch & Acceleration for Postdoctoral Associates. Saturday, August 15, 8:00 AM to 4:00 PM. Renaissance Boston Waterfront, Pacific Ballroom F&G. Sponsored by COACH. Learn how to assimilate fundamentals of responsible negotiation and communication skills. Attendees will examine the Best Alternative to a Negotiated Agreement (BANTA) concept as a tool to prepare and build confidence, as well as communication styles that are effective for women, projecting confidence, and using powerful rather than weak words. Discussions will focus on making the best impression in the job interview process, succeeding in the negotiating stage, and securing an academic appointment that will position you for career success. This workshop will be held concurrently with the COACH-the-COACHes workshop. Preregister at <http://coach.uoregon.edu>. Registration is free; travel assistance is available. For more information, contact Priscilla Lewis: coach@uoregon.edu, phone: 541-346-0116.

COACH-the-COACHes. Saturday, August 15, 8:00 AM to 4:00 PM. Renaissance Boston Waterfront, Pacific Ballroom F&G. Sponsored by COACH. This workshop is designed for women faculty who are interested in being trained to offer COACH workshops to graduate students and postdoctoral associates and who have attended COACH workshops in the past. COACH-the-COACHes is being offered in conjunction with the "Career Launch & Acceleration for Postdoctoral Associates" workshop. 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 presentations. The workshop will also provide attendees an opportunity to work directly

with the postdoctoral associates to practice skills in interviewing and negotiation. Participants must attend the full day of activities. The traditional COACH reception will follow the day's activities. Space is limited with priority given to early applicants and applicant qualifications. Apply at <http://coach.uoregon.edu>. For more information, contact Priscilla Lewis: coach@uoregon.edu, phone: 541-346-0116.

Basics of Entrepreneurship & Commercialization of Research.

Saturday, August 15, 8:30 AM to 5:00 PM. Renaissance Boston Waterfront, Mediterranean Room. Sponsored by COACH. Commercialization of research involves taking articles, documentation, know-how, patents, and copyrights created during research activities and getting them to the marketplace for financial and societal gain. This workshop will provide an overview of the basic pathways to commercialization, why an entrepreneur needs a minimum viable product (MVP), and the steps involved in customer and market validation. An overview of intellectual property options, legal issues associated with emerging ventures, team building, and creating and funding companies will be offered. Participants will also have the opportunity to examine their own entrepreneurial mind-set and create a customized plan for developing their entrepreneurial capabilities.

ACS PHYS Workshop for Undergraduate Students. Sunday, August 16, 8:30 AM to 12:30 PM. BCEC, 254A. This workshop will introduce students to the excitement of modern physical chemistry. PHYS symposium organizers or their designees will present 30-minute overview lectures providing technical and background context that will enable students to benefit from their attendance at subsequent physical chemistry symposia. This workshop is free and open to the public; no registration is necessary. Graduate-school-bound students are particularly encouraged to attend.

Wikipedia Edit-A-Thon. Wednesday, August 19, 1:30 to 5:30 PM. BCEC, 102B. Sponsored by the ACS Office of Public Affairs, Division of Chemical Information, and Committee on Public Relations & Communications. Join us for a Wikipedia training and editing session

to improve coverage of notable chemists and chemistry topics on Wikipedia. All are welcome to participate, newcomer and veteran alike. Attendees may come and go, but instruction will be provided during the first hour. Bring a laptop. Advance registration required. Contact Keith Lindblom in the ACS Office of Public Affairs at k_lindblom@acs.org or (202) 872-6214.



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 more informed decisions.

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

ACS CAREER FAIR

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

EMPLOYERS, are you looking to hire scientists and engineers? Then you need to attend the ACS Career Fair, open Sunday, August 16, 9:00 AM to 4:30 PM; Monday, August 17, 9:00 AM to 5:00 PM; and Tuesday, August 18, 9:00 AM to 5:00 PM. The career fair is the place where the best talent and the best employers in chemistry meet.

ON-SITE ACTIVITIES FOR JOB SEEKERS

Let the ACS Career Fair help you reach your career goals. ACS will help you prepare for your next career move by providing resources that make it possible to map out your personal job search strategy, strengthen your résumé, and build your interview skills, all with the support of career consultants. During the career fair, participants can take full advantage of the following:

- Networking opportunities
- Résumé reviews
- One-on-one career consulting
- Interview practice and skills building
- More than 20 career-related workshops
- Request live on-site 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 in the convention center beginning Sunday, August 16).

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

ONE-ON-ONE CAREER CONSULTING.

Individual 30-minute appointments with career consultants are available both on-site and online. These consults can help you strengthen your résumé, improve your interviewing skills, and design a job search or comprehensive professional growth strategy. Please bring a copy of your résumé or CV to all

appointments. All one-on-one on-site career consulting sessions will take place in the Résumé Review/Mock Interview area. Sign-up begins at 9:00 AM on Sunday, August 16, on a first-come, first-served basis.

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

Sunday, August 16

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

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

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

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

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

Monday, August 17

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

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

Working for Yourself, 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, August 18

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, August 19

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

EMPLOYERS—FIND THE TALENT YOU NEED AT THE ACS CAREER FAIR. 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 recruiters seeking to fill positions in all facets of chemistry, pharmaceuticals, and biotechnology.

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

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

LOOKING FOR A MORE TRADITIONAL CAREER FAIR EXPERIENCE? 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 online at www.acs.org/careers.

Employers will receive an e-mail confirmation and must visit the ACS Career Fair Information Booth 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.

ACS PROFESSIONAL EDUCATION SHORT COURSES

THE FOLLOWING short courses, specifically designed to improve the skills and marketability of chemical scientists and technicians, are offered in conjunction with the national meeting. ACS member, early 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 Boston, to obtain pricing details, or to view a full course catalog, visit www.proed.acs.org/boston. If you have questions, call 202-872-4508, fax 202-872-6336, or e-mail proed@acs.org.

EWorkflow Efficiencies: 2-D Liquid Chromatography & Novel Sample Preparation Techniques, August 14

1-D & 2-D NMR Spectroscopy: Structure Determination of Small-Molecule Organic Compounds, August 14–15

BIOLOGICAL/PHARMACEUTICAL/MEDICINAL CHEMISTRY

Application of Pharmacokinetics & Safety Pharmacology for Chemists in Drug Development, August 14–15

COMPUTERS/STATISTICS/ENGINEERING

Statistical Analysis of Laboratory Data, August 14–16

ORGANIC/PHYSICAL CHEMISTRY

1-D & 2-D NMR Spectroscopy: Structure Determination of Small-Molecule Organic Compounds, August 14–15

Dispersions in Liquids: Suspensions, Emulsions & Foams, August 14–15

POLYMER CHEMISTRY

Polymeric Coatings, August 14–15

Polymer Science & Technology, August 14–15

PROFESSIONAL DEVELOPMENT

Effective Technical Writing, August 14–15

Write Your Own Patent Applications, August 16

REGULATORY/ENVIRONMENTAL

CHAS NRCC CERTIFICATION EXAMS

WHAT: Certification exams of the National Registry of Certified Chemists

WHEN: Sunday, August 16, 8:00 AM to noon

WHERE: Seaport Hotel and World Trade Center

HOW: Advance registration and completion (with approval) of application must be done before July 31. Applications may be downloaded from www.nrcc6.org.

For additional information contact Russ Phifer by e-mail at rphifer@nrcc6.org.

Workflow Efficiencies: 2-D Liquid Chromatography & Novel Sample Preparation Techniques, August 14

Intellectual Property Strategies for Technical Professionals, August 16

Write Your Own Patent Applications, August 16

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 System course held at the ACS national meeting. The following four-hour facilitated courses require a fee of \$150 each for ACS members and \$300 each for non-members. Register for these courses when you register for the meeting. For more information and full course descriptions, visit www.acs.org/leadershipdevelopment.

Access meeting information and the On-site Program at www.acs.org/boston2015

Fostering Innovation. Sunday, August 16, 1:00 to 5:00 PM. Keeping pace in an environment of constant change requires innovation. Whether you are part of 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 success. Coming up with new ideas is challenging, and few of us have the tools and skills to do this effectively. This course will teach a proven, systematic process to generate ideas. You will learn your innovation style and how to stimulate innovative thinking among team members and colleagues.

Strategic Planning. Monday, August 17, 8:00 AM to noon. Gain understanding of the structure and contents of a strategic plan as well as the impact that strategy has on your work and an organization's success. You will learn how to become a "partner in planning" with other leaders as you develop a plan for your unit that aligns with the executive-level strategic goals.

Leading Without Authority. Tuesday, August 18, 8:00 AM to noon. Leading volunteers comes with many challenges, including having no direct authority over the members. Leaders need to be able to engage and influence members to get things done, even when they may put up barriers or have different viewpoints. Learn practical tools to help you gain cooperation without formal authority and motivate your colleagues or volunteers.

Collaborating Across Boundaries. Tuesday, August 18, 1:00 to 5:00 PM. Do you work with people from other departments or from other countries? As the world becomes more complex, the ability to reach across boundaries to work on projects and share information is critical to organizational success. It's not just a matter of communication but of genuine collaboration—working in partnership to achieve common goals, create innovative solutions, and share expertise. Learn strategies and tools to be more effective in leading collaborative efforts, and gain practical skills that you can apply immediately in the lab, at school, in the office, or at ACS.

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

Introduce new products and services

Highlight innovative applications for existing instrumentation

Build skills with specific tools and techniques

Please visit www.acs.org/boston2015 to register for their workshops.

Highlights

Exposition, BCEC, Halls A & B1

- Sunday, 6 – 8:30 PM
- Monday & Tuesday, 9AM – 5 PM

- Join us on Sunday from 6 – 8:30 PM for our 250th Celebration
- Meet the ACS president-elect candidates inside the exposition on Monday, from 1 – 4 PM
- Visit the Daily Prize Booth 255 Sunday through Tuesday for a chance to win a prize!

Monday, August 17

Cyber Security Awareness: How to Protect Yourself and Your Small Business

Sponsor: ACS Member Insurance Program, 9:30 AM – Noon
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 1

Designing a Distance Learning Lab Curriculum for Chemistry

Sponsor: Carolina Biological Supply Co., 9:30 AM – Noon
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 2

SciFinder Training

Sponsor: CAS, 12:30 PM – 3:00 PM
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 1

Origin 2015 User Group Meeting and Product Demo

Sponsor: OriginLab Corp. 3:30 PM – 6:00 PM
BCEC, Room 101

Tuesday, August 18

SciFinder Training

Sponsor: CAS, 9:30 AM – Noon
BCEC, Room 258B

What's New from Waters

Sponsor: Waters Corporation, 9:30 AM – Noon
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 2

The State-Of-The-Art In Infrared and Raman Analysis

Sponsor: Bruker, 12:30 PM – 3:00 PM
BCEC, Room 258B

CDD Vision Workshop

Sponsor: Collaborative Drug Discovery, 9:30 AM – Noon
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 1

FTIR, Atomic Spectroscopy, HPLC, GC, and Mass Spectrometry

Sponsor: Agilent Technologies, 9:30 AM – 6:00 PM
BCEC, Room 101

Research in Germany Science Lunch

Sponsor: Research In Germany, 12:30 PM – 3:00 PM
BCEC, Exhibit Halls A/B1, Exhibitor Workshop Room 1

Wednesday, August 19

Nanomaterials Analysis by X-ray Scattering Methods

Sponsor: PANalytical, 12:30 PM – Noon
BCEC, Room 101

Inhibitor Design Using MOE Structure-Based Drug Design Applications

Sponsor: Chemical Computing Group, 3:30 PM – 6:00 PM
BCEC, Room 101

EXPOSITION

SEE WHAT'S NEW INSIDE THE EXPOSITION. Visit the ACS National Exposition at the Boston Convention & Exhibition Center (BCEC), Halls A & B1, from Sunday, August 16, through Tuesday, August 18. The show hours will be Sunday, 6 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/boston2015 to learn more about exhibiting companies and to download product information.

Free Exhibitor Workshops. Free workshops will be hosted by exhibitors on the exposition floor and in private rooms inside the BCEC. These workshops will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications that may improve your productivity. Visit the exhibitor at their booth to reserve your seat.

Presentations, Prizes & Special Events. Visit the Daily Prize Booth, 255, on Sunday through Tuesday for a chance to win a prize. Also, don't forget to join us on Sunday from 6 to 8:30 PM for the 250th Attendee Welcome Celebration in the Town Center. Meet the ACS president-elect candidates inside the exposition on Monday, from 1 to 4 PM.

Internet & Technology. Use free Internet access and leave messages for one another at the Meeting Mail terminals located throughout the meeting. Also, enjoy free Wi-Fi service at the BCEC.

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, by mail, or in person at ACS Attendee Registration at the BCEC, North Lobby.

To celebrate the ACS 250th ACS National Meeting make plans to pick up your commemorative lapel pen inside the exposition.

Stop by the ACS ProShot Social Media Lounge inside the TownCenter for a FREE headshot, Sunday through Tuesday during the Exposition.

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/boston2015 to register for workshops.

Monday, August 17

Cybersecurity Trends: How To Protect Yourself and Your Small Business.

Sponsor: ACS Member Insurance Program, 9:30 AM to noon, Boston Convention & Exhibition Center (BCEC), Exhibit Halls A & B1, Exhibitor Workshop Room 1. Cyber-crime cost Americans \$800 billion last year. This workshop will identify practical approaches to improving cybersecurity for individuals and small businesses. An information technology expert who reviews small businesses' security systems will provide background on what drives cyber thieves and how to protect your business against

them. A speaker from the Cyber Division of the FBI will outline their priorities and identify resources to help protect against cyber threats. Attendees will also learn about insurance plans available to reduce business liability and protect individuals against ID theft.

Speakers: Jeffrey M. Williams, special agent, FBI Boston division; John Poff, director of security and chief technology officer, Pearl Technology; Dave Wasson, professional and cyber liability practice leader, Hays Cos. **Moderator:** Joseph E. Sabol, program chair, ACS Division of Small Chemical Businesses.

Wiley Introduction to Publishing for Early-Career Researchers. Sponsor: Wiley, 9:45 AM to noon, BCEC, Room 101. A one hour workshop session with Q&A covering how to publish with Wiley. Attend the workshop and learn how to critically assess and select a suitable journal for article publication, refine your paper to increase your chances of success, submit a manuscript and survive peer review, and apply practical techniques to increase the visibility of your article after it has been published. Workshop one starts at 9:45 AM. Due to popular demand, an additional workshop will run at 11 AM.

Designing a Distance Learning Lab Curriculum for Chemistry. Sponsor: Carolina Biological Supply Co., 9:30 AM to noon, BCEC, Exhibit Halls A & B1, Exhibitor Workshop Room 2. Help your online students learn the same critical science process skills as your classroom students. Carolina Science has transformed the hands-on labs you have used for years into distance learning labs that are reliable, safe, and affordable. Experience for yourself during this hands-on workshop how your students will easily learn the necessary lab skills and reinforce key concepts using Carolina Science Distance Learning kits. Begin to design your online lab course by reviewing more than 25 different chemistry investigations. Suitable for Gen Chem and GOB Chem courses.

Pinpoint Local Chemistry & Function—New AFM Capabilities for Photovoltaics, Batteries, Fuel Cells. Sponsor: Bruker, 12:30 to 3:00 PM, BCEC, Exhibit Hall A & B1, Exhibitor Workshop Room 2. In this workshop we will discuss new techniques in nanochemi-

cal characterization with atomic force microscopy related to photovoltaics, batteries, and fuel cells.

From Discovery to Practical Applications—Solving Real-World Challenges in Spectroscopy.

Sponsor: Thermo Scientific, 12:30 to 3:00 PM, BCEC, Room 101. This workshop will cover teaching and research applications of FTIR, Raman, and NMR spectroscopy. Join us for a hands-on opportunity to experience the latest in new instrumentation, software, and sample-handling techniques as we guide you through the latest trends in vibrational spectroscopy for more confident analyses.

SciFinder Skill Builder: Reference

Searching. **Sponsor:** CAS, 1:30 to 2:30 PM, BCEC, Exhibit Halls A & B1, Exhibitor Workshop Room 1. SciFinder training for new and experienced users.

Graphing & Analysis Using Origin

2015. **Sponsor:** OriginLab Corp., 3:30 to 6:00 PM, BCEC, Room 101. This workshop will focus on graphing and data analysis in our latest version, Origin 2015. The first half of the workshop will cover creating and customizing two-dimensional, 3-D, and specialized graph types; exporting and publishing graphs; saving templates and themes for repeat use; and batch plotting. The second half will cover data analysis including curve fitting, peak analysis, statistics, and batch analysis. A brief introduction to programming in Origin will also be covered.

Tuesday, August 18

CDD Vision Workshop. **Sponsor:** Collaborative Drug Discovery, 9:30 AM to noon, BCEC, Exhibit Halls A & B1, Exhibitor Workshop Room 1. CDD Vault is a multidomain information management system enabling users to organize chemical and biological data through a Web interface. CDD Vision expands the CDD Vault platform by providing dynamic data visualization, custom calculations, and predictive activity modeling. During this workshop, the benefits of this interactive, dynamic visualization will be presented with case studies in a multisite collaboration scenario.

What's New from Waters. **Sponsor:** Waters, 9:30 AM to noon, BCEC, Exhibit Halls A & B1, Exhibitor Workshop Room 2.

9:45 to 10:25 AM GPS for Glycan Analysis, Disruptive LC-MS Technologies & Workflows for Glycan & Glycoprotein Analysis

Learn about the advancing technologies and workflows for glycan sample preparation, separations, and analysis by mass spectrometry. During this session you will learn about two new technologies that will greatly enhance the ability of researchers to profile and characterize glycoproteins.

10:30 to 11:10 AM Simplified Sample Preparation

Learn about a simplified sample preparation technique for small molecules from complex sample matrices. The technique yields a cleaner sample with reduced matrix effects as well as saving labor and solvent by using fewer sample-processing steps.

11:15 to 11:55 AM Advances in LC Technology: Waters Introduces the Newest Addition to Its LC Portfolio

Learn how to preserve method equivalency for established LC methods while improving productivity and gain greater understanding of the impact of system dispersion on separation performance.

FTIR, Atomic Spectroscopy, HPLC, GC & Mass Spectrometry.

Sponsor: Agilent Technologies, 9:30 AM to 6:00 PM, BCEC, Room 101. Agilent will host a full-day workshop focusing on FTIR, atomic spectroscopy, HPLC, GC, and mass spectrometry topics. We will also host sessions on sample preparation, analytical method choices including HPLC columns, and optimization of your analytical process. During these interactive workshops, Agilent scientists will discuss how new technology and applications are advancing these analytical techniques. Both hardware and software advancements will be discussed with the overall goal to help users achieve the highest instrument performance across a broad range of applications.

The State-of-the-Art in Infrared and Raman Analysis.

Sponsor: Bruker, 12:30 to 3:00 PM, BCEC, Room 258B. The latest advances in FTIR and Raman instrumentation and applica-

tions will be reviewed in this seminar with a thorough discussion of authentication of art objects, fluorescence-free rapid portable Raman analysis, simultaneous mid- and far-IR analysis, reverse engineering using vibrational microscopy, and chemical imaging and depth profiling.

Examples of applications will include the authentication of a newly discovered Leonardo Da Vinci, Raman analysis of previously challenging samples with fluorescence interference, and the identification of layers in multilayer polymer films. The seminar will include a live demonstration of Bruker's new handheld Raman system and the novel Lumos FTIR microscope. Attendees are encouraged to bring samples for analysis.

SciFinder Skill Builder: Substance

Searching. **Sponsor:** CAS, 10:00 to 11:00 AM, BCEC, Room 258B. SciFinder training for new and experienced users.

Research in Germany Science Lunch.

Sponsor: Research in Germany, 12:30 to 3:00 PM, BCEC, Exhibit Halls A & B1, Exhibitor Workshop Room 1. Promoting scientific research in Germany with funding programs and testimonials.

New Applications in High-Resolution Accurate Mass (HR/AM) Mass Spectrometry.

Sponsor: Thermo Scientific, 12:30 to 3:00 PM, BCEC, Exhibit Halls A & B1, Exhibitor Workshop Room 2. For 10 years, Thermo Scientific Orbitrap technology has been transforming mass spectrometry. Now, the first-ever combination of high-resolution gas chromatography (GC) and high-resolution/accurate-mass (HR/AM) Orbitrap technology has been introduced in the new Q Exactive GC Orbitrap Mass Spectrometer. This system offers the quantitative power of a GC triple-quadrupole MS combined with the high precision, full-scan HR/AM capabilities available only in combination with Orbitrap technology. The Orbitrap Fusion Lumos Tribrid Mass Spectrometer was also recently introduced, offering expanded performance in advanced proteomics, biopharma, and metabolomics applications, including quantitation using isobaric tags, low-level PTM analysis, data-independent acquisition (DIA), and top-down proteomics. The

new instrument features enhanced sensitivity resulting in improved analyte detection, characterization, and quantitation.

Flow Chemistry Seminar. Sponsor: ThalesNano Nanotechnology Inc., 3:30 to 6:00 PM, BCEC, Room 258B. Education seminar on flow chemistry with industrial applications about safe and efficient synthesis and scale-up.

Wednesday, Aug. 19

Nanomaterials Analysis by X-ray Scattering Methods. Sponsor: PANalytical, 9:30 AM to noon, BCEC, Room 101. This workshop will focus on the analysis of nanosized (1- to 100-nm) materials using a laboratory diffractometer. A variety of distinct analysis techniques can be applied on the same diffractometer, such as conventional XRD, SAXS, PDF, in situ heating experiments, and GISAXS, that provide information about pore/particle size, ordering, crystalline

size, phase stability, thermal dependence of lattice parameters, and local atomic structure.

Inhibitor Design Using MOE Structure-Based Drug Design Applications. Sponsor: Chemical Computing Group, 3:30 to 6:00 PM, BCEC, Room 101. This hands-on course 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 modelling, binding pocket visualization, protein-ligand contact analysis, and the use of SAR for in situ modeling 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.

In Silico Modeling in Drug Discovery. Sponsor: Simulations Plus Inc., 12:30 to 3:00 PM, BCEC, Room 101. This course will describe the new functionality in version 8.0 of ADMET Predictor (substructure searching, duplicate checking, etc.) as well as the science behind the program. We will discuss the new pKa model, constructed in collaboration with Bayer AG, along with the predictive classification confidence measure we recently introduced and the predictive CYP sites and rates of metabolism models. The final section of the course will show how the log *P*, p*K*_a, solubility and other ADME property predictions can support physiologically based pharmacokinetic (PBPK) simulations in GastroPlus to assist with early exposure predictions and dose selection in animals and humans and how those predictions can be exported through KNIME or Pipeline Pilot to streamline modeling activities.

250th
Celebration

American Chemical Society National Meeting & Exposition



Innovation from Discovery to Application Thematic Program organized by Carston R. Wagner, Professor & Endowed Chair in Medicinal Chemistry, University of Minnesota College of Pharmacy and Executive Editor, *Molecular Pharmaceutics*

INNOVATION from Discovery to Application

Plenary Session

Sunday, August 16, 2015, 3:00 – 5:00 PM
Boston Convention & Exhibition Center
Ballroom West



Dr. Paula Hammond
Massachusetts Institute of Technology
Tailored Drug Release Surfaces for Regenerative Medicine and Targeted Nanotherapies

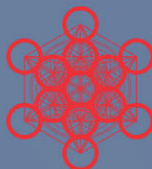


Dr. Pat Brown
Impossible Foods
Replacing the World's Most Destructive Industry



Dr. Karen Wooley
Texas A&M University
Targeted Applications as Inspirations to Develop Strategies toward Functionally-Sophisticated Nanoscopic Macromolecules with Diverse Compositions, Structures, and Properties





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 Fred Kavli Innovations in Chemistry Lecture



Boston Convention & Exhibition Center, Ballroom West

Monday, August 17, 2015

5:30 – 6:30 PM

Dr. George Whitesides
Harvard University

Problems, Puzzles, and Inevitabilities in Research

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

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

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

The Kavli Foundation Emerging Leader in Chemistry Lecture



Boston Convention & Exhibition Center, Ballroom West

Monday, August 17, 2015

4:00 – 5:00 PM

Dr. William Dichtel
Cornell University

The Spectacular Properties of Porous Polymers

Polymers with many small pores exhibit enormous surfaces areas that enable us to store gaseous fuels, rapidly transport ions, immobilize catalysts and modify their selectivity, detect trace substances, and remove contaminants from liquid or gas streams.

ACS Publications Editor/Author/Reviewer Reception in honor of Kavli Lecture Series Speakers
BCEC, Ballroom West Lobby, 6:30 – 7:30 PM





ACS Publications
Most Trusted. Most Cited. Most Read.

pubs.acs.org/catalysis

The 2015 ACS Catalysis Lectureship for the Advancement of Catalytic Science

1.5-Day Symposium

in honor of Drs. Morris Bullock, Daniel DuBois
and the PNNL Hydrogen Catalysis Team

Monday, August 17

8:00 am – 11:20 am and 1:00 pm – 4:45 pm

Tuesday, August 18

8:00 am – 11:30 am

Atlantic Ballroom 3 — Renaissance Boston Waterfront

*This Event is Co-Sponsored by the ACS Divisions of Catalysis
Science & Technology and Inorganic Chemistry*

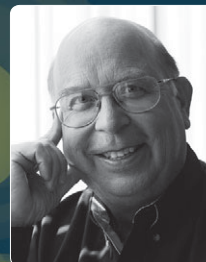
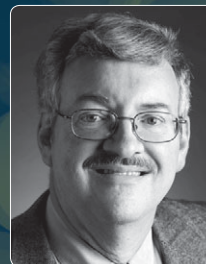


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research
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ACS Catalysis
IMPACT FACTOR

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 abstracts.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 service center located on Concourse Level 1, near Hall A of the Boston Convention & Exhibition Center (BCEC) that provides a range of services including copying, incoming and outgoing faxes, computer access, laser 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; 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 arrive together when 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 250th national meeting is now available at www.acs.org/boston2015. You can search by divisions or committees, symposia, speakers, or keywords from abstracts as well as presidential events and the multidisciplinary theme of “Innovation from Discovery to Application.”

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 on-site in Boston from August 16 to 20. 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 BCEC. You can have a USB flash drive shipped to you if you place your order before June 29, 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 www.proceedings.com/2256.html

Polymer Chemistry.

Kathy Mitchem, e-mail: kathyl@vt.edu



ACS
Chemistry for Life®

Boston 2015

Interdivisional
Poster Session
& Mixer

Monday, August 17th
Boston Convention & Exhibition 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. You can now access the **Sci-Mix** sessions on the free meeting mobile app. Download it today!

For more photo fun, prizes, and educational content, the Greener Meetings Team will be inside Sci-Mix. Join the fun...#ACSGreenerMeetings

TECHNICAL PROGRAM SUMMARY

Presidential Events

PRES

Diane Grob Schmidt, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Westin Boston Waterfront/Sheraton Boston Hotel/Boston Convention & Exhibition Center					
National Science Foundation's Centers for Chemical Innovation** IDA	D				
21st Century Chemistry Education: Formal & Informal**	P	A			
ACS Scholars: Rising Stars in Academe**		A			
ACS Scholars: Rising Stars in Industry**		P			
Transforming University-Industry Partnerships for an Innovative Future**			D		
Professional Legacy of Henry Hill* (PROF)	P				
The Chemistry Enterprise in 2015* (BMGT)		A			
Memories of Henry Hill: His Legacy in Science & in Professional Service* (HIST)		A			
Younger Chemists Exchanging More than Currency: First—Euros & Dollars; Next—Rupees, Rands & Reais* (YCC)		D			
Leadership Skills as a Strategic Advantage: The Chemist's Competitive Edge* (BMGT)		P			
The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)		P			
Henry A. Hill Centennial Symposium: Innovation in Polymer Science* (POLY)			D		
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		

Multidisciplinary Program Planning Group

MPPG

Meeting Theme: Innovation from Discovery to Application (IDA)

R. Wagner, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Innovation from Discovery to Application Plenary Session** IDA	P				
Innovation in Health & Medicine** IDA		A			

Multidisciplinary Program Planning Group (continued)

MPPG

Meeting Theme: Innovation from Discovery to Application (IDA)

R. Wagner, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Public Perception of the Chemistry Enterprise IDA		P			
The Fred Kavli Innovations in Chemistry Lecture IDA		P			
The Kavli Foundation Emerging Leader in Chemistry Lecture IDA		P			
The Future of Innovation Now** IDA		E			
Fifty Years of Innovation: The Legacy of the Westheimer Report** IDA			A		
Innovation in Materials for Emerging Uses** IDA			P		
Innovation in Chemical Synthesis** IDA				A	

Academic Employment Initiative

A E I

C. Kuniyoshi, J. Sostaric, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Academic Employment Initiative		E			

Division of Agricultural & Food Chemistry

AGFD

B. Park, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Bioactive Compounds from Fruits & Vegetables	D	A			
Phytonutrients: Thinking Beyond the "Essential" Nutrient Box	D				
Economically Motivated Food Adulteration: Interplay between Detection, Policy & Food Defense	D				
Modern Perspectives on Oxidation: Flavor Consequences in Foods & Beverages		P			
Food Toxicants Formed during Food Processing & Storage			D	A	

PROGRAM SUMMARY

Division of Agricultural & Food Chemistry (continued)

AGFD

B. Park, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Complex Coacervation: Principles & Applications**		D	D		
Metabolites & Metabolomics of Food Bioactives & Influence of Gut Microbiota: Chemistry & Health Effects		D			
Chemistry, Composition & Analysis of Dietary Supplements		P			
Sci-Mix		E			
Young Scientist Award Symposium			P		
Browned Flavors: Analysis, Formation & Physiology			D	A	
Recovery of Bioactive Compounds from Processing By-Products			D		
General Posters			P		
AGFD Division Award: Honoring Dr. Andrew Taylor			P		
Environmental Effect on Plant Volatile Formation & Nonvolatile Composition				D	
Challenges in Applied Flavor Sciences				D	
General Papers				P	A
Chemistry & Bioactivities of Natural Polymethoxyflavones				P	A
Undergraduate Research Posters* (CHED)		P			
The Future of Innovation Now* (MPPG)		E			
Journal of Agricultural & Food Chemistry Best Paper Awards* (AGRO)			A		
USDA-ARS Sterling B. Hendricks Memorial Lectureship: James H. Tumlinson* (AGRO)			A		
Current Topics in Chemical Safety Information* (CHAS)			D		
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		
Nanoparticles in Food, Agricultural & Environmental Settings* (COLL)					D

Division of Agrochemicals

AGRO

P. Rice, Program Chair

Boston Park Plaza Hotel & Towers	S	M	Tu	W	Th
Innovations in Agrochemical Discovery & Process Chemistry: 2015 Kenneth A. Spencer Award in Honor of Thomas Selby; 2015 AGRO Award for Innovation in the Chemistry of Agriculture in Honor of Tom Sparks				D	A
Combining Scientific Evidence for Health Policy & Regulation**	A				
Pesticide Dose: Effects on the Environment & Target & Non-Target Organisms**	D				
Insecticide Action on Ion Channels: A Tribute to Professor Toshio Narahashi	D				
Feeding the World Requires Pesticides & Maximum Residue Levels	D				
Protection of Agricultural Productivity, Public Health & the Environment	P				
Latest Trends in Environmental Fate & Exposure Assessments: Filling in Knowledge & Data Gaps across the Commodity Groups**	P				
Current Topics in Seed Treatment**	P				
Urban Agriculture: Turf, Ornamentals, Household Products & Water Re-Use**	P				
Global Research Needs: Identifying & Prioritizing Efforts To Sustain Environmental Quality**		A			
Metabolites from Endophytic Microorganism To Combat Biotic Stress in Crop Plants**		A			
Environmental Fate, Transport & Modeling of Agricultural Chemicals**		D			
Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications**		D			
Innovation in Metabolism, Bioavailability & Formulations Research Leading to the Discovery of Agrochemicals: Symposium Honoring Dr. Keith D. Wing; AGRO International Award for Research in Agrochemicals**		D			
Biochemical Biopesticides: Discovery & Regulation of New & Potential Products**		D			
Endangered Species Risk Assessment for Pesticides: Advances in Methods & Process**		P	D		
Sci-Mix		E			
Journal of Agricultural & Food Chemistry Best Paper Awards**			A		

PROGRAM SUMMARY

**Division of Agrochemicals
(continued)**

AGRO

P. Rice, Program Chair

Boston Park Plaza Hotel & Towers	S	M	Tu	W	Th
USDA-ARS Sterling B. Hendricks Memorial Lectureship: James H. Tumlinson**			A		
Immunochemistry Summit XII: Immunoassays & Other Bioanalytical Techniques**			D		
GMOs & the Entanglement of Intellectual Property Rights**			A		
Current Advances & Challenges of Arthropod Vector Control			D		
Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis & Ecological Effects**			D		
Pollinators & Agrochemicals**			D		
Pesticides & Hydrophobic Compounds in Sediment**				A	
Environmental Fate, Management & Mitigation of Nitrogen in Agricultural Systems**				A	
Degradation of Halogenated Compounds in the Environment**				D	D
Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage & Monitoring Data**				D	
Recent Advances in the Analysis of Environmental Contaminants in Foods & Feeds**				D	
Formulation Technologies for Improved Crop Protection**				D	
Structure Elucidation in Metabolism Studies: Plant, Animal & Soil**					P
Spray Application Technology**					D
Data to Decisions: Software Solutions for Modern Analytical Workflows**					P
Biomonitoring for Pesticide Exposures**					A
Hydrothermal Carbonization: Possibilities & Limits for Feedstocks, Processes & Applications* (ENVR)	D				E
National Science Foundation's Centers for Chemical Innovation* (PRES)	D				
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
Memories of Henry Hill: His Legacy in Science & in Professional Service* (HIST)		A			

**Division of Agrochemicals
(continued)**

AGRO

P. Rice, Program Chair

Boston Park Plaza Hotel & Towers	S	M	Tu	W	Th
ACS Scholars: Rising Stars in Academe* (PRES)	A				
Sensing of Environmentally Relevant Contaminants* (ENVR)	D			E	
ACS Scholars: Rising Stars in Industry* (PRES)	P				
The Future of Innovation Now* (MPPG)	E				
Reclamation, Remediation, Restoration: Novel Approaches to Environmental Challenges* (ENVR)			A	E	
Microorganism-Membrane Interactions: Towards Understanding Pathogen Removal & Membrane Biofouling* (ENVR)			A		
Transforming University-Industry Partnerships for an Innovative Future* (PRES)			D		
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		
Starting-Up & Spinning-Out: Commercializing Innovative Chemistry* (SCHB)			D		
Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas & Professor Mehmet A. Oturan* (ENVR)			P	DE	A
Computational Toxicology: From QSAR Models to Adverse Outcome Pathways* (CINF)					D
Detection & Fate of Health-Related Microorganisms in Water* (ENVR)					PE
Using Passive Sampling Techniques To Detect Organic Contaminants* (ENVR)					PE

*Cospponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

IDA: Innovation from Discovery to Application

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

PROGRAM SUMMARY

Division of Analytical Chemistry

A N Y L

D. Duckworth, Program Chair

Renaissance Boston Waterfront	S	M	Tu	W	Th
Analytical Chemistry Applications in Pharmaceutical Sciences	A				
Beyond Quant: Re-envisioning the Foundational Course in Analytical Chemistry	D				
Informatics 2.0 for the Analytical Sciences: Big Data, the Semantic Web & Metadata	P				
Forced Degradations in the Pharmaceutical Industry	P				
General Analytical	E				
Analytical Advances in Protein-DNA Thermodynamic Analysis		D			
Advances in Analytical Separations		D			
Addressing Challenges in Spectroscopy		D			
Sci-Mix		E			
2015 ACS Analytical Division Award Symposium			A		
Innovations in Analytical Chemistry & Their Application to National Security & Forensics* (CBRNE)			D	A	
Advanced Analytical Techniques for Early Cancer Screening			D		
Micro- & Nanoscale Innovations in Chromatography			P		
ACS Award in Analytical Chemistry: Honoring John R. Yates III			P		
Nanotechnology for Analytical Sensing & Spectroscopy-Based Applications				D	D
Analytical Advances in Mass Spectrometry				D	
Open-Air Analytical Measurements for Forensics, Health & Homeland Security				P	
New Developments & Applications of Electrochemistry					A
Challenges in Bioanalytical Chemistry					D
Current Topics in Seed Treatment* (AGRO)	P				
Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications* (AGRO)		D			
Undergraduate Research Posters* (CHED)		P			
Immunoassays & Other Bioanalytical Techniques: Immunochemistry Summit XII* (AGRO)			A		
Academic Innovations for Tomorrow's Industries: GSSPC Symposium* (CHED)			D		

Division of Analytical Chemistry (continued)

A N Y L

D. Duckworth, Program Chair

Renaissance Boston Waterfront	S	M	Tu	W	Th
Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis & Ecological Effects* (AGRO)			D		
Immunochemistry Summit XII: Immunoassays & Other Bioanalytical Techniques* (AGRO)			P		
Recent Advances in the Analysis of Environmental Contaminants in Foods & Feeds* (AGRO)				D	
Structure Elucidation in Metabolism Studies: Plant, Animal & Soil* (AGRO)					A
Data to Decisions: Software Solutions for Modern Analytical Workflows* (AGRO)					P

Division of Biological Chemistry

B I O L

C. Crews, V. Bandarian, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Young Investigator Symposium	A		P		
Current Topics in Biological Chemistry	E		E		
Pfizer Award in Enzyme Chemistry	P				
Gordon Hammes Award Lecture		A			
Repligen Award for the Chemistry of Biological Processes		P			
Sci-Mix		E			
Chemical Biology Approaches to Probe Ubiquitin-like Signaling			A		
Innovative Platforms for Drug Discovery, Diagnostics & Target Validation			P		
Eli Lilly Award in Biological Chemistry				A	
Graduate Student & Postdoctoral Symposium				P	
Advances in Oligonucleotide Therapeutics* (CARB)	D				
Metabolites from Endophytic Microorganisms To Combat Biotic Stress in Crop Plants* (AGRO)		A			
Innovation in Health & Medicine* (MPPG)		A			
Biochemical Biopesticides: Discovery & Regulation of New & Potential Products* (AGRO)		D			
Undergraduate Research Posters* (CHED)		P			

PROGRAM SUMMARY

Division of Business Development & Management

BMGT

K. Allen, J. Bryant, Program Chairs

Renaissance Boston Waterfront	S	M	Tu	W	Th
The Chemistry Enterprise in 2015**		A			
Leadership Skills as a Strategic Advantage: The Chemist's Competitive Edge**		P			
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)		A			
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		
Academic Innovations for Tomorrow's Industries: GSSPC Symposium* (CHED)			D		
Women in Innovation: Business & Commerce* (PROF)			P		

Division of Carbohydrate Chemistry

CARB

E. Rozners, Program Chair

Seaport Hotel and World Trade Center	S	M	Tu	W	Th
Advances in Oligonucleotide Therapeutics**	D				
Fundamental & Applied Aspects of Glyconanotechnology	D				
New Strategies & Applications of Aminoglycosides**		D			
Sci-Mix		E			
Glycolipid Immunostimulants**			D		
General Posters			E		
Carbohydrate Synthesis for Medicinal Chemistry & Biology				D	A
National Science Foundation's Centers for Chemical Innovation* (PRES)	D				
True Stories from Entrepreneurs: BRIC Edition* (SCHB)	P	A			
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
Memories of Henry Hill: His Legacy in Science & in Professional Service* (HIST)		A			
ACS Scholars: Rising Stars in Academe* (PRES)		A			
ACS Scholars: Rising Stars in Industry* (PRES)		P			

Division of Carbohydrate Chemistry (continued)

CARB

E. Rozners, Program Chair

Seaport Hotel and World Trade Center	S	M	Tu	W	Th
Transforming University-Industry Partnerships for an Innovative Future* (PRES)			D		
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		

Division of Catalysis Science & Technology

CATL

K. Ramasamy, Program Chair

Renaissance Boston Waterfront	S	M	Tu	W	Th
Nano Catalysis	D	D	D		
Symposium Honoring Gary Haller	D	D			
Role of the Outer Coordination Sphere on the Activity of Enzymes & Molecular Catalysts	D	D			
Metal Organic Frameworks for Catalysis Applications	D	D			
Single Atom Catalysis	D				
2015 ACS Catalysis Lectureship**		D	A		
Catalysis Poster Session		E			
Sci-Mix		E			
In Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles			A	D	P
SABIC Young Catalysis Investigator Award: Honoring Melanie Sanford			A		
Computational Catalysis			D	D	
Catalysis by Mixed Oxides			D	D	
CO ₂ Reduction & Utilization			P	D	A
Catalytic Upgrading of Biomass				D	P
Energy Storage Applications of Ammonia: Synthesis, Storage, Cracking & Utilization					A
General Catalysis					P
Biofuels for Powering the World: Discovery to Application* (ENFL)	D	A			
Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application* (ENFL)	D	D	A		

PROGRAM SUMMARY

Division of Catalysis Science & Technology (continued)

CATL

K. Ramasamy, Program Chair

Renaissance Boston Waterfront	S	M	Tu	W	Th
Advances in Ceria-Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion* (ENFL)	D	D	A		
Heterogeneous Catalysis for Environmental Applications* (ENVR)	P	D		E	
Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions* (COLL)		D	A		
International Symposium on Mesoporous Zeolites* (ENFL)				D	
Innovative Utilization Pathways for Natural Gas* (ENFL)				P	

Division of Chemical Education

CHED

I. Levy, I. Black, B. Rios-McKee, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
High School Program**	A				
Toxicology & Environmental Impact in the Chemistry Curriculum: Science & Strategies for Educators—State of the Art Symposium**	D	A			
General Papers	D			D	A
Undergraduate Research Papers**	D				
Education for Sustainable Development & Innovative Technologies across Culture**	P				
General Posters	E				
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits** <i>IDA</i>		A			
Citizens First! Using Real-World Contexts for Engaging Students in Learning Chemistry**		D			
Active Learning in the Chemistry Classroom		P	D		
Undergraduate Research Posters**		P			
Promoting Engaged Student Learning through the ACS Guidelines		P			
Incorporating Green Chemistry Innovations & Applications into the Classroom & Outreach**		P			
From Raw to Varoom: The Science behind Getting a Car on the Road** <i>IDA</i>		E			

Division of Chemical Education (continued)

CHED

I. Levy, I. Black, B. Rios-McKee, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Successful Student Chapters**		E			
Sci-Mix		E			
From Discovery to Application: Implementing the Last 50 Years of Innovation into the Undergraduate Chemistry Classroom			A		
Chemistry Education Research			D	A	
Academic Innovations for Tomorrow's Industries: GSSPC Symposium** <i>IDA</i>			D		
Process-Oriented Guided Inquiry Learning (POGIL)				A	
Teaching Organic Chemistry for Biology Majors				P	
Polymer Concepts in Inorganic Chemistry Courses**				P	
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
Wikipedia & Chemistry: Collaborations in Science & Education* (CINF)	P				
Younger Chemists Exchanging More Than Currency: First—Euros & Dollars; Next—Rupees, Rands & Reais* (YCC)			D		
Current Topics in Chemical Safety Information* (CHAS)				D	

Division of Chemical Health & Safety

CHAS

D. Decker, J. Pickel, F. Wood-Black, Program Chairs

Seaport Hotel and World Trade Center	S	M	Tu	W	Th
Lab Safety 25 Years after Promulgation of the OSHA Laboratory Standard**	P	A			
Chemical Health & Safety Awards**		P			
Current Topics in Chemical Safety Information** <i>IDA</i>			D		
Combining Scientific Evidence for Health Policy & Regulation* (AGRO)	A				
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
Transforming University-Industry Partnerships for an Innovative Future* (PRES)			D		

PROGRAM SUMMARY

Division of Chemical Information

C I N F

E. Davis, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
The Growing Impact of Big Data in the World of Chemical Information	A				
Substance Identifiers, Addressing the Challenges Presented by Chemically Modified Biologics: The Role of InChI & Related Technologies	A				
Applications of Cheminformatics to the Diverse World of Natural Products	A				
Visualizing Chemistry Data To Guide Optimization	P				
Wikipedia & Chemistry: Collaborations in Science & Education**	P				
CINF Scholarships for Scientific Excellence: Student Poster Competition	E				
CINFlash: Workflow Tools Lightning Round <i>IDA</i>	A				
Workflow Tools & Data Pipelining in Drug Discovery <i>IDA</i>		A			
Enabling Machines To “Read” the Chemical Literature: Techniques, Case Studies & Opportunities		D			
Retrosynthesis, Synthesis Planning, Reaction Prediction: When Will Computers Meet the Needs of the Synthetic Chemist?		D			
The Growing Impact of Openness in Chemistry: A Symposium in Honor of J. C. Bradley		P			
Sci-Mix		E			
Scientific Integrity: Can We Rely on the Published Scientific Literature?***			D		
Herman Skolnik Award Symposium** <i>IDA</i>			D		
Computational Toxicology: From QSAR Models to Adverse Outcome Pathways**				D	
Chemical Information Skills: The Essential Toolkit for Chemical Research				D	
Find the Needle in a Haystack: Mining Data from Large Chemical Spaces				D	
General Papers					D
Best in Class Computational Software by Integration* (COMP)	A				
Integrated Approaches in Structure-Based Drug Design* (COMP)	D				
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
Current Topics in Chemical Safety Information* (CHAS)			D		

Division of Chemical Toxicology

T O X I

A. C. Bryant-Friedrich, Program Chair

Westin Boston Waterfront	S	M	Tu	W	Th
Chemical Research in Toxicology Young Investigator Award Symposium	A				
General Poster Session	E				
Founders Award Lecture & Symposium	P				
Young Investigator Symposium		A			
New Approaches to the Study of Chemical Toxicology in Human Health: Accelerator Mass Spectrometry		P			
Sci-Mix		E			
The Exposome			A		
The Role of Gut Microbiota in Carcinogenesis			P		
Division of Chemical Toxicology Keynote Address				E	
General Papers				A	
DNA Polymerases: From Mutagenesis to Biotechnology				P	
Combining Scientific Evidence for Health Policy & Regulation* (AGRO)	A				
Global Research Needs: Identifying & Prioritizing Efforts To Sustain Environmental Quality* (AGRO)		A			
Innovation in Health & Medicine* (MPPG)		A			

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IDA: Innovation from Discovery to Application

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PROGRAM SUMMARY

Division of Chemistry & the Law

CHAL

K. Bianco, J. Hasford, J. Kennedy, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions	A				
Beyond the Bench: Careers in Intellectual Property	P				
Best Practices in Identifying, Protecting & Managing Your Intellectual Portfolio		A			
The Importance of Scientific Information in Patent-Related Endeavors		P			
Sci-Mix		E			
Developments in Pharmaceutical Patent Law			D		
Strategic Planning for Your IP Portfolio: Patents, Trade Secrets & Government Funding, What Should I Do?				D	
The Many Faces of CHAL: Where Chemistry Meets the Law					D
GMOs & the Entanglement of Intellectual Property Rights* (AGRO)			A		

Division of Colloid & Surface Chemistry

COLL

R. Nagarajan, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Basic Research in Colloids, Surfactants & Nanomaterials	D	D	A	D	D
Colloid-Polymer Architectures & Mixtures	D	D	A		
Biochemical Ligands at Interfaces: From Molecular-Scale Characterization to Devices	D	D			
<small>IDA</small> Theory & Modeling of Nanoparticles' Interactions with Biomolecules & Polymers	D				
Nanotheranostics for Cancer Applications	E			D	
Fundamental Research in Colloids, Surfaces & Nanomaterials	E				
Surface Modification to Control Cell/Surface Interactions		D	A		
Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions**		D	A		
30 Years of Langmuir: Looking Back & Forward			D		
Sci-Mix		E			

Division of Colloid & Surface Chemistry (continued)

COLL

R. Nagarajan, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Polymer & Biopolymer-Based Nanomaterials			A	D	D
Experimental & Computational Approaches to Reactions at the Surface of Colloidal Nano Materials, Facilitated by Photo Excitation & Charge Transfer			A		
Langmuir Lectures; NanoLetters Award Lecture; ACS Materials & Interfaces Award Lecture			P		
Nanomaterials for Defense & Homeland Security Applications				D	D
Metrology of Characterization, Simulation & Theory of Biomembranes				D	
Nanoparticles in Food, Agricultural & Environmental Settings**					D
Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility & Biological Impact* (PHYS)	D	D	A	D	A
Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies* (PHYS)	D	D	A	D	A
National Science Foundation's Centers for Chemical Innovation* (PRES)	D				
True Stories from Entrepreneurs: BRIC Edition* (SCHB)	P	A			
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
Memories of Henry Hill: His Legacy in Science & in Professional Service* (HIST)		A			
ACS Scholars: Rising Stars in Academe* (PRES)		A			
Complex Coacervation: Principles & Applications* (AGFD)		D	D		
The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)		P			
ACS Scholars: Rising Stars in Industry* (PRES)		P			
Transforming University-Industry Partnerships for an Innovative Future* (PRES)				D	
Starting Up & Spinning Out: Commercializing Innovative Chemistry* (SCHB)				D	
Big Chemistry from Small Businesses* (SCHB)					A

PROGRAM SUMMARY

Division of Computers in Chemistry

COMP

H. L. Woodcock, W. Cornell, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Best in Class Computational Software by Integration**	A				
Calculating pKas & Redox Potentials	D	D	D		
Molecular Mechanics	D	D			
Accelerated Discovery of Chemical Compounds: Design New Polymers & Inorganic Materials from Integration of Polymer Science, Materials Science & Informatics	D	P			
Designing Chemical Libraries for Screening: Past, Present & Future	D				
Integrated Approaches in Structure-Based Drug Design** <i>IDA</i>	D				
Measuring “Success” of Molecular Modeling Efforts	P				
Functional Polymers: Connecting Modeling & Experiment		A	D	D	A
Emerging Technologies in Computational Chemistry		A			
Quantum Chemistry		D	D	D	A
Molecular Dynamics Simulations in Drug Discovery		D	D		
Drug Discovery		P	D	D	A
Sci-Mix		E			
The OpenEye Outstanding Junior Faculty Award			E		
The Chemical Computing Group Excellence Award for Graduate Students			E		
NVIDIA GPU Award			E		
Poster Session			E		
Materials Science				D	A
Computational Study of Water				D	A

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Division of Computers in Chemistry (continued)

COMP

H. L. Woodcock, W. Cornell, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment* (PHYS)	D	D	A	A	
Electronic Structure Methods for Large Systems* (PHYS)	D	D	D	D	A
Molecular Biophysics: Revealing the Interplay between Different Forces & Effects in Biochemical Processes* (PHYS)	P	D	A	D	A
Undergraduate Research Posters* (CHED)		P			
Herman Skolnik Award Symposium* (CINF)			D		
Computational Toxicology: From QSAR Models to Adverse Outcome Pathways* (CINF)				D	

Division of Energy & Fuels

ENFL

A. Park, X. Wang, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Solar Energy & Solar Cells	D	A			
Biofuels for Powering the World: Discovery to Application**	D	A			
Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization & Storage**	D	A			
Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application**	D	D	A		
Porous Materials for Energy & Sustainability from Discovery to Application	D	D	D		
Advances in Ceria-Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion**	D	D	D		
Innovative Electrochemical Energy Storage	P	D	D	P	
Chemical Looping Innovation for Low-Carbon Energy	P	A			
Energy & Fuels Joint Award for Excellence in Publication: Honoring Phillip E. Savage	P				
Sci-Mix		E			
Energy & Fuels Storch Award in Fuel Science: Honoring Ripudaman Malhotra			D	A	
Advances in Chemistry of Energy & Fuels			P	D	A

PROGRAM SUMMARY

Division of Energy & Fuels (continued)

E N F L

A. Park, X. Wang, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
International Symposium on Mesoporous Zeolites**				D	
Advances in Analytical Methods for Petroleum Upstream Applications				D	
Innovative Utilization Pathways for Natural Gas**				P	
Next Generation Nanomaterials: Advances & Perspectives for Biomedicine, Energy & Environmental Protection* (ENVR)			D		
National Science Foundation's Centers for Chemical Innovation* (PRES)	D				
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
Memories of Henry Hill: His Legacy in Science & in Professional Service* (HIST)		A			
ACS Scholars: Rising Stars in Academe* (PRES)		A			
What's in Your Chemical Toolbox?*(SOCED)		P			
ACS Scholars: Rising Stars in Industry* (PRES)		P			
Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage & Materials* (ENVR)			D	DE	A
Transforming University-Industry Partnerships for an Innovative Future* (PRES)			D		
Academic Innovations for Tomorrow's Industries: GSSPC Symposium* (CHED)			D		
Advances in Chemistry for Carbon Capture, Utilization & Sequestration* (ENVR)				E	A

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Division of Environmental Chemistry

E N V R

D. Dionysiou, Program Chair

Boston Park Plaza Hotel & Towers	S	M	Tu	W	Th
Assessing Transformation Products by Non-Target & Suspected Target Screening: The New Frontier in Environmental Chemistry & Engineering	A				E
New Challenges in Water Quality, Treatment, Reuse & Sustainability: Chemistry & Application of Advanced Oxidation Processes for Removal of Contaminants of Concern & Transformation Products**	D	D	D	E	
Hydrothermal Carbonization: Possibilities & Limits for Feedstocks, Processes & Applications**	D				E
Advances in Drinking Water Disinfection: By-products' Occurrence, Formation, Treatment, Health Effects, Epidemiology & Regulation	D				E
Nano-enabled Environmental Technologies	D				E
Designing Safer Chemicals**	D				
Heterogeneous Catalysis for Environmental Applications**	P	D			E
Green Chemistry & the Environment**		D	A		E
Sensing of Environmentally Relevant Contaminants**		D			E
Advanced Materials & Technologies for Desalination & Wastewater Reuse		D			E
ACS Award for Creative Advances in Environmental Science & Technology: Honoring Dr. Paul B. Shepson		D			
Sci-Mix		E			
Reclamation, Remediation, Restoration: Novel Approaches to Environmental Challenges**			A		E
Microorganism-Membrane Interactions: Toward Understanding Pathogen Removal & Membrane Biofouling**			A		
Next Generation Nanomaterials: Advances & Perspectives for Biomedicine, Energy & Environmental Protection**			D		
Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage & Materials**			D	DE	A
Environmental Applications & Implications of Graphene-Based Nanomaterials			D		E

PROGRAM SUMMARY

Division of Environmental Chemistry (continued)

ENVR

D. Dionysiou, Program Chair

Boston Park Plaza Hotel & Towers	S	M	Tu	W	Th
Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas & Professor Mehmet A. Oturan**			P	DE	A
C. Ellen Gonter Awards Symposium			P		
The Debate: How Do We Respond to Climate Change?***			P		
Status & Trends of Biological & Persistent Organic Chemicals in the Great Lakes				A	
Anaerobic Sewage Treatment: Dissolved Methane & Nitrogen Control				AE	
Environmental Transformation of Nanoparticles: Processes, Mechanisms & Ecological Impacts				DE	A
Resource Recovery & Contaminant Elimination in Waste Streams of Increasing Concern				DE	A
Detection & Fate of Health-Related Microorganisms in Water**				PE	
Using Passive Sampling Techniques To Detect Organic Contaminants**				PE	
Advances in Chemistry for Carbon Capture, Utilization & Sequestration**				E	A
General Posters				E	
Biofuels for Powering the World: Discovery to Application* (ENFL)	D	A			
Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization & Storage* (ENFL)	D	A			
Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds* (PHYS)	D	D	D	D	A
Pesticide Dose: Effects on the Environment & Target & Non-Target Organisms* (AGRO)	D				
Latest Trends in Environmental Fate & Exposure Assessments: Filling in Knowledge & Data Gaps across the Commodity Groups* (AGRO)	P				
Current Topics in Seed Treatment* (AGRO)	P				
Urban Agriculture: Turf, Ornamentals, Household Products & Water Re-use* (AGRO)	P				
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)		A			

Division of Environmental Chemistry (continued)

ENVR

D. Dionysiou, Program Chair

Boston Park Plaza Hotel & Towers	S	M	Tu	W	Th
Global Research Needs: Identifying & Prioritizing Efforts To Sustain Environmental Quality* (AGRO)		A			
ACS Scholars: Rising Stars in Academe* (PRES)		A			
Environmental Fate, Transport & Modeling of Agricultural Chemicals* (AGRO)		D			
Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications* (AGRO)		D			
Endangered Species Risk Assessment for Pesticides: Advances in Methods & Process* (AGRO)		P	D		
Undergraduate Research Posters* (CHED)		P			
What's in Your Chemical Toolbox?* (SOCED)		P			
ACS Scholars: Rising Stars in Industry* (PRES)		P			
Immunochemistry Summit XII: Immunoassays & Other Bioanalytical Techniques* (AGRO)				D	
GMOs & the Entanglement of Intellectual Property Rights* (AGRO)				A	
Transforming University-Industry Partnerships for an Innovative Future* (PRES)				D	
Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis & Ecological Effects* (AGRO)				D	
Pollinators & Agrochemicals* (AGRO)				D	
Subsurface Geochemistry for Energy & the Environment* (GEOC)				P	D
Pesticides & Hydrophobic Compounds in Sediment* (AGRO)					A
Environmental Fate, Management & Mitigation of Nitrogen in Agricultural Systems* (AGRO)					A
Degradation of Halogenated Compounds in the Environment* (AGRO)					D D
Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage & Monitoring Data* (AGRO)					D
Recent Advances in the Analysis of Environmental Contaminants in Foods & Feeds* (AGRO)					D

PROGRAM SUMMARY

Division of Environmental Chemistry (continued)

ENVR

D. Dionysiou, Program Chair

Boston Park Plaza Hotel & Towers	S	M	Tu	W	Th
Formulation Technologies for Improved Crop Protection* (AGRO)				D	
Computational Toxicology: From QSAR Models to Adverse Outcome Pathways* (CINF)				D	
Spray Application Technology* (AGRO)					D
Data to Decisions: Software Solutions for Modern Analytical Workflows* (AGRO)					P
Biomonitoring for Pesticide Exposures* (AGRO)					A

Division of Fluorine Chemistry

FLUO

V. Petrov, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Radiochemistry**		D	A		

Division of Geochemistry

GEOC

Y. Jun, Program Chair

Seaport Hotel and World Trade Center	S	M	Tu	W	Th
Structure & Reactivity of Mineral-Fluid Interfaces		D	A		
Sci-Mix		E			
Subsurface Geochemistry for Energy & the Environment**			P	D	
General Geochemistry Session					A
Biogeochemical Cycling of Nutrients & Contaminants in Physically Complex Environments					A
Undergraduate Research Posters* (CHED)		P			
Transformation & Transport of Radionuclides in the Environment* (NUCL)			P		

Division of the History of Chemistry

HIST

S. Rasmussen, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Edwin Land & Instant Photography: Massachusetts's First National Historic Chemical Landmark	P				
Memories of Henry Hill: His Legacy in Science & in Professional Service**		A			
HIST Tutorial & General Papers**		P			
Sci-Mix		E			
HIST Award Symposium Honoring Christoph Meinel			P		
Professional Legacy of Henry Hill* (PROF)	P				
The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)		P			
Fifty Years of Innovation: The Legacy of the Westheimer Report* (MPPG)				A	
Henry A. Hill Centennial Symposium: Innovation in Polymer Science* (POLY)				D	

Division of Industrial & Engineering Chemistry

I & EC

P. Smith, Program Chair

Renaissance Boston Waterfront	S	M	Tu	W	Th
Symposium in Honor of the 2013 & 2014 ACS Fellows in the Division of Industrial & Engineering Chemistry	A				
Industrial & Engineering Fellow: Honoring Kenneth L. Nash	D	A			
Industrial & Engineering Fellow: Honoring Henry C. (Hank) Foley	P				
Industrial & Engineering Fellow: Honoring Gary M. Seabolt		P			
Sci-Mix		E			
Industrial & Engineering Chemistry Division Graduate Student Award Symposium			A		
Green Chemistry Makes a Difference: Pharmaceutical Industry/Academic Collaborations**			P		
General Posters			E		
General Papers				D	A
True Stories from Entrepreneurs: BRIC Edition* (SCHB)	P	A			

PROGRAM SUMMARY

Division of Industrial & Engineering Chemistry (continued) I & E C

P. Smith, Program Chair

Renaissance Boston Waterfront	S	M	Tu	W	Th
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)		A			
Undergraduate Research Posters* (CHED)		P			
Incorporating Green Chemistry Innovations & Applications into the Classroom & Outreach* (CHED)		P			
The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)		P			
Starting Up & Spinning Out: Commercializing Innovative Chemistry* (SCHB)			D		
Big Chemistry from Small Businesses* (SCHB)				A	
International Symposium on Mesoporous Zeolites* (ENFL)				D	

Division of Inorganic Chemistry I N O R

S. Koch, N. Radu, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Solid-State Inorganic Chemistry	A		E	A	
Main Group Chemistry	AE			A	
Chemistry of Materials	D	D	DE	D	
Bioinorganic Chemistry	AE	P	P	PE	
Organometallic Chemistry	DE		DE	DE	
Coordination Chemistry	D		PE	D	
Metalloenzyme Mechanisms	P	A			
Inorganic Catalysts	P			PE	
Inorganic Young Investigator Awards	P				
Synthetic Chemistry Approaches to Magnetic Materials	PE	D	A		
Lanthanide & Actinide Chemistry	E	A		A	

Division of Inorganic Chemistry (continued) I N O R

S. Koch, N. Radu, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Building Innovative Solid-State Materials through Solution Chemistry	E	P			
Nanoscience	E			D	
Environmental & Energy-Related Inorganic Chemistry	AE		A		
Inorganic Chemistry Lectureship		A			
Industrial Inorganic Chemistry: Innovation from Discovery to Applications		A			
Molecular Water Oxidation Catalysis		D	A		
High-Energy Organometallic Complexes: Reactivity Driving New Synthesis & Catalysis		P	D		
Metalloprotein Inhibitors: Drugs, Drug Candidates & New Targets at the Interface of Medicinal & Inorganic Chemistry		P			
Sci-Mix		E			
Inorganic Nanoscience Award			A		
Electrochemistry			AE		
Inorganic Spectroscopy			AE		
Transition-Metal-Catalyzed Olefin Polymerization: Toward Structure Control* (PMSE)	D	D	A		
2015 ACS Catalysis Lectureship* (CATL)		D	A		
Undergraduate Research Posters* (CHED)		P			
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)				D	
Innovation in Chemical Synthesis* (MPPG)					A
International Symposium on Mesoporous Zeolites* (ENFL)					D
Polymer Concepts in Inorganic Chemistry Courses* (CHED)					P

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PROGRAM SUMMARY

Division of Medicinal Chemistry

MEDI

W. Young, S. Plumlee, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
NeuroInflammation	A				
Evolution of Natural Product Research in Drug Discovery	A				
General Orals	D		P	D	
Protein-Protein Interactions	P				
General Posters	E			E	
Ophthalmic Drug Discovery	A				
Emerging Antibody Drug Conjugates: Applications of Medicinal Chemistry	A				
Advances in Predictive Toxicology	D				
Strategies in the Design & Characterization of Allosteric Inhibitors	P				
Cancer Immunotherapy: The Next Big Thing for Small Molecules	P				
Sci-Mix	E				
Medicinal Chemistry Toolbox: Understanding the Roles of Inducible Pockets, Water & Small Structural Changes			A		
MEDI Award Symposia			A		
Deuterated Drugs			P		
Case Studies of Successful Drugs			P		
Targeted Covalent Inhibitors				A	
Recent Advances in Heart Failure				A	
First-Time Disclosures				P	
Integrated Approaches in Structure-Based Drug Design* (COMP)	D				
Advances in Oligonucleotide Therapeutics* (CARB)	D				
Innovation from Discovery to Application Plenary Session* (MPPG)	P				
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)	A				
Innovation in Health & Medicine* (MPPG)	A				
Radiochemistry* (FLUO)	D	A			
New Strategies & Applications of Aminoglycosides* (CARB)	D				
Undergraduate Research Posters* (CHED)	P				
The Future of Innovation Now* (MPPG)	E				

Division of Medicinal Chemistry (continued)

MEDI

W. Young, S. Plumlee, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Transforming University-Industry Partnerships for an Innovative Future* (PRES)			D		
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		
Glycolipid Immunostimulants* (CARB)			D		
Herman Skolnik Award Symposium* (CINF)			D		
Innovation in Chemical Synthesis* (MPPG)				A	
Computational Toxicology: From QSAR Models to Adverse Outcome Pathways* (CINF)				D	

Division of Nuclear Chemistry & Technology

NUCL

J. Terry, D. Hobart, Program Chairs

Seaport Hotel and World Trade Center	S	M	Tu	W	Th
Analytical Chemistry in Nuclear Technology	P	D			
Transformation & Transport of Radionuclides in the Environment**			P		
General Topics in Nuclear & Radiochemistry				D	

Division of Organic Chemistry

ORGN

M. McIntosh, R. Broene, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
New Reactions & Methodology	D	D	D	D	
Molecular Recognition & Self-Assembly	D	D			
Asymmetric Reactions & Syntheses	D	D			
Nanomaterials	D				
Peptides, Proteins & Amino Acids	D				
Small Splash, Big Waves: Research at Primarily Undergraduate Institutions	P				
JOC/OL Lectureship Symposium	P				
Asymmetric Reactions & Syntheses; Chemistry of Fullerenes, Carbon Nanotubes & Graphene; Materials, Devices & Switches; Nanomaterials; Physical Organic	E				
Magnetically Recyclable Nanocatalysts		A			

PROGRAM SUMMARY

**Division of Organic Chemistry
(continued)**

ORGN

M. McIntosh, R. Broene, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Process Chemistry: New Developments in Pharmaceutical Process Development		A			
Teva Pharmaceuticals Scholars Grant Symposium		A			
Young Investigator Symposium		D			
Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species		P	D		
Green Chemistry Makes a Difference: Pharmaceutical Industry/Academic Collaborations		P			
Tetrahedron Prize for Creativity in Organic Chemistry Symposium		P			
Sci-Mix		E			
Metal-Mediated Reactions & Syntheses			D	D	
Materials, Devices & Switches			D	P	
Total Synthesis of Complex Molecules			D		
Young Academic Investigator Symposium			D		
Cope Award Symposium			D		
Biologically Related Molecules & Processes; Innovation from Discovery to Application; Metal-Mediated Reactions & Syntheses; Molecular Recognition & Self-Assembly; Peptides, Proteins & Amino Acids			E		
Frontiers of Functional Interfaces				A	
On the Importance of Synthetic Organic Chemistry in Drug Discovery				A	
Heterocycles & Aromatics				D	A
Biologically Related Molecules & Processes				D	A
Technical Achievements in Organic Chemistry Symposium				D	
Heterocycles & Aromatics; New Reactions & Methodology				E	
Flow Chemistry & Continuous Processes					A
Chemistry of Fullerenes, Carbon Nanotubes & Graphene					A
Advances in Oligonucleotide Therapeutics* (CARB)	D				
Professional Legacy of Henry Hill* (PROF)	P				

**Division of Organic Chemistry
(continued)**

ORGN

M. McIntosh, R. Broene, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Innovation in Metabolism, Bioavailability & Formulations Research Leading to the Discovery of Agrochemicals: Symposium Honoring Dr. Keith D. Wing, AGRO International Award for Research in Agrochemicals* (AGRO)		D			
Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage & Materials* (ENVR)			D	DE	A
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		
Glycolipid Immunostimulants* (CARB)			D		
Green Chemistry Makes a Difference: Pharmaceutical Industry/Academic Collaborations* (I&EC)			P		
Innovation in Chemical Synthesis* (MPPG)					A
Formulation Technologies for Improved Crop Protection* (AGRO)				D	
Using Passive Sampling Techniques To Detect Organic Contaminants* (ENVR)					PE

Division of Physical Chemistry

PHYS

E. Sibert, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability & Spectroscopic Signatures <i>IDA</i>	D	A	A	D	A
From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment**	D	D	A	A	
Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility & Biological Impact**	D	D	A	D	A
Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies** <i>IDA</i>	D	D	A	D	A
Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds** <i>IDA</i>	D	D	D	D	A

PROGRAM SUMMARY

**Division of Physical Chemistry
(continued)**

PHYS

E. Sibert, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Electronic Structure Methods for Large Systems**	D	D	D	D	A
Materials for Heat to Energy Conversion <i>IDA</i>	D	D			
Physical Chemistry of Clusters & Nanoparticles <i>IDA</i>	D	P	A	D	A
Molecular Biophysics: Revealing the Interplay between Different Forces & Effects in Biochemical Processes**	P	D	A	D	A
Hydrophobicity, Ion Solvation & Interfaces: Theory, Simulations & Experiments		D	A	D	A
Sci-Mix		E			
Award Symposium			P		
Poster Session				E	
Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage & Materials* (ENVR)			D	DE	A
Academic Innovations for Tomorrow's Industries: GSSPC Symposium* (CHED)			D		
Innovation in Materials for Emerging Uses* (MPPG)			P		

Division of Polymer Chemistry

POLY

T. White, D. Boday, M. Jeffries-El, K. Mitchem, Program Chairs

Westin Boston Waterfront	S	M	Tu	W	Th
Protein-Like Structure & Activity in Synthetic Systems	D	A	AE		
Surface Modification of Polymeric Materials	D	A	E		
Silicones	D	D	DE		
General Topics: New Synthesis & Characterization of Polymers	D	D	E	D	D
Herman Mark Scholars Award Symposium in Honor of Stuart Rowan	D				
Ring Opening Polymerization		A	E		D
Biomacromolecules/Macromolecules Young Investigator Award		P			
Herman Mark Award Symposium in Honor of Timothy Lodge		P			
Industrial Innovations in Polymer Chemistry		P			
Sci-Mix		E			

**Division of Polymer Chemistry
(continued)**

POLY

T. White, D. Boday, M. Jeffries-El, K. Mitchem, Program Chairs

Westin Boston Waterfront	S	M	Tu	W	Th
Value of Basic Research in Solving Industrial Polymer Problems			A		
Henkel Award for Outstanding Graduate Research in Polymer Chemistry			A		
Henry A. Hill Centennial Symposium: Innovation in Polymer Science**			D		
Value of Basic Research to Industrial Polymer Science—A Senior Chemist's Perspective			A		
Multicomponent & Sequential Reactions in Polymer Science: Efficient Synthesis of Structurally Diverse Polymers			PE	D	A
Ionic Liquids in Polymer Design: From Energy to Health			PE	D	D
Charles Overberger Award Symposium in Honor of Krzysztof Matyjaszewski				D	
Herman Mark Young Scholars Award Symposium in Honor of Bradley Olsen				D	
Innovation from Discovery to Application Plenary Session* (MPPG)	P				
Professional Legacy of Henry Hill* (PROF)	P				
Memories of Henry Hill: His Legacy in Science & in Professional Service* (HIST)	A				
Undergraduate Research Posters* (CHED)		P			
The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)		P			
From Raw to Varoom: The Science behind Getting a Car on the Road* (CHED)		E			
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)				D	
Academic Innovations for Tomorrow's Industries: GSSPC Symposium* (CHED)				D	
Innovation in Materials for Emerging Uses* (MPPG)				P	
Joint PMSE/POLY Poster Session* (PMSE)				E	
Polymer Concepts in Inorganic Chemistry Courses* (CHED)					P
Joint PMSE/POLY Awards Reception & Plenary Lecture* (PMSE)					E

PROGRAM SUMMARY

Division of Polymeric Materials: Science & Engineering

PMSE

C. Soles, C. Stafford, A. Tsou, Program Chairs

Westin Boston Waterfront	S	M	Tu	W	Th
Eastman Chemical Student Award in Applied Polymer Science	A				
Transition-Metal-Catalyzed Olefin Polymerization: Toward Structure Control**	D	D	A		
Advanced Materials for High Performance Formulations <i>IDA</i>	D	D			
Phase Separation & Morphology Development in Polymers	D	D			
Patterning Materials for Bio-Interface	D				
Journal of Polymer Science Award Symposium	P				
Materials for Printed Electronics		D	D	A	
New Advances in Nanostructured Polymeric Membranes for Filtration		D	D		
Sci-Mix		E			
Celebrating 50 Years of Polymer Science & Engineering			D	D	
Roy W. Tess Award: Honoring Jamil Baghdachi			D		
Adhesion Science & Adhesive Materials			P	D	D
Joint PMSE/POLY Poster Session**			E		
General Papers/New Concepts in Polymeric Materials				D	D
Joint PMSE/POLY Awards Reception & Plenary Lecture**				E	
Professional Legacy of Henry Hill* (PROF)	P				
Innovation from Discovery to Application Plenary Session* (MPPG)	P				
Undergraduate Research Posters* (CHED)		P			
From Raw to Varoom: The Science behind Getting a Car on the Road* (CHED)		E			
The Future of Innovation Now* (MPPG)		E			
Henry A. Hill Centennial Symposium: Innovation in Polymer Science* (POLY)			D		
Innovation in Materials for Emerging Uses* (MPPG)			P		
Polymer Concepts in Inorganic Chemistry Courses* (CHED)				P	

Division of Professional Relations

PROF

R. D. Libby, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Professional Legacy of Henry Hill**	P				
Getting Your First Industrial Job**		A			
Chemical Angel Network: Chemists Investing in Chemical Companies** <i>IDA</i>		P			
Checklist for Turning Thirty**			A		
Women in Innovation: Business & Commerce** <i>IDA</i>			P		
Opportunities for U.S./Cuba Collaboration in Chemistry, Chemical Engineering & Chemistry Education* (IAC)	A				
National Science Foundation's Centers for Chemical Innovation* (PRES)	D				
True Stories from Entrepreneurs: BRIC Edition* (SCHB)	P	A			
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
The Chemistry Enterprise in 2015* (BMGT)		A			
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)		A			
Memories of Henry Hill: His Legacy in Science & in Professional Service* (HIST)	A				
Managing Transitions* (WCC)		A			
ACS Scholars: Rising Stars in Academe* (PRES)		A			
Younger Chemists Exchanging More Than Currency: First—Euros & Dollars; Next—Rupees, Rands & Reais* (YCC)		D			
Leadership Skills as a Strategic Advantage: The Chemist's Competitive Edge* (BMGT)		P			
The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)		P			
ACS Scholars: Rising Stars in Industry* (PRES)		P			
Transforming University-Industry Partnerships for an Innovative Future* (PRES)			D		
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		
Starting-Up & Spinning-Out: Commercializing Innovative Chemistry* (SCHB)			D		

PROGRAM SUMMARY

Division of Professional Relations (continued)

PROF

R. D. Libby, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Henry A. Hill Centennial Symposium: Innovation in Polymer Science* (POLY)			D		
Big Chemistry from Small Businesses* (SCHB)				A	

Division of Small Chemical Businesses

SCHB

J. Sabol, Program Chair

Westin Boston Waterfront	S	M	Tu	W	Th
Entrepreneurs' Poster Session <i>IDA</i>	A				
True Stories from Entrepreneurs: BRIC Edition**	P	A			
The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector** <i>IDA</i>		P			
Sci-Mix		E			
Starting-Up & Spinning-Out: Commercializing Innovative Chemistry** <i>IDA</i>			D		
Big Chemistry from Small Businesses** <i>IDA</i>				A	
National Science Foundation's Centers for Chemical Innovation* (PRES)	D				
Professional Legacy of Henry Hill* (PROF)	P				
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)		A			
Memories of Henry Hill: His Legacy in Science & in Professional Service* (HIST)	A				
ACS Scholars: Rising Stars in Academe* (PRES)		A			
Chemical Angel Network: Chemists Investing in Chemical Companies* (PROF)		P			
ACS Scholars: Rising Stars in Industry* (PRES)		P			
GMOs & the Entanglement of Intellectual Property Rights* (AGRO)			A		
Transforming University-Industry Partnerships for an Innovative Future* (PRES)			D		
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace* (IAC)			D		
Women in Innovation: Business & Commerce* (PROF)			P		

International Activities Committee

I A C

H. N. Cheng, A. Rimando, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Opportunities for U.S./Cuba Collaboration in Chemistry, Chemical Engineering & Chemistry Education**	A				
International Entrepreneurship: How To Start a Business & Thrive in the Global Marketplace**			D		
True Stories from Entrepreneurs: BRIC Edition* (SCHB)	P	A			
Younger Chemists Exchanging More Than Currency: First—Euros & Dollars; Next—Rupees, Rands & Reais* (YCC)			D		

Society Committee on Education

SOCED

G. Muller, Program Chair

Boston Convention & Exhibition Center	S	M	Tu	W	Th
What's in Your Chemical Toolbox?***		P			
High School Program* (CHED)	A				
Undergraduate Research Papers* (CHED)	D				
21st Century Chemistry Education: Formal & Informal* (PRES)	P	A			
Undergraduate Research Posters* (CHED)		P			
Incorporating Green Chemistry Innovations & Applications into the Classroom & Outreach* (CHED)		P			
Successful Student Chapters* (CHED)		E			

Women Chemists Committee

W C C

A. Debaille, K. Woznick, Program Chairs

Sheraton Boston Hotel	S	M	Tu	W	Th
Managing Transitions**		A			
Women in Innovation: Business & Commerce* (PROF)			P		

PROGRAM SUMMARY

Younger Chemists Committee

Y C C

A. Gavrilenko, T. Matos, Program Chairs

Seaport Hotel and World Trade Center	S	M	Tu	W	Th
Younger Chemists Exchanging More Than Currency: First—Euros & Dollars; Next—Rupees, Rands & Reais**		D			
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)		A			
Getting Your First Industrial Job* (PROF)		A			
ACS Scholars: Rising Stars in Academe* (PRES)		A			
Green Chemistry & the Environment* (ENVR)		D	A	E	
Leadership Skills as a Strategic Advantage: The Chemist's Competitive Edge* (BMGT)		P			
ACS Scholars: Rising Stars in Industry* (PRES)		P			
Checklist for Turning Thirty* (PROF)			A		
Starting-Up & Spinning-Out: Commercializing Innovative Chemistry* (SCHB)			D		
Women in Innovation: Business & Commerce* (PROF)			P		

Consultative Committee on Metrology in Chemistry & Biology

CCQM

W. May, R. Wielgosz, Program Chairs

Boston Convention & Exhibition Center	S	M	Tu	W	Th
Chemistry & the International System of Weights & Measures				D	

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

IDA: Innovation from Discovery to Application

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

TOXI

Division of Chemical Toxicology

A. Bryant-Friedrich, Program Chair

Note:

Times represent the start of oral presentations and numbers represent poster numbers.

3. Locate the session name

SUNDAY MORNING

Section A

Westin Boston Waterfront
Harbor Blrm II

2. Locate the day

4. Locate the time or poster #

Chemical Research in Toxicology Young Investigator Award Symposium

P. J. Beuning, Organizer, Presiding

8:00 Award Presentation.

5. Locate the venue and room for each session

8:15 **TOXI 1.** Multiple conformations of a chimeric Y-family polymerase define a pathway for docking primer-template



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- Learn about the newest ACS Journals from ACS Publications, including Editors' Choice
- Discuss how to achieve your career goals with ACS Career Navigator™
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- Enter contests and receive giveaways, including tablets, gift cards, photos and more!



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EXHIBIT HOURS

Sunday, March 22 • 6:00 pm – 8:30 pm

Monday, March 23 • 9:00 am – 5:00 pm

Tuesday, March 24 • 9:00 am – 5:00 pm

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.

FULL TECHNICAL PROGRAM

TWENTY-NINE OF THE SOCIETY'S technical divisions and four committees are hosting original technical programming during the meeting. More than 9,000 papers have been accepted for this meeting.

Each organizing group's programming is detailed on the following pages.

Nearly 4,000 chemical professionals and students are expected to attend the ever-popular Sci-Mix Interdivisional Poster Session & Mixer on Monday,

August 17 from 8:00 to 10:00 PM at the Boston Convention & Exhibition Center, Hall C. More than 500 noteworthy poster presentations, networking with colleagues, and light refreshments make up this enjoyable event.

Organizing Group	Acronym	Page
PRESIDENTIAL & CROSS-DIVISION PROGRAMMING		
Presidential Events	PRES	TECH-70
Multidisciplinary Program Planning Group	MPPG	TECH-71
Academic Employment Initiative	AEI	TECH-72

DIVISION PROGRAMMING

Agricultural & Food Chemistry	AGFD	TECH-74
Agrochemicals	AGRO	TECH-80
Analytical Chemistry	ANYL	TECH-89
Biochemical Technology	BIOT	TECH-95
Biological Chemistry	BIOL	TECH-95
Business Development & Management	BMGT	TECH-98
Carbohydrate Chemistry	CARB	TECH-99
Catalysis Science and Technology	CATL	TECH-101
Cellulose & Renewable Materials	CELL	TECH-110
Chemical Education	CHED	TECH-110
Chemical Health & Safety	CHAS	TECH-118
Chemical Information	CINF	TECH-119
Chemical Toxicology	TOXI	TECH-123
Chemistry & the Law	CHAL	TECH-125
Colloid & Surface Chemistry	COLL	TECH-126
Computers in Chemistry	COMP	TECH-136
Energy & Fuels	ENFL	TECH-144
Environmental Chemistry	ENVR	TECH-153
Fluorine Chemistry	FLUO	TECH-166
Geochemistry	GEOC	TECH-166
History of Chemistry	HIST	TECH-168
Industrial & Engineering Chemistry	I&EC	TECH-169

Organizing Group	Acronym	Page
Inorganic Chemistry	INOR	TECH-171
Medicinal Chemistry	MEDI	TECH-185
Nuclear Chemistry & Technology	NUCL	TECH-195
Organic Chemistry	ORGN	TECH-196
Physical Chemistry	PHYS	TECH-209
Polymer Chemistry	POLY	TECH-221
Polymeric Materials Science & Engineering	PMSE	TECH-230
Professional Relations	PROF	TECH-239
Rubber	RUBB	TECH-240
Small Chemical Businesses	SCHB	TECH-240

COMMITTEE PROGRAMMING (In order of appearance)

Committee on Chemical Safety	CCS	TECH-241
Committee on Corporation Associates	CORP	TECH-242
Committee on Divisional Activities	DAC	TECH-242
Committee on Economic and Professional Affairs	CEPA	TECH-242
Committee on Environmental Improvement	CEI	TECH-242
Committee on Ethics	ETHC	TECH-242
Committee on Minority Affairs	CMA	TECH-243
Committee on Nomenclature, Terminology and Symbols	NTS	TECH-243
Committee on Science	COMSCI	TECH-243
International Activities Committee	IAC	TECH-243
Senior Chemists Committee	SCC	TECH-243
Society Committee on Education	SOCED	TECH-244
Women Chemists Committee	WCC	TECH-244
Younger Chemists Committee	YCC	TECH-244
Consultative Committee on Metrology in Chemistry and Biology	CCQM	TECH-245

PRES

Presidential Events

Diane Grob Schmidt, Program Chair

SUNDAY MORNING

Section A

Westin Boston Waterfront
Burroughs RoomNational Science Foundation's
Centers for Chemical InnovationCospponsored by AGRO, CARB,
COLL, ENFL, PROF and SCHB

S. Dasgupta, Organizer, Presiding

8:30 PRES 1. NSF Centers for Chemical
Innovation Program overview. K.J. Covert**8:40 PRES 2.** Solar fuels. H.B. Gray**9:10 PRES 3.** Center for Enabling
New Technologies Through
Catalysis. K.I. Goldberg**9:40 PRES 4.** Center for Selective C-H
Functionalization. H.M. Davies**10:10** Intermission.**10:40 PRES 5.** Center for Chemistry at
the space-time limit. V.A. Apkarian**11:10 PRES 6.** Center for Chemical
Evolution. N.V. HudOpportunities for US/Cuba
Collaboration in Chemistry, Chemical
Engineering and Chemistry EducationSponsored by IAC, Cospponsored
by COMSCI, PRES and PROF

SUNDAY AFTERNOON

Section A

Westin Boston Waterfront
BurroughsNational Science Foundation's
Centers for Chemical InnovationCospponsored by AGRO, CARB,
COLL, ENFL, PROF and SCHB

S. Dasgupta, Organizer, Presiding

1:30 PRES 7. Center for Sustainable
Materials Chemistry. D.A. Keszler**2:00 PRES 8.** Overview of Center for
Aerosol Impacts on climate and the
environment. K.A. Prather, V.H. Grassian**2:30 PRES 9.** The Center for Sustainable
Polymers. M.A. Hillmyer

Technical program information
known at press time.
The official technical program
for the 250th ACS National
Meeting is available at:
www.acs.org/boston2015

Section A

Westin Boston Waterfront
GalleriaNational Science Foundation's
Centers for Chemical InnovationCospponsored by AGRO, CARB,
COLL, ENFL, PROF and SCHB

S. Dasgupta, Organizer

3:00 - 6:00**PRES 10.** Spontaneous formation and assem-
bly of potentially prebiotic nucleosides
in water. B. Cafferty, M. Chen, D.M. Fialho,
I. Gállego, R. Krishnamurthy, N.V. Hud**PRES 11.** Investigations on the emergence of
peptides on the prebiotic earth. J. Forsythe**PRES 12.** Potential emergence of RNA
from chimeric pre-RNA scaffolds.
T.C. Eftthymiou, K. Kim, J.V. Gavette, B. Cafferty,
C.L. Musetti, N.V. Hud, R. Krishnamurthy**PRES 13.** Surface tension measure-
ments of individual submicron sized
sea spray aerosol particles. H. Morris,
O. Laskina, V.H. Grassian, A.V. Tivanski**PRES 14.** Sustainable poly(lac-
tide)-based multiblock copolymers
with improved mechanical proper-
ties. T. Panthani, I. Lee, F.S. Bates**PRES 15.** Autocatalytic self-polym-
erization of biorenewable mono-
mers. B.J. Tiegs, G.W. Coates**PRES 16.** Novel porous and reusable β -cyclo-
dextrin sorbent for the instant removal
of organic contaminants from water.
A. Alsbaiee, B.J. Smith, L. Xiao, W. Dichtel**PRES 17.** New insights into the hetero-
geneous chemistry of nitric acid with
sea spray aerosol particles. C. Lee,
J. Trueblood, V.H. Grassian, K.A. Prather**PRES 18.** Control of biological activity
on distinct organic containing par-
ticle types in sea spray aerosols.
X. Wang, C. Sultana, J. Trueblood, T. Hill,
C. Lee, O. Laskina, C. Bealle, K. Moore,
P.J. DeMott, V.H. Grassian, K.A. Prather**PRES 19.** Solution-cast electronic
oxide films from aqueous all-inor-
ganic molecular precursors: Solution
chemistry, design principles, and
applications. S.W. Boettcher, M. Kast,
A. Nadarajah, P. Plasmeyer, D. Clayton,
D. Lepage, S.E. Hayes, K. Archila, L. Enman,
D.A. Keszler, J. Wager, M. Lonergan, C. Page**PRES 20.** Alkanes to aromatics:
Catalytic dehydroaromatization.
A.M. Steffens, A.S. Goldman**PRES 21.** Nanopatterning with inorganic
clusters. S. Saha, S.R. Decker, J.M. Amador,
F. Luo, R. Frederick, S.G. Ferron, M.D. Nyman,
G.S. Herman, E.L. Garfunkel, D.A. Keszler**PRES 22.** Biochemical origins of sea-
water and sea spray aerosol compo-
sition. J. Michaud, C. Lee, C. Sultana,
A. Rabines, M. Kim, R. Williams, F. Malfatti,
F. Azam, R.S. Pomeroy, T. Bertram, A. Allen,
K.A. Prather, M.D. Burkart**PRES 23.** Prebiotic phosphorylation of nucle-
osides by meteoritic minerals. M.A. Pasek**PRES 24.** Controlled ring-opening
polymerization of cyclic ester-
acetals to polyesteracetals and
polyhydroxyalkanoates. A. Neitzel,
M. Petersen, E. Kokkoli, M.A. Hillmyer**PRES 25.** Chemical theory and computations
in the CSMC: Predicting metal hydroxo
cluster stabilities, cluster spectroscopic
properties and structural and electronic
properties of amorphous metal oxide
solids. L. Wills, B. Hanken, T.J. Mustard,
I. Chang, A.F. Oliveri, M. Jackson Jr,
W. Wang, W. Liu, D. Fast, M. Dolgos, C. Fang,
D.W. Johnson, J. Wager, D.A. Keszler, P. Cheong**PRES 26.** Innovative tools for complex
mixture analysis at the Center for
Chemical Evolution. F.M. Fernandez**PRES 27.** New frontiers in group
V chemistry. M.D. Nyman**PRES 28.** New frontiers in synthesis
and solid-state NMR spectroscopy
of group 13 clusters and com-
plexes. B.A. Hammann, Z. Ma, K. Wentz,
M.K. Kamunde-Devonish, W. Wang, M. Jackson
Jr, D.A. Keszler, D.W. Johnson, S.E. Hayes**PRES 29.** Incorporating glucose and
castor oil derivatives into linear,
shape-memory polymers. L.M. Lillie,
W.C. Shearouse, T.M. Reinke, W.B. Tolman**PRES 30.** Low-pressure homoge-
neous hydrogenation of CO₂ to
methanol under basic conditions.
N.M. Rezaee, C.A. Huff, M.S. Sanford**PRES 31.** Heterogeneous nucleation of ice
on alcohol monolayers. Y. Qiu, V. Molinero**PRES 32.** Optimizing and understand-
ing photon absorption and charge
transport of BiVO₄ photoanodes for
solar water splitting. G.A. Galli, K. Choi**PRES 33.** Theoretical and experimental study
of the optoelectronic properties of tanta-
lum nitride (Ta₃N₅) for photoelectrochem-
ical (PEC) water splitting. I. Narkeviciute**PRES 34.** Oxidation chemistry facilitated by a
hexacarboxamide cryptand. J. Stauber**PRES 35.** Discovery and characterization of
transition metal phosphides as electrocat-
alysts and photocatalysts for the hydrogen
evolution reaction. N.S. Lewis, R.E. Schaak**PRES 36.** Advances in heterogeneous
tungsten catalysts for use in tandem
alkane metathesis. P.E. Sues**PRES 37.** Molecules, materials, and mecha-
nisms for solar fuel production. H.B. Gray**PRES 38.** Atom-efficient catalytic
methods for reduction and oxida-
tion of carbonyls. T. Brewster**PRES 39.** Chemical imaging and
spectroscopy of single molecules
with a tunable femtosecond laser
coupled RF-STM. W. Cao**PRES 40.** Optimizing C-H functionaliza-
tion catalysis. D. Morton, H.M. Davies**PRES 41.** Mechanistic studies of
Pd-catalyzed enantioselective
iodination. D.G. Blackmond**PRES 42.** Overview of new directions in
directed C-H functionalization. D. Morton**PRES 43.** Understanding selectivity in
C-H functionalization. K. Liao**PRES 44.** Overview of late-stage C-H
functionalization strategies. K. White,
M. Movassaghi, A.R. Narayan**PRES 45.** Single molecule vibra-
tional dynamics in time and fre-
quency domain. N. Tallarida**PRES 46.** Ultrafast pump-probe force micros-
copy with nanoscale resolution. E. Potma**PRES 47.** Using surface-enhanced
Raman to study chemistry at the
space-time limit. L.E. Buchanan

Section B

Boston Convention & Exhibition Center
Room 15821st Century Chemistry Education:
Formal and InformalCospponsored by AGRO, CARB, CHAS, CHED,
CINF, COLL, ENFL, PROF and SOCED

G. M. Bodner, Organizer

I. Montes, Organizer, Presiding

1:30 Introductory Remarks.**1:40 PRES 48.** A community for
teachers of chemistry by teach-
ers of chemistry. B.P. Sitzman**2:10 PRES 49.** Young chemists in action:
The benefits of informal chemis-
try education. S.B. Mitchell**2:40 PRES 50.** Promoting excellence in
chemistry teaching through in-service
professional development. J.D. Bernstein**3:10** Intermission.**3:20 PRES 51.** Making connections:
Mentoring, networking, and present-
ing makes a difference for us and
others as educators. L.E. Slocum**3:50 PRES 52.** Teacher-tested, but stu-
dent-blackbox online professional devel-
opment for chemistry teachers. W. Hunter**4:20 PRES 53.** Engaging researchers
and students as partners in educa-
tion and outreach. C.L. Alpert**4:50** Concluding Remarks.Edwin Land and Instant Photography:
Massachusetts' First National
Historic Chemical Landmark

Sponsored by HIST, Cospponsored by PRES

Professional Legacy of Henry Hill

Sponsored by PROF, Cospponsored by
CEPA, CMA, ETHC, HIST†, ORGN,
PMSE, POLY†, PRES and SCHB†True Stories from Entrepreneurs:
BRIC EditionSponsored by SCHB, Cospponsored by
CARB, COLL, I&EC, IAC, PRES and PROF

MONDAY MORNING

Section A

Sheraton Boston Hotel
Back Bay A

ACS Scholars: Rising Stars in Academe

Cospponsored by AGRO, CARB, CMA†,
COLL, ENFL, ENVR, PROF, SCHB and YCC

A. Poggi, L. M. Watkins, Organizers

C. Gutierrez, Presiding

8:30 Introductory Remarks.**8:55 PRES 54.** ACS Scholar: Fikile Brushett
(Massachusetts Institute of Technology).**9:20 PRES 55.** ACS Scholar: Lesley-Ann
Giddings (Middlebury College).**9:45** Intermission.**10:00 PRES 56.** ACS Scholar: Nicholas
D. Ball (Pomona College).**10:25 PRES 57.** ACS Scholar: Fatima Rivas
(St. Jude Children's Research Hospital).**10:50 PRES 58.** ACS Scholar:
Joshua S. Figueroa (University
of California San Diego).**11:15** Questions and Answers.**11:30** Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 158

21st Century Chemistry Education: Formal and Informal

Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF and SOCED

I. Montes, *Organizer*

G. M. Bodner, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 **PRES 59.** Inspiring and motivating chemistry learning through visualization and rich contexts. P.G. Mahaffy

9:10 **PRES 60.** Strategies to effectively incorporate learner-centered instruction into chemistry service courses. M. Oliver-Hoyo

9:40 **PRES 61.** Opportunities of formal and informal chemistry education at the two-year college. A.K. El-Ashmawy

10:10 Intermission.

10:20 **PRES 62.** Encouraging diversity in the chemical sciences. C. Gutierrez

10:50 **PRES 63.** Informal STEM education: Theory to outcome. M.L. Miller

11:20 **PRES 64.** Overcoming popular myths about education. G.M. Bodner

11:50 Concluding Remarks.

Memories of Henry Hill: His Legacy in Science and in Professional Service

Sponsored by HIST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES‡, PROF and SCHB

The Chemistry Enterprise in 2015

Sponsored by BMGT, Cosponsored by PRES and PROF

True Stories from Entrepreneurs: BRIC Edition

Sponsored by SCHB, Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais

Sponsored by YCC, Cosponsored by CHED, IAC, PRES and PROF

MONDAY AFTERNOON**Section A**

Sheraton Boston Hotel
Back Bay A

ACS Scholars: Rising Stars in Industry

Cosponsored by AGRO, CARB, CMA‡, COLL, ENFL, ENVR, PROF, SCHB and YCC

A. Poggi, L. M. Watkins, *Organizers*

R. L. Lichter, *Presiding*

1:45 Introductory Remarks.

2:10 **PRES 65.** ACS Scholar: Amber O. Evans, Ph.D. (BASF Corporation).

2:35 **PRES 66.** ACS Scholar: Kimberly Ortiz (Dow Chemical).

3:00 Intermission.

3:15 **PRES 67.** ACS Scholar: Antonio Ubiera (GlaxoSmithKline).

3:40 **PRES 68.** ACS Scholar: Tashica Williams Amirgholizadeh, Ph.D., J.D. (Gilead Sciences, Inc).

4:05 **PRES 69.** ACS Scholar: Dr. Jalonne L. White-Newsome (Director of Federal Policy).

4:30 Questions and Answers.

4:45 Concluding Remarks.

Leadership Skills as a Strategic Advantage: The Chemist's Competitive Edge

Sponsored by BMGT, Cosponsored by CEPA, PRES‡, PROF and YCC

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector

Sponsored by SCHB, Cosponsored by CMA, COLL, HIST, I&EC, POLY, PRES and PROF

Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais

Sponsored by YCC, Cosponsored by CHED, IAC, PRES and PROF

TUESDAY MORNING**Section A**

Westin Boston Waterfront
Burroughs

Transforming University-Industry Partnerships for an Innovative Future

Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

L. Graziano, *Organizer*

C. Ribes, *Organizer, Presiding*

8:15 Introductory Remarks.

8:30 **PRES 70.** Future of industrial – academic partnerships. J. Ringer

8:50 **PRES 71.** Spectrum of engagement for research, collaboration, and innovation. J. Garton

9:10 Questions and Answers.

9:25 **PRES 72.** Making the most of university-industry alliances. C.J. Hawker

9:45 **PRES 73.** Alignment, development, and sustainment of the strategic research partnership. D. Fortner

10:05 **PRES 74.** Role of the federal government. A. Boccanfuso

10:25 Questions and Answers.

10:40 Intermission.

10:50 **PRES 75.** University-industry collaboration: A proliferation of new models. A. Westervelt

11:10 **PRES 76.** Public research universities: Engines for innovation and growth. H.C. Foley

11:30 **PRES 77.** P&G's perspective on strengthening university/industry partnerships. E. Sawicki

11:50 Questions and Answers.

12:05 Concluding Remarks.

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Sponsored by POLY, Cosponsored by HIST, PMSE‡, PRES and PROF‡

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES‡, PROF and SCHB

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

TUESDAY AFTERNOON**Section A**

Westin Boston Waterfront
Burroughs

Transforming University-Industry Partnerships for an Innovative Future**Energizing and Education**

Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

C. Ribes, *Organizer*

L. Graziano, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **PRES 78.** Creating structures for fruitful university- industrial research partnerships. K.J. Stebe

1:55 **PRES 79.** National network for manufacturing innovation. M. Molnar

2:15 **PRES 80.** Building a co-creation system for focused innovation. J. von Briesen

2:35 **PRES 81.** Engaging Value Chain members to improve new product launch success. J.S. de Wit

2:55 Questions and Answers.

3:10 Intermission.

3:20 **PRES 82.** Balancing the university's overarching policy for openness and dissemination of information with industry's need for confidentiality for translational R. D. Waldman

3:40 **PRES 83.** University of Cincinnati Simulation Center: A UC Engineering and P&G collaboration. B. Rudd

4:00 Questions and Answers.

4:15 Panel Discussion.

4:50 Concluding Remarks.

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Sponsored by POLY, Cosponsored by HIST, PMSE‡, PRES and PROF‡

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES‡, PROF and SCHB

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

WEDNESDAY MORNING**Big Chemistry from Small Businesses**

Sponsored by SCHB, Cosponsored by COLL, I&EC, PRES and PROF

MPPG**Multidisciplinary Program Planning Group**

C. R. Wagner, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Transforming University-Industry Partnerships for an Innovative Future (see PRES, Tuesday)

SOCIAL EVENTS:

MPPG Representatives Reception, 3:30 PM: Saturday

BUSINESS MEETINGS:

MPPG Representatives Business Meeting, 2:30 PM: Saturday

SUNDAY AFTERNOON**Section A**

Boston Convention & Exhibition Center
Ballroom West

Innovation from Discovery To Application Plenary Session

Cosponsored by BIOT, MEDI, PMSE and POLY

C. R. Wagner, *Organizer, Presiding*

3:00 Introductory Remarks.

3:10 **MPPG 1.** Tailored drug release surfaces for regenerative medicine and targeted nanotherapies. P.T. Hammond

3:45 Introduction of Speaker.

3:50 **MPPG 2.** A chemist's foray into translational medicine. P.G. Schutz

4:25 Introduction of Speaker.

4:30 **MPPG 3.** Targeted applications as inspirations to develop strategies toward functionally-sophisticated nanoscopic macromolecules with diverse compositions, structures, and properties. K.L. Wooley

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MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 102A/B

Innovation in Health and Medicine

Cosponsored by BIOL, BIOT, MEDI and TOXI

R. DiMarchi, *Organizer, Presiding*

9:00 MPPG 4. Total chemical synthesis used to develop a D-protein antagonist of VEGF-A: X-ray structure of the heterochiral {VEGF-A+D-protein antagonist} complex by racemic crystallography. S. Kent

9:30 MPPG 5. Setting a course for biomedical innovation in the 21st century. A.D. Palkowitz

10:00 Intermission.

10:30 MPPG 6. Identification and validation of cell type selective drug targets. S. Hitchcock

11:00 MPPG 7. Integration of tissue engineering and systems biology in drug development. L. Griffith

11:30 MPPG 8. Novel synthetic strategies for insulin and related peptide. F. Liu, A.N. Zaykov, R. DiMarchi, J. Mayer

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 102A

Public Perception of the Chemistry Enterprise

How Scientists Can Effectively Communicate To the Public

N. E. Blount, B. Campos-Seijo, A. T. Yarnell, *Organizers*

S. R. Morrissey, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 MPPG 9. How scientists can effectively communicate to the public. S.R. Morrissey

Section A

Boston Convention & Exhibition Center
Room 102A

Public Perception of the Chemistry Enterprise

Chemistry Reacts To Chemophobia: A Problem of Public Perception and/or Communication?

N. E. Blount, B. Campos-Seijo, A. T. Yarnell, *Organizers*

S. R. Morrissey, *Organizer, Presiding*

2:20 MPPG 10. Chemistry reacts to chemophobia: A problem of public perception and/or communication? S.R. Morrissey

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:

www.acs.org/boston2015

Section A

Boston Convention & Exhibition Center
Room 102A

Public Perception of the Chemistry Enterprise

A Poisoner's Guide To Communicating Chemistry

N. E. Blount, B. Campos-Seijo, S. R. Morrissey, A. T. Yarnell, *Organizers*

D. S. Gottfried, *Presiding*

3:10 MPPG 11. Poisoner's guide to communicating chemistry. D. Blum

Section A

Boston Convention & Exhibition Center
Ballroom West

The Kavli Foundation Emerging Leader in Chemistry Lecture

C. R. Wagner, *Organizer*

D. G. Schmidt, *Presiding*

4:00 Introductory Remarks.

4:05 MPPG 12. Spectacular properties of porous polymers. W. Dichtel

Section A

Boston Convention & Exhibition Center
Ballroom West

The Fred Kavli Innovations in Chemistry Lecture

C. R. Wagner, *Organizer*

D. G. Schmidt, *Presiding*

5:00 Introductory Remarks.

5:35 MPPG 13. Problems, puzzles, and inevitabilities in research. G.M. Whitesides

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Chemical Innovation and Design (CID) Talks: The Future of Innovation Now

Cosponsored by AGFD, AGRO, BIOT, MEDI, PMSE and SCHB

C. R. Wagner, *Organizer, Presiding*

8:30 MPPG 14. Consumer products from sugarcane: Renewable fuels, fragrances, emollients, and tires. R. Jain

8:50 MPPG 15. Biology is too important to be left to biologists. A. Edwards

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 205A

Fifty Years of Innovation: The Legacy of the Westheimer Report

Cosponsored by HIST†

R. A. Egolf, *Organizer, Presiding*

8:35 Introductory Remarks.

8:45 MPPG 16. Opportunities and needs: The Westheimer view of chemistry in the 1960's and beyond. R.A. Egolf

9:15 MPPG 17. Innovation in condensed matter chemistry. G.D. Patterson

9:45 MPPG 18. Medicinal chemistry in and after the Westheimer report: Recommendations and ripples. N.D. Heindel

10:15 Intermission.

10:30 MPPG 19. Fifty years of computational chemistry. K.N. Houk

11:00 MPPG 20. Bridging the divide: A tale of the merger of computational chemistry and structural biology in enzyme design. S.L. Mayo

11:30 MPPG 21. The Breslow-Tirrell Report. R. Breslow

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 205A

Innovation in Materials for Emerging Uses

Cosponsored by PHYS, PMSE and POLY

K. L. Wooley, *Organizer, Presiding*

1:30 MPPG 22. Colloidal quantum dot light emitters: From fundamental discoveries to applications as light emitters. P. Alivisatos

2:00 MPPG 23. Innovation in materials for emerging uses: Breakthroughs in imprint lithography and 3D additive fabrication. J.M. Desimone

2:30 MPPG 24. Recent success stories in commercial functional materials. C.J. Hawker

3:00 Intermission.

3:30 MPPG 25. Spherical nucleic acids: A new paradigm in nucleic acid therapeutics. C.A. Mirkin

4:00 MPPG 26. By indirections find directions out: Understanding the effects of order in disordered materials. M.A. Ratner

4:30 MPPG 27. Chemical sensors enabled by complex electronic materials. T.M. Swager

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 205A

Innovation in Chemical Synthesis

Cosponsored by INOR, MEDI and ORGN

J. Aube, *Organizer, Presiding*

9:00 MPPG 28. Studies in natural product synthesis. P.S. Baran

9:30 MPPG 29. Challenges in the synthesis and analysis of oligosaccharides. N.L. Pohl

10:00 Intermission.

10:30 MPPG 30. Synthesis design using flow chemistry. T.F. Jamison

11:00 MPPG 31. Discovery and invention of new chemical reactions using photoredox catalysis. D.W. MacMillan

11:30 MPPG 32. Polymer mechanochemistry and the concept of the mechanophore. J. Moore

AEI

Academic Employment Initiative

C. Kuniyoshi and J. Sostaric, *Program Chairs*

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Academic Employment Initiative

C. Y. Kuniyoshi, J. Z. Sostaric, *Organizers*

8:00 - 10:00

AEI 1. Operation potato shield declassified: Metabolite profiling, antioxidant assessment, and solid-state NMR compositional analysis of wound-healing tissues from different potato cultivars. K. Dastmalchi, L.R. Kallash, V.C. Phan, W. Huang, O. Serra, R. Stark

AEI 2. 8-Hydroxyquinoline based nanoscavenger for the dispersion preconcentration of trace elements in contaminated waters. M. Algaradah

AEI 3. Modes of regulation in platelet activation. S.A. Finkenstaedt-Quinn, S. Ge, S.M. Gruba, C.L. Haynes

AEI 4. Integrating origins-of-life chemistry and analytical training at a primarily undergraduate institution. J.G. Forsythe

AEI 5. New variable temperature solution-solid interface scanning tunneling microscope. A. Jahanbeka, U. Mazur, K. Hips

AEI 6. Computer programming in the chemistry laboratory. J. Radney

AEI 7. RC constant based label free biomarkers detection. P. Ramiah Rajasekaran

AEI 8. Interfacial processes in energy storage and conversion devices. H. Tavassol

AEI 9. Withdrawn.

AEI 10. Withdrawn.

AEI 11. Toward an inhibitor for fatty acid binding protein 5. M. Doud, N. Noy, G. Tochtrop

AEI 12. Iron homeostasis is a target of nickel toxicity in *E. coli*. G. Ford, C. Washington-Hughes, N.V. Ozonma, F.W. Ouiten

AEI 13. Using biophysical chemistry to modulate the activity of aldehyde dehydrogenases and Amot family proteins. A.C. Kimble Hill, H.I. Petrasche, C.D. Wells, T.D. Hurley

AEI 14. Synthetic (An)ionophores: From theory to applications. S.A. Kostina

AEI 15. Functional mimic approach from biological reaction to design efficient electrocatalysts for H₂ oxidation. N. Kumar, S. Raugel, B. Ginovska-Pangovska, M. Dupuis

AEI 16. Mechanistic studies and kinetics on F₄₂₀H₂: NADP⁺ oxidoreductase from *Archaeoglobus fulgidus*. C.Q. Le, T.Q. Nguyen, E. Joseph, M.S. Hossain, F.W. Foss, K.L. Johnson-Winters

AEI 17. Illumination of the therapeutic potential and physiological roles of insulin-degrading enzyme using the first physiologically active inhibitor. J. Maiani, A.K. McFedries, Z. Foda, R.E. Kleiner, M.A. Seeliger, A. Saghatelyan, D.R. Liu

AEI 18. Engineering electron transfer among bacteria for improved bioenergy and biofuels. N.S. Malvankar

- AEI 19.** Quantitative proteomics of nitroxidative post-translational modifications. **T. Rhoads**
- AEI 20.** Treating Tamoxifen resistant breast cancer by inhibiting protein degradation. **J.A. Smith**
- AEI 21.** Development of an isotopic approach for detailing heparin sequences. **Q. Guo, V.N. Reinhold**
- AEI 22.** Isotope targeted glycoproteomics (IsoTaG): A mass-independent platform for intact N- and O-glycopeptide discovery. **C.M. Woo, A.T. Iavarone, D. Spicciarich, K.K. Palaniappan, C.R. Bertozzi**
- AEI 23.** Observations of dynamic restructuring of nanoporous gold during selective alcohol coupling reactions. **B. Zugic, M.L. Personick, R.J. Madix, C.M. Friend**
- AEI 24.** Innovation of peer learning. **N.H. Marashi**
- AEI 25.** Realm of colloidal interactions and assembly: A pathway toward programmable metamaterials. **B. Bharti, K. Kaneko, G.H. Fhindenegg, O.D. Velev**
- AEI 26.** Advancing the technologies for nanoparticles in living systems. **G.B. Braun**
- AEI 27.** Withdrawn.
- AEI 28.** Nanomaterials and devices for active interplay with the biological environment. **A. Pallaoro**
- AEI 29.** DNA nanostructures: Template tools for nanoelectronics. **M. Rahman, A. Mangalam, D. Neff, M.L. Norton**
- AEI 30.** Withdrawn.
- AEI 31.** Computational approaches to elucidate fundamental electron and energy transfer processes in complex supramolecular systems. **L.A. Fredin**
- AEI 32.** Dissecting the ion atmosphere surrounding nucleic acids. **G.M. Giambasu, D.M. York, D.A. Case**
- AEI 33.** Challenges in characterizing and predicting the activity of transition metal exchanged zeolites. **F. Goeltl, P. Mueller, P. Uchupalainun, P. Sautet, I. Hermans**
- AEI 34.** Calculation of protein-ligand binding affinities via a polarizable model. **M.L. Laury, J.W. Ponder**
- AEI 35.** Novel, cell-trained approach to biological target-guided chemical tools and its application to *Mycobacterium tuberculosis*. **A.L. Perryman, X. Wang, S. Li, S.D. Paget, T.P. Stratton, A.J. Olson, S. Ekins, J. Freundlich**
- AEI 36.** Data-driven paradigm for encoding chemical intuition. **E.O. Pyzer-Knapp**
- AEI 37.** Nanomaterials: Possible ways for computational assessment and data mining towards rational design of new materials. **B. Rasulev**
- AEI 38.** Computational materials design for sustainable energy and biomedical systems. **S.V. Sambasivarao**
- AEI 39.** Realistic and affordable ab initio calculations for electrochemistry. **K. Schwarz**
- AEI 40.** Modeling and design of large RNAs. **S. Somarowthu, A.M. Pyle**
- AEI 41.** New electronic structure theory methods and high-throughput computational screening algorithms for catalytic processes. **K.D. Vogiatzis**
- AEI 42.** Understanding singlet fission and other physical processes related to organic photovoltaics using theoretical models. **S. Yost, M.P. Head-Gordon**
- AEI 43.** Multifunctional nanomaterials at the water-energy nexus. **N. Aich**
- AEI 44.** Investigating and exploiting the interaction between graphene and hydrated ions. **D.G. Dressen, J. Golovchenko**
- AEI 45.** Green chemistry through electrocatalysis. **A.B. Laursen**
- AEI 46.** Pore scale microbial biogeography in petroleum hydrocarbon contaminated soils. **A. Akbari, S. Ghoshal**
- AEI 47.** Applications of organometallic complexes to organic transformations: Tandem experimental and computational studies. **K.D. Field, M. Emmert, A.S. Goldman**
- AEI 48.** Optimizing the electrocatalytic reduction of CO₂ by Re- and Mn-based bipyridine complexes with supramolecular assembly. **C.W. Machan, S.A. Chabolla, C.P. Kubiak**
- AEI 49.** Chemistry and reactivity of hydrogen on γ -molybdenum nitride. **E.A. Mader, B.M. Wyratt, J.R. Gaudet, D. Pardue, A. Marton, S. Rudic, T. Cundari, J.M. Mayer, L.T. Thompson**
- AEI 50.** Oxidation reactivity of a chelated cobalt fluoroalkoxide complex. **A.J. Arduengo, S.P. Kelley, W.J. Marshall, J.W. Runyon**
- AEI 51.** Band-edge modulation of p-Si(111) and integration of H₂ catalyst with p-Si(111). **J. Seo**
- AEI 52.** Nano confinement effects on metal ions or nanoparticles catalysts. **J. Shen**
- AEI 53.** Advances in the use of gel permeation chromatography (GPC) to nanocrystals: Purification, solvent change, and surface modification. **Y. Shen, R. Tan, M.Y. Gee, A. Roberge, A.B. Greytak**
- AEI 54.** Solar fuel production by photosensitizer-protein-molecular catalyst biohybrids. **S. Soltan, J. Niklas, P.D. Dahlberg, K.L. Muffort, O. Poluektov, D.M. Tiede, L.M. Utschig-Johnson**
- AEI 55.** Paramagnetic transition metal complexes: From research to application and education. **P.B. Tsitovich**
- AEI 56.** Stable luminescent metal-organic frameworks for sensing and light emitting applications. **Q. Zhang**
- AEI 57.** Organometallic and noncluster chemistry of iridium. **M. Zhou, R.H. Crabtree, A.S. Goldman, R.G. Finke**
- AEI 58.** Synthesis of 18F-labeled inhibitor of indoleamine 2,3-dioxygenase for positron emission tomography imaging. **N.M. Evdokimov, P. Clark, G. Flores, O. Witte, M.E. Jung, M. Phelps**
- AEI 59.** Computer-aided drug design and development: A research program designed to produce novel research and enhance undergraduate education. **M.J. Ferracane**
- AEI 60.** Beyond morphine: Mu opioid/NOP and mu opioid/NPFF bifunctional small molecules as analgesics with reduced dependence and tolerance liabilities. **V.B. Journigan**
- AEI 61.** Novel applications of ionic liquids. **W. Medina-Ramos**
- AEI 62.** Withdrawn.
- AEI 63.** Amber Thaxton: Synthetic organic chemist. **A.N. Thaxton**
- AEI 64.** Heterogeneous catalysis: Synthesis and spectroscopy of supported metal oxide catalysts for natural gas upgrading. **C.A. Carroero**
- AEI 65.** Light-induced rotational dynamics in photoresponsive molecular rotor. **A. Aytou, M.A. Garcia-Garibay**
- AEI 66.** Signal transduction within supramolecular materials. **M.B. Baker**
- AEI 67.** Design and development of novel synthetic methods for application toward the synthesis of natural products. **R. Lamon-Bishop**
- AEI 68.** Mild palladium-catalyzed cyanation of (hetero)aryl halides and triflates in aqueous media. **D.T. Cohen, S.L. Buchwald**
- AEI 69.** Metalloradical catalysis for stereoselective organic synthesis. **X. Cui, X. Xu, L. Jin, P.X. Zhang**
- AEI 70.** Theoretical insights of mechanisms and stereoselectivities in organocatalysis by amino acid and cinchona alkaloid derivatives. **Y. Lam**
- AEI 71.** Development of cooperative Lewis acid catalysts for asymmetric Henry reactions, expedient library synthesis toward medical molecules, and development of bridged D₂-symmetric chiral amidoporphyrin catalysts for highly enantio-switchable, intramolecular C(sp³)-H radical amination. **K. Lang, S. Hong, D.W. MacMillan, P.X. Zhang**
- AEI 72.** Trialkylphosphine-derived palladacycle as a catalyst in the selective cross-dimerization of two terminal alkynes. **M.G. Lauer, O.M. Gobble, K.H. Shaughnessy**
- AEI 73.** Carbon-rich architectures: Design, synthesis, and applications. **D. Lehnher, W. Dichtel**
- AEI 74.** Structure, morphology, and reversible mechanotropic properties of molecular gels derived from (*R*)-12-hydroxystearic acid as gelator. **A.V. Mallia**
- AEI 75.** N,N-dimethylaminobenzyl boronate esters functionalization into diamines. **K.A. McGarry, A. Duenas, T.B. Clark**
- AEI 76.** Experimental and theoretical studies: Selective metal-catalyzed C-H functionalization. **S.R. Neufeldt**
- AEI 77.** Opening a new front in the battle against α -synuclein aggregation: An effort to combat Parkinson's disease through targeted delivery of antioxidant molecules attached to polyphosphazene polymers. **P.W. Peterson**
- AEI 78.** Regio- and stereocontrolled allylic substitutions with organocuprates on α -substituted- β,γ -unsaturated esters and cyanohydrin phosphates. **A. Picado, R. Dieter**
- AEI 79.** From organofluorine chemistry to bioinorganic chemistry: Methodology, mechanistic studies, and applications. **F. Wang**
- AEI 80.** Inspiring diversity: Strategies for the classroom and the flask. **R. Whittaker**
- AEI 81.** Withdrawn.
- AEI 82.** Supramolecular approaches for improving reactivity and selectivity in transition metal catalyzed transformations. **M. Young**
- AEI 83.** Collective behaviors of self-assembled matters in chemistry. **T. Adachi**
- AEI 84.** Methionine enkephaline simulation using the statistical temperature molecular dynamics algorithm. **S.C. Begay**
- AEI 85.** From gas-phase to heterogeneous reaction: Applications in combustion to astrochemistry. **B.B. Dangi, R. Kaiser, K.M. Ervin**
- AEI 86.** Ultra coarse-graining and dynamic force matching: Path to realistic coarse-grained modeling. **A. Davtyan, J.F. Dama, A. Sinitskiy, H. Andersen, G.A. Voth**
- AEI 87.** Computational studies of proton transfer and proton-coupled electron transfer in chemical and biological systems. **P. Goyal, Q. Cui, S. Hammes-Schiffer**
- AEI 88.** New innovative ways for waste water cleaning. **C. Janssen**
- AEI 89.** Physical mechanisms involved in viral infection and replication. **D. Li**
- AEI 90.** Single aerosol particle studies in a temperature-controlled optical trap. **J. Lu, R. Signorell**
- AEI 91.** Energetics and dynamics of electrons in conjugated molecule. **T. Mani, D.C. Grills, J.R. Miller**
- AEI 92.** Thermodynamically motivated sintering model of ceramics. **N. Mohan**
- AEI 93.** Computational catalysis for green chemistry and sustainable technology. **A. Pelzer**
- AEI 94.** Scanning tunneling microscopy studies of low-dimensional materials for use in next generation electronic devices. **R. Quardokus**
- AEI 95.** Processing and properties of novel semiconductor glasses with a focus on teaching, mentoring, and innovative ways to promote STEM. **C.M. Schwarz**
- AEI 96.** Exciton dynamics in disordered organic films. **L. Shi, A.P. Willard**
- AEI 97.** Effect of dislocations on optical and transport properties of organometal halide perovskites. **P. Tyagi**
- AEI 98.** Biofunctional polymeric materials for drug delivery and tissue engineering. **M.A. Azagarsamy**
- AEI 99.** Functional polymers for bio- and industrial applications: Synthesis, properties, and engineering. **M. Gkikas**
- AEI 100.** Polymerization and electrochemistry in biosensing. **P. He**
- AEI 101.** Controlling the morphology in blended polymer systems: From fundamentals to applications. **R. Hickey, T. Gillard, M. Irwin, T.P. Lodge, F.S. Bates**
- AEI 102.** Dynamic materials: Putting chemistry into motion. **L.D. Zarzar, J. Aizenberg, T.M. Swager**
- AEI 103.** Withdrawn.
- AEI 104.** Polymer matrix composites using covalently modified carbon nanotube materials. **J.S. Baker, M.A. Meador**
- AEI 105.** Efficient synthesis of unimolecular polymers with absolute control over mass, monomer sequence, and stereochemistry. **J.C. Barnes, D. Ehrlich, A. Gao, F.A. Leibfarth, Y. Jiang, E. Zhou, T.F. Jamison, J.A. Johnson**
- AEI 106.** Design and synthesis of advanced polymeric materials. **A.M. Diccio, G.W. Coates, r. langer, G. Traverso**
- AEI 107.** Materials design via supramolecular engineering: From folding polymers to assembling colloids. **E. Elacqua, M. Weck**
- AEI 108.** Selective CO₂ adsorption by a phthalocyanine porous polymer. **V. Neti**
- AEI 109.** Orthogonal engineering of block copolymers: Tools, techniques, and applications. **M. Quadir**

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AGFD

Division of Agriculture and Food Chemistry

B. Park, Program Chair

OTHER SYMPOSIA OF INTEREST:

Journal of Agricultural and Food Chemistry Best Paper Awards (see AGRO, Tuesday)

Innovations in Agrochemical Discovery and Process Chemistry: 2015 Kenneth A Spencer Award in Honor of Thomas Selby and 2015 AGRO Award for Innovation in the Chemistry of Agriculture in honor of Tom Sparks (see AGRO, Wednesday, Thursday)

SOCIAL EVENTS:

AGFD Awards Banquet, 6:00 PM: Tuesday

BUSINESS MEETINGS:

AGFD Special Committee Meeting, 12:00 PM: Sunday

AGFD Executive Committee Meeting, 5:00 PM: Sunday

AGFD Future Programs Planning Meeting, 12:00 PM: Monday

AGFD Business Meeting, 12:00 PM: Tuesday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center Room 212

Phytonutrients: Thinking Beyond the "Essential" Nutrient Box

B. Burton-Freeman, I. Edirisinghe, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 1. Chemistry and analysis of polyphenols in food and human samples. E. Richling, M. Schantz, D. Mueller, D. Scherbl, T. Erk, H. Bergmann

8:35 AGFD 2. Anthocyanins in the blood: Where are they going and how do they get there? J.A. Vinson, I. Alshdoukhi

9:05 AGFD 3. Understanding factors that influence the bioavailability and kinetic profile of strawberry anthocyanins: A focus on meal timing and fasted-fed state status. A. Sandhu, I. Edirisinghe, B. Burton-Freeman

9:35 Intermission.

9:50 AGFD 4. Absorption, distribution, metabolism, and excretion of orange juice flavanones in humans. A. Crozier

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10:20 AGFD 5. Cocoa flavanols – chemical nature, analysis, and fate during processing. X. Wu

10:50 AGFD 6. Comparison of polyphenolics and secoiridoids in California-style black ripe olives and dry salt-cured olives using UHPLC/MS/MS. J. Zweigenbaum, E. Melliou, A.E. Mitchell

11:20 Concluding Remarks.

Section B

Boston Convention & Exhibition Center Room 213

Bioactive Compounds from Fruits & Vegetables

L. Cisneros-Zevallos, F. Tomas-Barberan, *Organizers*C. Osorio Roa, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 7. Phenolic acid profiles of Fuji, Golden Delicious, Granny Smith, and Pink Lady apples. A.E. Mitchell

8:30 AGFD 8. Influence of different deposition forms of carotenoids in plant foods on their bioavailability. R. Schweiggert, R. Carle

8:55 AGFD 9. Application of different analytical systems for the characterization of food bioactives. D. Giuffrida, F. Cacciola, M. Utzas, M. Beccaria, P. Donato, P. Dugo, L. Mondello

9:20 AGFD 10. Effects of thermal and enzymatic treatment on polyphenol profiles during bilberry juice production. F. Weber, P. Heffels, F. Blüthle, D. Kaumans, A. Schieber

9:45 Intermission.

10:05 AGFD 11. Biological effects of anthocyanins from fruits. E. Richling, M. Schantz, M. Baum, T. Bakuradze, D. Mueller

10:30 AGFD 12. Transport and uptake of anthocyanins in gastric tissue and their effect on the gastric inflammatory response: Developing an in vitro model using the NCI-N87 gastric cell line. A. Atnip, M. Giusti, J. Bomser

10:55 AGFD 13. Optimized and validated method for the characterization and quantification of bioactive ellagitannins in pomegranate and other fruits and nuts. F. Tomas-Barberan, R. Garcia-Villalba, K. Aaby, T. Kouvumäki, M. Heinonen, E. Pelvan, C. Alasalvar, G. Jacobs, S. Saha, J. Espin, P. Kroon

Section C

Boston Convention & Exhibition Center Room 209

Economically Motivated Food Adulteration: Interplay Between Detection, Policy, & Food Defense

J. Moore, P. F. Scholl, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 14. Olive oil authenticity and adulteration: Analytical tools and standards. R. Cantrill

8:35 AGFD 15. USP skim milk powder advisory group: The development of a toolbox of methods to detect food adulteration. R.L. Magaletta, J.C. Moore

9:05 AGFD 16. Development of field screening methods using surface enhanced Raman spectroscopy (SERS). L.C. Pogue, N.P. Sardesai, B.J. Yakes, S. Barcelo, M. Yamakawa, A. Rogacs, Z. Li, A. Shareef

9:35 Intermission.

9:45 AGFD 17. Meat fraud and speculation: From vulnerability assessment to analytical methods. G. Cottenet

10:15 AGFD 18. DNA-based species identification of seafood. A. Eiseheid, S. Stadig, S. Handy, F.S. Fry, J. Deeds

10:45 AGFD 19. Honey adulteration: Methods currently applied in the routine control of commercial samples, analytical challenges, legal and regulatory aspects. L. Elflein

11:15 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center Room 212

Phytonutrients: Thinking Beyond the "Essential" Nutrient Box

B. Burton-Freeman, I. Edirisinghe, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 20. Is volunteer stratification necessary in clinical trials with phenolic phytochemicals? F. Tomas-Barberan

1:35 AGFD 21. Predicting the mechanism of anthocyanin-induced insulin sensitization with molecular modeling. D. Minh

2:05 AGFD 22. Grape seed extract authentication. M.A. Kelm, S. Kupina, A. Shrikhande

2:35 Intermission.

2:50 AGFD 23. Withdrawn.

3:20 AGFD 24. Anthocyanin metabolism and transport across the blood brain barrier. P.E. Milbury

3:50 Concluding Remarks.

Section B

Boston Convention & Exhibition Center Room 213

Bioactive Compounds from Fruits & Vegetables

C. Osorio Roa, F. Tomas-Barberan, *Organizers*
L. Cisneros-Zevallos, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 25. Bioactive compounds for cancer prevention and health aging. R.H. Liu

1:30 AGFD 26. Withdrawn.

1:55 AGFD 27. Using untargeted metabolomics to profile tomato products intended for clinical trials. M.J. Cichon, K.M. Riedel, S. Schwartz

2:20 AGFD 28. Cranberry oligosaccharides decrease biofilm formation by uropathogenic *Escherichia coli*. J. Sun, J.P. Marais, C. Khoo, N.P. Seeram, K. Laplante, D.C. Rowley

2:45 Intermission.

3:05 AGFD 29. Antioxidant and anti-inflammatory activity of protein hydrolysates from germinated black bean cotyledons. L. Lopez-Barrios

3:30 AGFD 30. Potential antimicrobial and anticarcinogenic properties of *Rhoeo discolor* (*Tradescantia spathacea*) extracts. R. Garcia-Varela

Section C

Boston Convention & Exhibition Center Room 209

Economically Motivated Food Adulteration: Interplay Between Detection, Policy, & Food Defense

J. Moore, P. F. Scholl, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 31. Analytical puzzle of allergenic peanut and almond residues in spices: Was adulteration the root cause? S.L. Taylor, J.L. Baumert, S. Wijerathne

1:40 AGFD 32. Using fraud history to inform food fraud vulnerability assessments. J.C. Moore, K. Everstine

2:15 Intermission.

2:25 AGFD 33. Food fraud mitigation framework for industry and regulators. K. Everstine, J. Moore

3:00 AGFD 34. You can't test your way to safety. S. Kennedy

3:35 Concluding Remarks.

Section D

Boston Convention & Exhibition Center Room 211

Modern Perspectives on Oxidation: Flavor Consequences in Foods & Beverages

K. Tandon, *Organizer*R. Elias, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 35. Impact of antioxidants on the formation of volatile secondary lipid oxidation products in oil-in-water emulsions. E. Bakota, J.K. Winkler-Moser, H. Hwang

1:30 AGFD 36. Performance stability of nonmigratory metal chelating active packaging materials in model food systems. M. Roman, F. Tian, Y. Ogiwara, E.A. Decker, J.M. Goddard

1:55 AGFD 37. Unravelling chemical pathways for wine aging: Role of quinones as intermediaries in wine oxidation as "Strecker degradation reagents". A.C. Silva Ferreira, C. Oliveira, A. Monforte, A. Silva

2:20 AGFD 38. Changes to oat secondary lipid oxidation products as a function of initial moisture content. M.J. Morello, T. Rakofsky

2:45 AGFD 39. Complications of analyzing acetaldehyde as a wine oxidation product. A.L. Waterhouse, A. Peterson

3:10 Concluding Remarks.

MONDAY MORNING

Section A

Boston Convention & Exhibition Center Room 212

Complex Coacervation: Principles & Applications

Financially supported by The Dow Chemical Company

Cosponsored by COLL†

P. L. Dubin, S. L. Perry, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 40. Complex coacervation: Principles and simple theories. R. de Vries

8:45 AGFD 41. Polyelectrolyte complex-coacervate continuum. J.B. Schlenoff, Q. Wang

9:15 AGFD 42. Electrostatic complexes between (bio)polyelectrolytes and nanoparticles. Effect of the chain persistence length over particle diameter ratio. F. Boue

9:45 Intermission.

10:10 AGFD 43. Multivalent counterion-induced bridging of polyelectrolyte chains. B.K. Brettmann, N. Laugel, P. Pincus, M.V. Tirrell

10:30 AGFD 44. New opportunities for complex coacervation control exposed by bridging the gap between two classical models. C.E. Sing, M. Radhakrishna

11:00 AGFD 45. Complex coacervates for enzyme encapsulation and stabilization. B.D. Olsen, A. Obermeyer, C. Mills, X. Dong, W. Shi

11:30 AGFD 46. Effect of multivalent ions on hydrated polyelectrolyte multilayers. D. Reid, A. Kavarthapu, J.L. Lutkenhaus

Section B

Boston Convention & Exhibition Center Room 213

Bioactive Compounds from Fruits & Vegetables

L. Cisneros-Zevallos, C. Osorio Roa, *Organizers*

F. Tomas-Barberan, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 47. Characterization of the activity of dietary organosulfides from vegetables as natural donors of hydrogen sulfide in cell line model. D. Huang, D. Liang, C. Wang, H. Wu, R. Tomco

8:30 AGFD 48. Characterization of tomato volatiles by headspace-solid-phase micro extraction. G. Jayaprakasha, B. Patil

8:55 AGFD 49. Bioactives from berries and their by-products. F. Shahidi

9:20 AGFD 50. Establishing biochemical justification for the value of fruit pomace a path from discovery to application. J.W. Finley

9:45 Intermission.

10:05 AGFD 51. Organic resveratrol: Natural occurrence and sunlight phototransformations. A.A. Gakh, A. Sosnov

10:30 AGFD 52. Preservation of anthocyanins in solid lipid nanoparticles: Optimization of microemulsion dilution method by Plackett Burman and Box Behnken design. R. Ravanfar, A. Tamadan, M. Niakousari, M. Moein

10:55 AGFD 53. DOPC liposomes doped with octadecylferulate. K. Evans, D.L. Compton, J.A. Laszlo

11:20 Concluding Remarks.

Section C

Boston Convention & Exhibition Center Room 209

Food Toxicants Formed During Food Processing & Storage

S. Wang, L. L. Yu, *Organizers, Presiding*

8:30 AGFD 54. Reactive carbonyl species: Will they be the next food safety issue? C. Ho

9:05 AGFD 55. Formation and reduction of furan in various food model systems. J. Her, M. Kim, K.G. Lee

9:40 AGFD 56. Influence of California-style black ripe olive processing methods on acrylamide formation. A.E. Mitchell

10:15 Intermission.

10:30 AGFD 57. Free radical mediated 3-MCPD fatty acid ester formation and the potential catalytic effect of Fe. Z. Zhang, B. Gao, X. Zhang, H. Shi, L.L. Yu

11:05 AGFD 58. Chemodiversity and biosynthesis of cereulide, the food-born emetic toxin of *Bacillus cereus*. T. Hofmann, S. Marxen, T.D. Stark, A. Rutschle, G. Luecking, E. Frenzel, S. Scherer, M. Ehling-Schulz

Section D

Boston Convention & Exhibition Center Room 211

Metabolites & Metabolomics of Food Bioactives & Influence of Gut Microbiota: Chemistry and Health Effects

S. Sang, F. Shahidi, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 59. Food phenolics, their bioactivities, and their metabolites. F. Shahidi

8:40 AGFD 60. Interplays between microbiota and plant bioactives. C.O. Chen

9:15 AGFD 61. 2-Way interaction of dietary polyphenols with gut microbiota and effects on human health. F. Tomas-Barberan

9:50 Intermission.

10:10 AGFD 62. Biotransformation of cranberry A-type proanthocyanidins: Influence on gut microbiota and immune function. J.W. Soares, K. Racicot, L.A. Doherty, S. Ardiciacono, E. Apostolidis, C.O. Chen

10:45 AGFD 63. Metabolism of oat avenanthramides by gut microbiota. S. Sang, P. Wang, H. Chen

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center Room 212

Complex Coacervation: Principles & Applications

Financially supported by The Dow Chemical Company

Cosponsored by COLL†

P. L. Dubin, *Organizer*

S. L. Perry, Y. Wang, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 AGFD 64. Artificial cells in picoliter droplets. W. Huck

1:50 AGFD 65. Biomimetic micro-compartmentalization by aqueous phase separation. C.D. Keating

2:20 AGFD 66. Directing the phase behavior of biopolyelectrolyte complexes. L. Leon Gibbons, S.L. Perry, M.J. Lueckheide, J. Vieregger, R.A. Klein, N. Pacalin, M.V. Tirrell

2:50 Intermission.

3:15 AGFD 67. Design and construction of higher-order structure and function in coacervate-based protocells. S. Mann

3:45 AGFD 68. Biomimetic effects on actin cytoskeletal filament growth. S.L. Perry, P. McCall, S. Srivastava, D. Kovar, M. Gardel, M.V. Tirrell

4:15 AGFD 69. In vitro reconstitution of a nonmembrane-bound RNA-protein compartment. S. Saha, A. Hyman

4:45 AGFD 70. Coacervation of mussel-inspired zwitterionic adhesives. H. Waite, B. Ahn

Section B

Boston Convention & Exhibition Center Room 213

Chemistry, Composition & Analysis of Dietary Supplements

M. Sukan, *Organizer*

K. Goodner, Y. Kim, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 71. Heavy metals and aflatoxins in various herbal medicines and health functional foods. K.G. Lee

1:25 AGFD 72. Reactions between polyphenolic dietary supplements and other biomolecules dictate bioactivity, bioavailability and analysis. A.E. Hagerman

1:45 AGFD 73. Rosemary: From nature to table. M. Jordan, C. Martinez-Conesa, S. Bañon, J. Sotomayor

2:05 AGFD 74. Simple UPLC-MS to monitor the presence of pomegranate in pomegranate juices. C. Mathon, A. Green, C.K. Larive

2:25 Intermission.

2:40 AGFD 75. New methods and antioxidants to prevent oxidation of omega-3 oil supplements. M. Phaner, H. Hwang, J.K. Winkler-Moser, E.L. Bakota, S.X. Liu

3:00 AGFD 76. Facile synthesis and characterization of curcumin metformin adduct: Potentially important gamma-secretase inhibitor for Alzheimer disease. B. Dayal

3:20 AGFD 77. Coffee-based dietary supplements contain kaurane diterpenoid glycosides inhibiting adenine nucleotide translocase in mitochondria and reduce respiration. R. Lang, T. Fromme, A. Beusch, T. Lang, M. Klingspor, T. Hofmann

3:40 AGFD 78. Multivitamin and mineral supplements: An overview of key product issues. E.T. Finocchiaro

4:00 Concluding Remarks.

Section C

Boston Convention & Exhibition Center Room 209

Food Toxicants Formed During Food Processing & Storage

S. Wang, L. L. Yu, *Organizers, Presiding*

1:00 AGFD 79. Generation of reactive oxidative species during thermal and UV processing of sugars. R.V. Tikekar

1:35 AGFD 80. Lipid oxidation as a source of diverse food toxicants. B.E. De Meulenaer

2:10 AGFD 81. Evaluation of temperature effect on the concentration levels of polycyclic aromatic hydrocarbons (PAHs) in edible vegetable oil. O.S. Olatunji, B.O. Opeolu, O.S. Fatoki, B.J. Kimba

2:45 Intermission.

3:00 AGFD 82. Effects of thermal and high pressure processing on chemical migration in food contact polymers. J.L. Koontz, Y. Song, Y. Zhou, K. Pillai, K. Zhao, R.O. Juskelis

3:35 AGFD 83. FDA update on acrylamide, furan, and other processing toxicants. L. Jackson

Section D

Boston Convention & Exhibition Center Room 211

Metabolites & Metabolomics of Food Bioactives & Influence of Gut Microbiota: Chemistry and Health Effects

S. Sang, F. Shahidi, *Organizers, Presiding*

1:00 AGFD 84. Metabolic and colonic microbiota transformation may alter the bioactivities of dietary food bioactives. C. Ho, M. Pan, F. Shahidi

1:35 AGFD 85. Metabolites of wheat phytochemicals as the exposure biomarkers of whole grain wheat intake. Y. Zhu, S. Sang

2:10 AGFD 86. Gastrointestinal biotransformation of resveratrol and pterostilbene in mice. Y. Sun, M. Song, F. Li, Y. Cao, H. Xiao

2:45 Intermission.

3:05 AGFD 87. Biological importance of fucoxanthin and its metabolites. K. Miyashita, M. Hosokawa, N. Mikami, Y. Kokai

3:40 AGFD 88. Are anthocyanins PPAR α agonists? A.M. Rimando, S. Khan, C. Mizuno, G. Ren, S. Mathews, H. Kim, W. Yokoyama

4:15 Concluding Remarks.

Section E

Boston Convention & Exhibition Center Room 212

Complex Coacervation: Principles & Applications

Financially supported by The Dow Chemical Company

Cosponsored by COLL†

P. L. Dubin, S. L. Perry, *Organizers, Presiding*

12:00 - 2:00

AGFD 89. Effect of supercharging on coacervation between proteins and polyelectrolytes. A. Obermeyer, C. Mills, X. Dong, B.D. Olsen

AGFD 90. Effect of charge patterning on polypeptide-based complex coacervation. L. Chang, S.L. Perry

AGFD 91. Liquid-to-solid transitions in polyelectrolyte complexes. Y. Liu, H.H. Winter, S.L. Perry

AGFD 92. Polypeptide complexation: From bulk coacervates to nanoscale assemblies. D. Priftis, L. Leon, K.O. Margossian, A. Trophikova, M.V. Tirrell

AGFD 93. Polyelectrolyte complex formation in acetone-water mixture. H. Acar, S. Srivastava, D. Priftis, J. Cabaral, M.V. Tirrell

Undergraduate Research Posters

Agricultural and Food Chemistry

Sponsored by CHED, Cosponsored by AGFD and SOCED

MONDAY EVENING

Section A

Boston Convention & Exhibition Center Hall C

Sci-Mix

B. Park, *Organizer*

8:00 - 10:00

26, 30, 57. See previous listings.

136, 150, 153, 209, 221, 227, 229, 242-243, 245, 248-249, 251-252, 254-257, 259, 291, 305. See subsequent listings.

Chemical Innovation and Design (CID) Talks: The Future of Innovation Now

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Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 212

**Complex Coacervation:
Principles & Applications**

*Financially supported by The
Dow Chemical Company*

Cosponsored by COLL†

S. L. Perry, *Organizer*

P. L. Dubin, S. Mann, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 94. Chirality-selected phase behavior in complexes of ionic polypeptides. M.V. Tirrell

8:35 AGFD 95. Marine sandcastle worm-inspired medical adhesives based on liquid-liquid phase separation. R. Stewart, M. Sima, R. O'Hara

9:05 AGFD 96. Self-assembled nanostructures from block copolymers for biomedical application. Y. Anraku

9:35 Intermission.

10:00 AGFD 97. Beyond elastin: New peptide polymers that exhibit aqueous coacervation. A. Chilkoti

10:30 AGFD 98. Directing encapsulated stem cell fate via in situ forming, growth factor-loaded coacervate microparticle-embedded hydrogels. E. Alsberg, O. Jeon

11:00 AGFD 99. Coacervates of ionic polysaccharides for tissue engineering. O. Karabiyik, E. Kilic Iljilik, G. Kose, A.B. Kayitmazer

11:30 AGFD 100. Complex coacervates as protein delivery vehicles: Preserved activity, controlled release rate, and in vivo efficacy. N. Johnson, W. Chen, Y. Wang

Section B

Boston Convention & Exhibition Center
Room 213

**Browned Flavors: Analysis,
Formation, & Physiology**

P. H. Schieberle, *Organizer*

M. Granvogl, D. G. Peterson, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 101. Using real time measurement of galvanic electrode potentials to clock the course of Maillard reactions. G.P. Rizzi

8:35 AGFD 102. Different reaction pathways generate aroma-active amino acid degradation products during fermentation, roasting and eating of cocoa. P.H. Schieberle

9:05 AGFD 103. On the role of Amadori-rearrangement products as precursors of aroma-active Strecker aldehydes in cocoa. S. Hartmann, P. Schieberle

9:35 Intermission.

Technical program information
known at press time.

The official technical program
for the 250th ACS National
Meeting is available at:

www.acs.org/boston2015

9:55 AGFD 104. Formation of Strecker aldehydes and biogenic amines as a consequence of carbonyl-amine reactions initiated by oxidized lipids. R. Zamora, M. Leon, F.J. Hidalgo

10:25 AGFD 105. Food-borne taste modulators from Mother Nature and culinary art. T. Hofmann

10:55 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 209

**Food Toxicants Formed During
Food Processing & Storage**

S. Wang, L. L. Yu, *Organizers, Presiding*

8:30 AGFD 106. Improved detection methods for food toxin with nanotechnology. B. Park, B. Wang, B. Xu

9:05 AGFD 107. Lipid rafts may involve in TFA-induced apoptosis and inflammation of human umbilical vein endothelial cells. Z. Deng, H. Rao, B. Qiu, B. Liu, J. Li

9:40 AGFD 108. 3-MCPD 1-monopalmitate induces apoptosis in NRK-52E cells via activation of p53-JNK pathway. G. Huang, M. Liu, H. Shi, X. Sun, L.L. Yu

10:15 Intermission.

10:30 AGFD 109. Stable isotope labeling experiments — a useful tool to identify formation pathways of food-borne toxicants. M. Granvogl

11:05 AGFD 110. Chemoprotection effect of catechins on detoxicity of dietary acrylamide in mercapturic acid adduct level in rats. Y. Zhang, J. Cheng, Q. Wang, X. Chen

Section D

Boston Convention & Exhibition Center
Room 211

**Recovery of Bioactive Compounds
from Processing By-Products**

S. Talcott, *Organizer*

L. Howard, Y. Kim, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 111. Utilization of agricultural by-products in healthful food products: Organogelators, antioxidants, and spreadable products. H. Hwang, J.K. Winkler-Moser, E.L. Bakota, S.X. Liu

8:35 AGFD 112. Extraction and analysis of high-value compounds in agricultural and forest byproducts using water, ethanol, and carbon dioxide at elevated temperature and pressure as solvents. V. Abrahamsson, S. Al-Hamimi, F. Jumaah, J. Liu, M. Plaza, M. Sun, M. Sandahl, C. Turner

9:05 AGFD 113. Components responsible for the functional properties of corn fiber gum. M.P. Yadav

9:35 Intermission.

9:55 AGFD 114. Hemp waste as a potential source of valuable chemicals. A. Hunt, T. Attard, C. Bainier, M. Reinaud, A. Lanot, S. McQueen-Mason, J. Clark

10:25 AGFD 115. Pressurized liquid sequential and direct extraction of phytochemicals from Dancy tangerines for their comprehensive characterization by LC-DAD-ESI-HR-MS. G. Jayaprakasha, B. Patil

10:55 AGFD 116. Orange peel by-products as a source of bioactive compounds. J.A. Manthey, R.G. Cameron

**Current Topics in Chemical
Safety Information**
**Use Cases for Chemical
Safety Information**

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**International Entrepreneurship:
How To Start a Business and
Thrive in the Global Marketplace**

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ORGN, POLY, PRES†, PROF and SCHB*

**Journal of Agricultural and Food
Chemistry Best Paper Awards**

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**USDA-ARS Sterling B. Hendricks
Memorial Lectureship:
James H. Tumlinson**

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TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 212

**Complex Coacervation:
Principles & Applications**

Cosponsored by COLL†

P. L. Dubin, S. L. Perry, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 AGFD 117. Interaction/coacervation between food proteins: Mechanisms and potential application. S. Bouhallab, G. Tavares, A. Chapeau, P. Hamon, T. Croguerneac

1:50 AGFD 118. Assembly of protein/polysaccharide complexes-based Pickering emulsions for nutraceutical delivery. Q. Huang

2:20 AGFD 119. Formation of a coacervate film across the oil-water interface: Stabilization of emulsions. H. Montelliet, M. Kleijn, F. Leermakers, J. Sprakel

2:50 Intermission.

3:15 AGFD 120. Complex coacervation in heteroprotein systems: A special form of macromolecular liquid-liquid phase separation. D. Seeman, P.L. Dubin

3:45 AGFD 121. Complex coacervation with oppositely charged polymer and surfactant: Determination factor in the morphology of coacervated complexes during the dilution process. M. Miyake

4:15 AGFD 122. Optimization of milk protein-native gum (tragacanth and Persian gums) interactions: Complex coacervation and soluble complexes. S. Abbasi, F. Azarkia

4:45 AGFD 123. Study of complex coacervation of gelatin A with sodium carboxymethyl cellulose/sodium alginate/carrageenan: Formation of smart microparticles and encapsulation. N. Devi, T. Maji, D. Kakati

Section B

Boston Convention & Exhibition Center
Room 213

**Browned Flavors: Analysis,
Formation, & Physiology**

M. Granvogl, *Organizer*

D. G. Peterson, P. H. Schieberle, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 124. Variation in Maillard reaction product formation in oats from 13 cultivars. M.J. Morello, B.C. Vastano

1:35 AGFD 125. Characterization of key aroma-active compounds in raw and roasted mustard seeds (*Sinapis alba* L.). M. Granvogl, E. Ortner, P.H. Schieberle

2:05 AGFD 126. Defining mechanisms of flavor development in foodstuffs. D.G. Peterson, L. Zhang, S. Kokkinidou

2:35 Intermission.

2:55 AGFD 127. Formation of reactive fragmentation products during Maillard degradation of higher sugars. M.A. Glomb, M. Smuda, C. Henning

3:25 AGFD 128. Characterization of color formation in juice products. L. Paravisini, D.G. Peterson

3:55 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 209

Young Scientist Award Symposium

C. J. Brine, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 129. Development and applications of surface-enhanced Raman spectroscopy in food science. L. He

1:35 AGFD 130. Primary expectations of secondary metabolites. J. Lee

2:05 AGFD 131. Concentration of propolis extract using hydrophobic membrane. C. Leo

2:35 Intermission.

2:50 AGFD 132. Utilization of in vitro and in vivo gastrointestinal models in the production of optimum functional food formulations. Y. Ting, Y. Jiang, C. Ho, Q. Huang

3:20 AGFD 133. High-resolution mass spectrometry for the exploration of novel plant sterol conjugates. L. Nystroem

3:50 AGFD 134. Integrated advanced multi-omics strategies: A new paradigm for agricultural and medicinal plant biotechnology. J. Marques, D.S. Dalisay, M. Costa, B. Herman, L.B. Davin, N.G. Lewis

4:20 Concluding Remarks.

Section D

Boston Convention & Exhibition Center
Room 211

**Recovery of Bioactive Compounds
from Processing By-Products**

S. Talcott, *Organizer*

L. Howard, Y. Kim, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 135. Recovery and development of value-added applications of fruit juice processing byproducts. Y. Zhao

1:35 AGFD 136. Eco-innovative polyphenol extraction using subcritical water from red and white pomace, coupled with purification by membrane processes. S. Yammine, X. Vitrac, R. Rabagliato, M. Mietton Peuchot, R. Ghidossi

2:05 AGFD 137. Incorporation of pressurized fluid technology in the recovery of bioactive constituents from pomace processing wastes. J.W. King, L. Howard

2:35 Intermission.

2:55 AGFD 138. Physicochemical challenges to recover polyphenolics from Concord grapes skins. S. Talcott

3:25 AGFD 139. Comparison between antioxidant potentials of extracts from black chokeberry pomace and walnut husk using supercritical carbon dioxide and ethanol. **J. Wenzel**, T. Dixon, E. Tucker, L. Burrows, N. Dwarshuis, E. Hossink, L. Wang, M. Ammerman, C. Samaniego

Section E

Boston Convention & Exhibition Center Room 212

AGFD Division Award: Symposium in honor of Dr. Andrew Taylor

K. D. Deibler, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 AGFD 140. Acrylamide — a challenge to food scientists in industry and academia. **D.S. Mottram**

1:35 AGFD 141. 2,5-Diketopiperazines — interesting markers of reaction or compounds with sensory and bioactive properties? **N.C. Da Costa**, M.Z. Chen

2:00 AGFD 142. On-line aroma monitoring with mass spectrometry and link to flavor release and flavor perception. **J. Le Quere**

2:25 Intermission.

2:40 AGFD 143. Separation and concentration of trace high-impact odorants using multidimensional gas chromatography-mass spectrometry-olfactometry with integrated preparative fraction collection. **L. Jones**, K. Chu, B. White, A. Ward

3:05 AGFD 144. Encapsulation, multimodal perception, and its applications. **G. Reineccius**

3:30 AGFD 145. Modelling mass transfer under simulated nasal conditions — innovative laboratory experimental systems. **M. Yabuki**, D. Scott, L. Briand, A.J. Taylor

3:55 AGFD 146. Biology of taste: Studies of the order Carnivora. **G.K. Beauchamp**, P. Jiang

4:20 Concluding Remarks.

Section A

Boston Convention & Exhibition Center Room 251

Complex Coacervation: Principles & Applications

Cosponsored by COLT†

P. L. Dubin, S. L. Perry, *Organizers, Presiding*

1:00 - 3:00

AGFD 147. Understanding colloidal stability and thermal transitions in polyelectrolyte complexes. **Y. Zhang**, D. Reid, E. Yildirim, H.S. Antila, R. Zhang, M. Sammalkorpi, J.L. Lutkenhaus

AGFD 148. Thermal transition in polyelectrolyte complexes via LCST mechanism. **E. Yildirim**, Y. Zhang, R. Zhang, J.L. Lutkenhaus, **M. Sammalkorpi**

AGFD 149. Polyelectrolyte complexes of DNA and polypeptides. **M.J. Lueckheide**, L. Leon, J. Viereg, M.V. Tirrell

AGFD 150. Complexation of linear poly(ethylene imine)/poly(acrylic acid) and branched poly(ethylene imine)/metal ions: The effect of ionic strength, molar ratio, and pH. **H. Zhang**, N. Zacharia

AGFD 151. Hydrogen bonded polymer complexes with hydrophobic associations. **Y. Gu**, R.A. Weiss, **N. Zacharia**

Section A

Boston Convention & Exhibition Center Halls A/B1

General Posters

B. Park, *Organizer*

3:00 - 5:00

AGFD 152. Mineral nutrient profile of orange juice. **M. Azik**, D. McLean

AGFD 153. Residual effects of low and/or high temperature treatment at mature green stage on volatile production of tomatoes at following ripeness stages. **L. Wang**, B. Elizabeth, A. Plotto, J. Brecht, Z. Yu, **J. Bai**

AGFD 154. Use of foliar fungicide spray for control of HLB-related pre-harvest fruit drop. **W. Zhao**, **J. Bai**, G. McCollum, T. Gottwald, A. Plotto, B. Elizabeth

AGFD 155. Self-assembly of two-way nanotubes by proteolysis of wheat bran albumins with protease V8, in presence of calcium ions. **G. Chaquilla-Quilca**, **R.R. Balandran-Quintana**, J.A. Azamar-Barrios, G. Ramos Clamont-Montfort, A.M. Mendoza-Wilson, J.N. Mercado-Ruiz, T.J. Madera-Santana, Y.L. Lopez-Franco

AGFD 156. Synthesis of wheat bran albumin nanoparticles by a cold gelation/desolvation method. **J.G. Luna-Valdez**, **R.R. Balandran-Quintana**, J.A. Azamar-Barrios, G. Ramos Clamont-Montfort, A.M. Mendoza-Wilson, J.N. Mercado-Ruiz, T.J. Madera-Santana, A. Rascon-Chu

AGFD 157. Improvements in the measurement of chlorophylloids in soybean oil. **A.C. Litin**, D.D. Brooks

AGFD 158. Impact of food preparation on total phenolic contents and anti-oxidant capacities of regularly consumed botanicals. **L. Yu**, **B. Gao**, T.T. Wang, L.L. Yu

AGFD 159. Effects of home-based preparation approaches in determining the release of bioactivity compounds in fruits and vegetables. **B. Gao**, L. Yu, T.T. Wang, L.L. Yu

AGFD 160. Determination of the heavy metals in the health functional foods by inductively-coupled plasma/atomic emission spectrometry. **J. Hong**, C. Lim, Y. Chang, C. Lim, T. Kang

AGFD 161. Multiresidue analysis of pesticides in commercial agricultural products using LC-MS/MS. **S. Won**, S. Kim, N. Kang, Y. Kang, D. Kim, H. Chang, D. Kim, I. Jung, S. Woo, S. Kim, J. Park, H. Yoon

AGFD 162. Antimicrobial peptide segments from soy protein for use in food safety. **N. Xiang**, Y. Lyu, A. Bhunia, **G. Narsimhan**

AGFD 163. Flavonol glycosides in wild and cultivated berries of two major subspecies of sea buckthorn and influence of growth sites. **X. Ma**, O. Laaksonen, H. Kallio, B. Yang

AGFD 164. Flavonol glycosides in leaves of different varieties of black currant, green currant, red currant, white currant and changes of growing season, growth location, leaf position. **W. Yang**, H. Kallio, B. Yang

AGFD 165. Pilot-scale bioreactor production and long term stability of feruloyl soy glycerides. **D.L. Compton**, J.R. Goodell, S. Grall, K. Evans

AGFD 166. Synthesis and lead discovery of pyrazolocyclohexanol derivatives. **G. Aiying**, C. Liu, Y. Xie, Z. Huang, J. Wang, X. Wang, Q. Sun, X. Sun, J. Yang, Y. Wu

AGFD 167. Withdrawn.

AGFD 168. Withdrawn.

AGFD 169. Withdrawn.

AGFD 170. Withdrawn.

AGFD 171. Design, synthesis, and insecticidal evaluation of novel insecticidal aryloxy dihaloropropane derivatives. **j. Yang**, C. Liu, M. Li, X. Chang, **G. Aiying**, Q. Wu, Y. Song

AGFD 172. Synthesis, characterization, and fungicidal activity of some new N-phenyl benzothiazolamine derivatives. **G. Aiying**, C. Liu, H. Li, Q. Sun, X. Sun, J. Wang, Y. Xie, F. Yang, J. Yang

AGFD 173. Synthesis and herbicidal activity of novel substituted 3-(pyridin-2-yl) benzenesulfonamide derivatives. **Y. Xie**, H. Chi, **G. Aiying**, C. Liu, H. Ma

AGFD 174. Synthesis and insecticidal activity study of 2-(2,6-dichlorobenzamido)-4-thiazolecarboxamide derivatives. **Y. Xie**, S. Xu, **G. Aiying**, L. Wang, C. Liu

AGFD 175. Adulteration and its detection of black raspberry products. **J. Lee**

AGFD 176. Effect of fresh and commercially processed orange juice on the oxidative status in healthy humans. **J.Q. Silveira**, T.B. Cesar, A.M. Nasser, J.A. Manthey, B. Elizabeth

AGFD 177. Luteolin-mediated apoptosis in leukemia cells involves PTTG1 oncoprotein and differential responses. **H. Tien**, P. Chen, J. Chen, M. Wu, J. Yen

AGFD 178. Development of lecithin emulsion gel to enhance the oral bioaccessibility of nobiletin. **Y. Ting**, Y. Pan, Q. Huang

AGFD 179. Updated exposure assessment for 4-methylimidazole (4-MEI) for the U.S. population based on quantitative data from foods. **D.E. Folmer**, D.L. Doell, H.S. Lee, G.O. Noonan, S.E. Carberry

AGFD 180. In-vitro digestion properties of Pickering emulsions stabilized by starch nanocrystals. **R. Liang**, Y. Jiang, C. Yang

AGFD 181. Tanshinone IIA modulates cell-surface LDLR level and LDL uptake via suppression of PCSK9 gene expression in HepG2 cells. **H. Chen**, M. Wu, P. Chen, Y. Chen, M. Tai, J. Yen

AGFD 182. Novel SERS-based approach to detect hydrogen peroxide scavenging activity. **W. Qian**

AGFD 183. Simultaneous analysis of unregistered pesticides in Korea by liquid chromatography-tandem mass spectrometry. **S. Lee**, J. Hwang, S. Jeon, J. Kim, Y.D. Lee, H. Kim, H. Lee, M. Jang, G. Lee

AGFD 184. Combination of pre-column nitro-reduction and ultra-performance liquid chromatography with fluorescence detection for the sensitive quantification of 1-nitronaphthalene, 2-nitrofluorene, and 1-nitropyrene in meat products. **K. Deng**, W. Chan

AGFD 185. Updated exposure estimate for FD&C color additives for the U.S. population. **D.L. Doell**, D.E. Folmer, H.S. Lee, K.M. Butts, S.E. Carberry

AGFD 186. Withdrawn.

AGFD 187. Saponins quantification in pigmented chickpeas cultivars. **A.K. Milan**, S.R. Serna Saldívar, J. Gutierrez

AGFD 188. Development and validation of analytical method of furan in seven different types of food matrices using SPME-GC/MS. **Y. Seok**, S. Jeong, J. Her, K.G. Lee

AGFD 189. Analytical advances in food-technology by establishment of a 14-C food-technology lab and kitchen. **M. Kotthoff**, M. Bücking

AGFD 190. Carotenoid composition analysis in fruit of rose hip (*Rosa glauca*) by HPLC-DAD-APCI-MS. **L. Zhong**, K. Gustavsson, M. Olsson

AGFD 191. Convenient, inexpensive measurement of free and copper-complexed hydrogen sulfide in wine. **Y. Chen**, J. Jastrzebski, I. Ryona, G.L. Sacks

AGFD 192. Interaction between caseinophosphopeptides and theaflavin-3,3'-digallate and its impact on the antioxidant activity of theaflavin-3,3'-digallate. **Y. Jiang**, Y. Ting, J. Li, Q. Huang

AGFD 193. Micronanopores in diatomite fabricated by high energy electron beam and hydrothermal treatment to control the loss of pesticide. **X. Zhang**, Z. Wu

AGFD 194. Determination of protein-bound metabolites of nitrofurans by combining on-line precolumn derivatization and high performance liquid chromatography with fluorescence detection. **W. Yinan**, W. Chan

AGFD 195. HPLC-MS of hesperidin metabolites in rat urine. **D. Gonçalves**, M. Rodrigues, T. Cesar, J.A. Manthey

AGFD 196. Spectrofluorimetric study of the interaction of the mycotoxin citrinin with gold nanoparticles. **M. Appell**, **W. Bosma**

AGFD 197. Inhibitory effects of edible berry extracts on the formation of advanced glycation endproducts. **H. Ma**, W. Liu, J.A. Dain, N.P. Seeram

AGFD 198. Pomegranate polyphenols inhibit the formation of advanced glycation endproducts and aggregation of beta amyloid. **H. Ma**, W. Liu, D.B. Niesen, J.A. Dain, N.P. Seeram

AGFD 199. Standardized food grade maple syrup extract (MSX) imparts lipid lowering and anti-inflammatory effects in mature differentiated mouse and human adipocytes. **P. Nahar**, A.L. Slitt, N.P. Seeram

AGFD 200. Natural product derived brain absorbable RAGE inhibitors for Alzheimer's disease: The case of the urolithins. **D.B. Niesen**, N. Shah, H. Ma, N.P. Seeram

AGFD 201. Beyond L-DOPA: Bioactives in *Mucuna pruriens* for the treatment of Parkinson's disease. **C. Hessler**, D.B. Niesen, H. Ma, N.P. Seeram

AGFD 202. Methylglyoxal induced cell cytotoxicity inhibitory and scavenging properties of a standardized food grade maple syrup extract (MSX). **W. Liu**, Z. Wei, H. Ma, J.A. Dain, Z. Shaikh, N.P. Seeram

AGFD 203. 3'-Hydroxypterostilbene simultaneously induces apoptosis and autophagy in human prostate cancer cells. **H. Tsai**, T. Huang, C. Ho, Y. Chen

AGFD 204. Withdrawn.

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- AGFD **205.** Withdrawn.
- AGFD **206.** Effects of KCl substitution on textural properties of Queso Fresco. M.H. Tunick
- AGFD **207.** Biological activities of diterpenoids from *Hyptis verticillata*. R.B. Porter
- AGFD **208.** Study of the encapsulation of aroma compounds from starch emulsions by reversed flow gas chromatography (RFGC). J. Kapolos, A. Koliadima, G. Karaiskakis
- AGFD **209.** Stereochemical determination of methamidophos and ruelene, organophosphorus compounds. M.C. Chiu, K. Tami, C. Kinahan, A. Ng, G. Proni
- AGFD **210.** Analysis of carcinogenic 4(5)-methylimidazole in various commercially available foods and beverages. S. Lee, J. Her, M. Jung, K.G. Lee
- AGFD **211.** Metabolic exploration about blueberry, raspberry, and blackberry. W. Kim, J. Pyo, J. Her, K.G. Lee
- AGFD **212.** Formation and reduction of furan in soy sauce (ganjnag) according to the time of addition of food additives. M. Kim, J. Her, J. Lee, K.G. Lee
- AGFD **213.** Validation of an analytical method for quantification of Benzo(a)pyrene in two different types of food matrices using GC/MS. S. Park, J. Jeong, J. Her, K.G. Lee
- AGFD **214.** Formation and reduction of ethyl carbamate in soybean paste (Doenjang) model system. S. Lee, H. Song, J. Her, K.G. Lee
- AGFD **215.** Development of an analytical method for quantification of biogenic amines in fermented soybean paste (Doenjang). Y. Kim, J. Lee, J. Her, K.G. Lee
- AGFD **216.** Oil lipolysis process controlled by formation of Pickering emulsion. W. Jin, Y. Jiang, B. Li, Q. Huang
- AGFD **217.** Use of fat compost from dairy industry wastewater as a new organic amendment for pepper (*Capsicum annuum* L.) crop. M. Fiasconaro, M. Lovato, C. Martin
- AGFD **218.** Anti-inflammatory effect of resveratrol metabolite, δ -viniferin, on LPS-stimulated murine macrophage. P. Hsieh, M. Pan, C. Ho
- AGFD **219.** Density functional theory study of the formation mechanism of acrylamide with glyoxal and asparagine as precursors. F.M. Tao, J. Wu, Z. Wang
- AGFD **220.** Characterization and quantification of flavonoids and organic acids throughout fruit development in American cranberry (*Vaccinium macrocarpon*) using HPLC and AP/MS/MS. Y. Wang, J. Johnson-Cicalese, A.P. Singh, N. Vorsa
- AGFD **221.** Flavor chemical analysis of shrimp from near-shore Louisiana Gulf Coast estuaries. K.H. Driggers
- AGFD **222.** Time-resolved determination of physicochemical quantities for physically adsorbed or chemisorbed aroma compounds on starch granules, by inverse gas chromatography. A. Koliadima, J. Kapolos, G. Karaiskakis
- AGFD **223.** Early detection of milk spoilage via volatile organic compound analysis using multidimensional gas chromatograph/mass spectrometry. K. Rochford
- AGFD **224.** Structural properties of B-type procyanidin oligomers and their ability to scavenge free radicals: A DFT study. A.M. Mendoza-Wilson, S.I. Castro-Arredondo, R.R. Balandran-Quintana
- AGFD **225.** Determination of the antiradical and chelating potential of a phenolic extract and a procyanidin-rich fraction of apple peel by experimental and computational methods. A.M. Mendoza-Wilson, A. Espinosa-Plascencia, R. Robles-Burgueño, R.R. Balandran-Quintana, M.d. Bermudez-Almada
- AGFD **226.** New active packaging film from natural resources. A. Machado
- AGFD **227.** Development of a novel biomagnetic separation method for rapid detection of *Escherichia coli* by phage display technique. Z. Wang
- AGFD **228.** Withdrawn.
- AGFD **229.** Synthesis of quinolactamide, penicillamine, and their analogs as potential insecticides. S. Rasapalli, R. Mastrolia
- AGFD **230.** Inhibitory activity of *Enterococcus faecalis* PL9003 on oxidation and melanogenesis. Y. Lee, H. Lee
- AGFD **231.** Studies on the discovery of agriculturally active compounds from marine endophytic fungi. H. Sun, C. Wang, Q. Song, Y. Tang, Y. Xia
- AGFD **232.** Study of vitro digestion on desiccated coconut. H. Wu, J. Xiong, J. Ye
- AGFD **233.** Quantitation of chiral heterocyclic key aroma compounds in cooked *Alliaceae* varieties using a stable isotope dilution assay. M. Flaig, M. Granvogl, P.H. Schieberle
- AGFD **234.** Peri-receptor modulation of the human salivary proteome by taste stimuli. T. Stolle, M. Bader, T. Hofmann
- AGFD **235.** Modeling the leachability of pH-dependent ionizable organic contaminants from municipal sewage sludge. A. Venkatesan, R.U. Halden
- AGFD **236.** Alkaloid profiles of hairy root cultures of *Catharanthus roseus* differ when generated by different strains of *Agrobacterium rhizogenes*. J. de la Parra, N. Rizvi, R.A. Kautz, P. Wang, R. Giese, C.W. Lee-Parsons
- AGFD **237.** Ensuring coffee freshness in portioned coffee system. L. Poisson, S. Legrand, Y. Wyser, F. Mestdagh, B. Folmer, J. Kerler
- AGFD **238.** Red shortening: Characterization and utilization in formulating novel functional biscuits. H. Abou Gharbia
- AGFD **239.** 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 **240.** Withdrawn.
- AGFD **241.** Capillary electrophoresis coupled with inductively-coupled plasma mass spectrometry as an analytical tool for arsenic speciation in rice. H. Qu, T. Mudalige, S. Linder
- AGFD **242.** Prevention and treatment of *Staphylococcus aureus* biofilm formation using Russian Propolis ethanol extracts. J. Bryan, C. Traba, M.J. Castaldi
- AGFD **243.** Orange juice reduces oxidative stress and inflammatory markers in patients with chronic hepatitis C. D.R. Gonçalves, C.G. Lima, P.S. Ferreira, P.I. Costa, T.B. Cesar
- AGFD **244.** Characterization of constituents from cranberry non-dialyzable material that inhibit bacterial co-aggregation and adhesion. K. Penndorf, C.C. Neto, M. Feldman, S. Meron-Sudai, Z. Rones, D. Steinberg, M. Fridman, I. Ginsburg, I. Ofek, E. Weiss
- AGFD **245.** Inhibition of colon cancer growth and inflammation in cellular and mouse models by cranberry extracts (*Vaccinium macrocarpon*). S. Frade, A. Liberty, A. Tata, X. Wu, M. Song, X. Cai, H. Xiao, C.C. Neto
- AGFD **246.** NMR-based metabolomic analysis and quantification of phytochemical constituents in North American cranberry fruit (*Vaccinium macrocarpon*). A. Milstead, L. Xue, K.L. Colson, C.C. Neto
- AGFD **247.** Dietary exposure of nonphthalate-based plasticizers from use in food contact material. L.T. Cureton, A.B. Bailey
- AGFD **248.** Preparation of metal chelating active food packaging materials by laminated photografting. J.Z. Lin, M. Roman, F. Tian, E.A. Decker, J.M. Goddard
- AGFD **249.** Rapid detection of *Salmonella* using a redox cycling-based electrochemical method. D. Wang, A. Kinchla, S.R. Nugen
- AGFD **250.** Metal oxide gas sensor array combined with a miniaturized gas chromatographic system for fast detection of volatile quality indicators. M. Kothhoff, M. Bücking, J. Bruckert, M. Bauersfeld, J. Wöllenstein
- AGFD **251.** Metabolomics application for rapid screening and authentication of Asian palm civet coffee (Kopi Luwak). U. Jumhawan, S. Putri, Y. Yusianto, T. Bamba, E. Fukusaki
- AGFD **252.** Withdrawn.
- AGFD **253.** Modeling the human colon: An automated multistage fermentation approach. L.A. Doherty, S. Arcidiacono, K. Racicot, J.W. Soares
- AGFD **254.** Antioxidant activity and inhibition of amylase by Washington navel oranges. S. Kommein, B. Patil
- AGFD **255.** Determination of microbial volatile organic compounds patterns from virulent and hypovirulent *Cryphonectria parasitica* isolates by headspace-SPME-GC-MS. J. She, M. King, B. Stokes, Y. Jiang, R. Baird, T.E. Mlnsa
- AGFD **256.** Kinetic stability of bean and pea proteins: Effect on protein digestibility and bean resistance to environmental conditions. K. Xia, J. Wilcox, S. Pittelli, W. Colon
- AGFD **257.** Antioxidative compounds from *Garcinia buchananii* stem bark. M. Salger, T.D. Stark, J. Wakamatsu, T. Hofmann
- AGFD **258.** Innovative microwave-assisted procedure for the extraction and purification of policosanols from beeswax. V. Brighenti, A. Chiossi, A. Venturini, F. Pellati
- AGFD **259.** Determination of hydrogen bonding acidity values and distribution coefficients for flavonoids with multiple hydroxyl substituents. C.E. Earp, W.L. Whaley, M.H. Abraham
- AGFD **260.** Characterization and phytoremediation of a crude oil contaminated wetland. E.O. Nwaichi, L. Opara, P. Nwoha
- AGFD **261.** Stabilization of whey protein isolate (WPI) by sugar beet pectin (SBP) through a Maillard-type reaction in solution. P.X. Qi, Y. Xiao
- AGFD **262.** Adsorption of clay microparticles at the interface of PEG/dextran aqueous biphasic systems: Formation of clay-stabilized aqueous-organic emulsion droplets. F. Pir-Cakmak, C.D. Keating
- AGFD **263.** Rechargeable antimicrobial N-halamine coatings for food contact surfaces. L.J. Bastarrachea, J.M. Goddard
- AGFD **264.** Sodium diffusion in potatoes. J.K. Pandya, A. Kinchla
- AGFD **265.** Determination of furan levels in commercial orange juice products and its correlation to the sensory and physicochemical characteristics. M. Kim, M. Kim, K.G. Lee
- AGFD **266.** Optimization of essential oils properties by enzymatic modification of their chemical composition: Toward sustainable processes for the production of new fragrant ingredients. S. Antonietti
- AGFD **267.** Analytical chemistry, formation, reduction, chemoprevention, and in vivo exposure of acrylamide. Y. Zhang
- AGFD **268.** Synthesis and development of a new respiratory inhibition-type fungicide. W. Lee, J. Kim, H. Shin, I. Hwang
- AGFD **269.** Differentiation of red Port wines categories according to their volatile carbonyl compounds. N. Moreira, I. Vasconcelos, F. Rogerson, P. Guedes de Pinho
- AGFD **270.** Influence of plant-based protein diet on orange-spotted grouper (*Epinephelus coioides*) white muscle proteome profile. Y. Ko, C. Liou, F. Huang, B. Kazlowski, S. Shu, Y. Tan, Y. Luo, I. Sie

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 212

Challenges in Applied Flavor Sciences

L. Jones, J. W. Marshall, A. J. Taylor, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 AGFD 271. Food's combinatorial odor codes — new knowledge on how nature recruits volatiles to make our foods smell so good. A. Dunkel, M. Steinhaus, M. Kothhoff, B. Nowak, D. Krautwurst, P. Schieberle, T. Hofmann

8:40 AGFD 272. Application of sensors to commercial flavour analyses. M. Thornton, M. Bueno-Fernandez, J. Addison, K. Chu, L. Jones

9:00 AGFD 273. Insights into the chemical composition of processed food products. A.J. Taylor, N. Wollmann, J.W. Marshall

9:30 Intermission.

9:50 AGFD 274. Needle in a haystack: Flavor analysis in complex food systems. J.W. Marshall, T. Andy, A. Obee

10:20 AGFD 275. From model food to real food systems: Advances and challenges in relating sensory measurements to in vivo flavor release. J. Le Quere, E. Guichard, P. Schlich

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

10:50 AGFD 276. Mechanism of flavor release from a pet food: Learnings and challenges.

P. Mohapatra, C. Cox, B. Bennett

11:10 AGFD 277. Withdrawn.

Section B

Boston Convention & Exhibition Center
Room 213

Browned Flavors: Analysis, Formation, & Physiology

D. G. Peterson, P. H. Schieberle, *Organizers*

M. Granvogel, *Organizer, Presiding*

V. Somoza, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD 278. Covalent polyphenol-protein interactions — challenges and research needs. S. Rohn

8:35 AGFD 279. Do dietary Maillard reaction products play a role in the progression of noncommunicable diseases? V. Somoza, A. Holik

9:05 AGFD 280. Kinetic modeling of acrylamide formation during the finish-frying of french fries with variable sugar content. D.P. Balagiannis, J.K. Parker, J. Higley, T. Henson, G. Smith, B.L. Wedzicha, D.S. Mottram

9:35 Intermission.

9:55 AGFD 281. Producing low acrylamide risk potatoes: A three-year public/private sector collaborative project focused on genetics, agronomy, and storage. N. Halford

10:25 AGFD 282. Flavor and Acrylamide Formation. J.S. Elmore

10:55 AGFD 283. Reducing the acrylamide-forming potential of wheat and rye. T. Curtis, J. Postles, N. Halford

11:25 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 209

Environmental Effect on Plant Volatile Formation & Nonvolatile Composition

M. C. Qian, A. M. Rimando, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 AGFD 284. Impact of water deficit on volatile composition of grapes and wine. M.C. Qian, K. Shellee

8:55 AGFD 285. Influence of sunlight exposure on Pinot noir grape and wine volatile composition. M.C. Qian, F. Yuan

9:20 AGFD 286. Not your ordinary terroir — the role of pathogenesis related proteins (PRPs) in limiting tannin extraction across winegrape varieties and regions. L.F. Springer, G.L. Sacks

9:45 Intermission.

10:00 AGFD 287. Accumulation of exogenous volatiles in *Vitis vinifera* fruit and leaves as nonvolatile glycoconjugates. K. Wilkinson, R. Ristic, J. Culbert, L. Van der Hulst, A. Pardo-Garcia, G. Alonso, R. Salinas, N. Lloyd, Y. Hayasaka

10:25 AGFD 288. Changes in orange juice flavor volatile and non-volatile compounds in response to citrus greening or Huanglongbing (HLB) disease and disease management strategies.

B. Elizabeth, A. Plotto, J. Bai, J.A. Manthey, S. Raitore, H. Yang, S. Deterre, S. Dea

10:50 AGFD 289. Postharvest practices to alleviate flavor loss of tomatoes under current marketing systems.

J. Bai, B. Elizabeth, A. Plotto, L. Wang

11:15 AGFD 290. Molecular assessment of metabolome changes in carrots (*Daucus carota* L.) induced by abiotic stress challenges. C. Dawid, A. Dunkel, T. Nothnagel, D. Ulrich, B. Singlinger, D. Günzkofer, T. Hofmann

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 212

Challenges in Applied Flavor Sciences

L. Jones, J. W. Marshall, A. J. Taylor, *Organizers, Presiding*

1:00 AGFD 291. Flavour formation in skimmed milk powder in a low-moisture model system. A. Stewart, A. Ryan, A. Grandison, J.K. Parker

1:20 AGFD 292. Use of gas chromatography with quadrupole time-of-flight mass spectrometry (GC/Q-ToF) to compare odor formation in meat and model meat systems following the addition of precursor flavors. L. Jones, J. Addison, N. Hawkins, K. Ridgway

1:40 AGFD 293. Parameters impacting flavour profile and shelf-life of dairy ingredients. M. Trotn, A. Czepa, B. Suess, P.R. Guillet, J. Pfeifer

2:00 AGFD 294. Sensory and instrumental analysis of sweet potato fries. J.K. Parker, S. Lignou, J.S. Elmore, D.P. Balagiannis, J. Higley, G.L. Smith, D.S. Mottram

2:20 AGFD 295. 1-p-Menth-8-thiol, the grapefruit character impact volatile, is a thermally generated artifact in citrus juices. F. Jabapurwala, J. Lin, R.L. Rouseff

2:40 Intermission.

3:00 AGFD 296. Chiral mono-terpene profile in Pinot Gris and Riesling wines determined by head phase-solid phase micro-extraction-multidimensional gas chromatography-mass spectrometry (HS-SPME-MDGC-MS). M. Song, Y. Xia, E. Tomasino

3:20 AGFD 297. Understanding the effects of ethanol-flavor interactions on flavor perception in alcoholic beverages. C. Ickes, K.R. Cadwallader

3:40 AGFD 298. Enantiomeric analysis of volatile chiral compounds in ready-to-drink tea beverages during storage using multidimensional gas chromatography. F. He, Y.L. Qian, M.C. Qian

4:00 AGFD 299. Changes in the key aroma compounds of Shiitake and Oyster mushrooms induced by a thermal treatment. P. Schmidberger, P. Schieberle

Section B

Boston Convention & Exhibition Center
Room 213

Chemistry and Bioactivities of Natural Polymethoxyflavones

C. Ho, *Organizer*

S. Li, M. Pan, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 300. Molecular mechanisms of disease chemoprevention by polymethoxyflavones.

M. Pan, C. Lai, C. Lo, S. Li, C. Ho

1:30 AGFD 301. Lipid-lowering activity of citrus polymethoxylated flavones is mediated by down-regulation of lipogenic genes. Z. Chen, L. Lei

1:55 AGFD 302. Citrus polymethoxyflavones and monodemethylated polymethoxyflavones inhibit adipogenesis in 3T3-L1 adipocytes. S. Lin, P. Chen, M. Pan, S. Li, C. Ho, C.Y. Lo

2:20 AGFD 303. Anti-adipogenesis effect of 5-demethylnobiletin and its acetylated derivative in 3T3-L1 preadipocyte model. Y. Tung, G. Wei, S. Li, M. Pan, C. Ho

2:45 Intermissions.

3:00 AGFD 304. Polymethoxyflavones from aged orange peels: Extraction, formulation, and bioefficacy. Q. Huang

3:25 AGFD 305. Withdrawn

3:50 AGFD 306. Gastrointestinal biotransformation enhances biological effects of polymethoxyflavones. M. Wang, M. Song, X. Wu, Z. Gao, F. Xu, Y. Cao, H. Xiao

Section C

Boston Convention & Exhibition Center
Room 209

Environmental Effect on Plant Volatile Formation & Nonvolatile Composition

M. C. Qian, A. M. Rimando, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 AGFD 307. Metabolite profiling of barley grain: Impact of induced drought stress. K. Engel, A. Lanzinger, T. Frank, G. Reichenberger, M. Herz

1:45 AGFD 308. Effect of growing environment on the characteristics of soybeans for food uses. S.K. Chang, S. Meng

2:10 AGFD 309. Growing conditions affect flavonoid concentration and yield in American skullcap (*Scutellaria lateriflora*). D.A. Shannon, A. Similien, A.M. Rimando, E. van Santen, C.W. Wood, N. Joshee, B.W. Kemppainen

2:35 Intermission.

2:50 AGFD 310. Chemical characterization of pigments in three guava (*Psidium guajava*) Colombian varieties. I. González, A. Melendez, F. Heredia, C. Osorio Roa

3:15 AGFD 311. Fresh ginger vs. dry ginger: The impact of temperature on the bioactive components in ginger. S. Sang

3:40 AGFD 312. Differentiating organic and conventional oregano using ultra-performance liquid chromatography mass spectrometry (UPLC-MS), headspace gas chromatography with flame ionization detection (headspace-GC-FID), and flow injection mass spectrum (FIMS) fingerprints combined with multivariate data analysis. B. Gao, W. Lu, L.L. Yu

Section D

Boston Convention & Exhibition Center
Room 211

General Papers

B. Park, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 313. Detection of *Escherichia coli* in drinking water using T7 bacteriophage-conjugated magnetic probe. J. Chen, Z. Jiang, S.D. Alcaine, V.M. Rotello, S.R. Nugen

1:30 AGFD 314. Electrospun water soluble nanofibers for dehydration and storage of bacteriophage for decontamination of agricultural water. C. Koo, S.R. Nugen

1:55 AGFD 315. Withdrawn.

2:20 AGFD 316. In-product anti-counterfeiting agrochemicals using phase change nanoparticles. M. Wang, M. Su

2:45 AGFD 317. Functional diet ginger (*Zingiber officinale Roscoe*, Zingiberaceae). H. Wang

3:10 Intermission.

3:25 AGFD 318. Is our salad safe? Efficacy of disinfection techniques to decontaminate spinach leaves and reduce cross-contamination. N. Kinsinger, S.L. Walker

3:50 AGFD 319. Authentic milk powder variance study and detection of melamine adulteration using Raman spectroscopy and chemometrics. S. Karunathilaka, S. Farris, M. Mossoba, B.J. Yakes

4:15 AGFD 320. Thermal dependence of riboflavin photodegradation in amorphous sucrose matrices. Y.L. Wang, M. Corradini, R.D. Ludescher

4:40 AGFD 321. Investigating the potato's defensive shield: Metabolites profiling and solid-state NMR compositional analysis of suberin-enriched wound-healing tissues. K. Dastmalchi, L.R. Kallash, V.C. Phan, W. Huang, O. Serra, R. Stark

5:05 Concluding Remarks.

THURSDAY MORNING

Section B

Boston Convention & Exhibition Center
Room 213

Chemistry and Bioactivities of Natural Polymethoxyflavones

M. Pan, *Organizer*

C. Ho, S. Li, *Organizers, Presiding*

8:00 AGFD 322. Neuroprotective effect of heptamethoxyflavone in the mouse brain. S. Okuyama, Y. Amakura, M. Yoshimura, T. Yoshida, A. Sawamoto, M. Nakajima, Y. Furukawa

8:25 AGFD 323. Citrus polymethoxyflavones preventing the development of Alzheimer's disease by regulating A β metabolism. L. Guo, L. Wang, W. Zhang, H. Li, S. Li

8:50 AGFD 324. 5-Demethylnobiletin synergistically enhances the anticancer activity of paclitaxel in non-small cell lung carcinoma (NSCLC). C. Lin, S. Li, C. Ho

9:15 Intermission.

9:30 AGFD 325. 5-Acetyloxy-6,7,8,4'-tetramethoxyflavone, a tangeretin derivative, inhibits cell growth in human prostate cancer PC-3 cells. Y. Chen, Y. Chen, J. Guo, T. Huang, S. Li, C. Ho

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- 9:55 AGFD 326. Distribution investigation of polymethoxyflavones in citrus peels. T. Long, L. Xu, H. Zhao, C. Ho, S. Li
- 10:20 AGFD 327. Chemistry and nutraceutical properties of polymethoxyflavones from citrus peels. S. Li, C. Ho, M. Pan
- 10:45 Concluding Remarks.

Section D

Boston Convention & Exhibition Center
Room 209

General Papers

- B. Park, *Organizer, Presiding*
- 8:00 Introductory Remarks.
- 8:05 AGFD 328. Biomimicking the stratum corneum to engineer edible oleogel. T. Wang
- 8:30 AGFD 329. Water alkalinity and hardness in beer brewing. R. Barth
- 9:20 AGFD 331. Influence of molecular structure on interactions of dietary polyphenols and an immunodominant gluten peptide. C. Van Buiten, C.N. Pacheco, E. Hatzakis, R. Elias
- 9:45 Intermission.
- 10:00 AGFD 332. Sugar dialdehydes as glutaraldehyde analogs for cross-linked and immobilized chymotrypsin. D.E. Wong, J.M. Goddard
- 10:25 AGFD 333. DNA-comprising iron oxide/silica particles as tags against extra virgin olive oil adulteration. M. Puddu, D. Paunescu, W.J. Stark, R.N. Grass
- 10:50 AGFD 334. Biological soil quality indicators and conditioners in the phytoremediation of crude oil polluted agricultural soil. E.O. Nwaichi, L.I. Opara, E.O. Anosike
- 11:15 AGFD 335. *Ginkgo biloba*: A new look at an old plant. J.D. Williams, G.R. Boyce
- 11:40 Concluding Remarks.

Nanoparticles in Food, Agricultural, & Environmental Settings

Sponsored by COLL, Cosponsored by AGFD‡

THURSDAY AFTERNOON

Nanoparticles in Food, Agricultural, & Environmental Settings

Sponsored by COLL, Cosponsored by AGFD‡

AGRO

Division of Agrochemicals

P.Rice, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

- The Growing Impact of Big Data in the World of Chemical Information (see CINF, Sunday, Monday)
- Biofuels for Powering the World: Discovery to Application (see ENFL, Sunday, Monday)
- Micro and Nanoscale Innovations in Chromatography (see ANYL, Tuesday)
- Cope Award Symposium (see ORGN, Tuesday)
- Nanoparticles in Food, Agricultural, & Environmental Settings (see COLL, Thursday)
- Biogeochemical Cycling of Nutrients & Contaminants in Physically Complex Environments (see GEOC, Thursday)

SOCIAL EVENTS:

- Graduate Student Luncheon, 12:00 PM: Monday
- Sterling B. Hendricks Reception, 11:30 AM: Tuesday
- AGRO Awards Social, 6:00 PM: Wednesday

BUSINESS MEETINGS:

- Business Meeting, 5:00 PM: Sunday
- Programming-Blues and Brews, 5:15 PM: Tuesday

SUNDAY MORNING

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Insecticide Action on Ion Channels: A Tribute to Prof. Toshio Narahashi

D. M. Soderlund, *Organizer*

K. Dong, V. L. Salgado, *Organizers, Presiding*

- 8:25 Introductory Remarks.
- 8:30 AGRO 1. Dr. Toshio Narahashi, the light traveling through ion channels. X. Zhao, J. Yeh
- 8:55 AGRO 2. Ion channels as insecticide targets. D.M. Soderlund
- 9:20 AGRO 3. Molecular mechanisms of action of pyrethrum and pyrethroid insecticides. D. Ke, P. Xu, Y. Du, K.R. Chauhan
- 9:45 AGRO 4. Relative activity on ion channels and mechanism of action of bifenthrin. D. Gammon, Z. Liu, S.F. El-Naggar, A. Chandrasekaran
- 10:10 Intermission.
- 10:30 AGRO 5. Functional reconstitution of sodium channels in vitro for studies of insecticide action. D.M. Soderlund, J. Tan, R.A. Araujo, B. He
- 10:55 AGRO 7. Potassium channels as under-exploited targets for insecticide design. J.R. Bloomquist, M. Totrov, P.R. Carlier
- 11:20 AGRO 6. Mapping insecticide receptors in two lipid-exposed domain interfaces of sodium channels. B. Zhorov, Y. Du, Y. Nomura, K. Dong
- 11:45 AGRO 8. Insect ryanodine receptors as molecular targets for diamide insecticides. B.J. Troczka, A.J. Williams, M. Williamson, L.M. Field, P. Luemmen, E.T. Davies
- 12:10 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Combining Scientific Evidence for Health Policy and Regulation

Cosponsored by CHAS and TOXI

E. Mundt, K. A. Mundt, *Organizers, Presiding*

- 8:50 Introductory Remarks.
- 8:55 AGRO 9. Accounts table, a tool for structuring the integration and interpretation of evidence regarding causation of toxic effects from chemical exposure. L. Rhomberg
- 9:20 AGRO 10. Integration of mechanistic and epidemiologic evidence in the identification and classification of human carcinogens. P. Boffetta, K.A. Mundt
- 9:45 AGRO 11. Weight of evidence and quantitative data integration using multicriteria decision analysis. I. Linkov, J. Keisler
- 10:10 Intermission.
- 10:30 AGRO 12. New model to track strawberry harvester activity and predict pesticide exposure. W. Jiang, D. Richmond, B. Hernandez, S. Yanga
- 10:55 AGRO 13. Consideration of the weight of evidence in local antipesticide initiatives: The Montgomery County, Maryland experience. S.Z. Cohen, D.A. Goldstein, C. Burns, S.M. Haelfner
- 11:20 AGRO 14. Pesticide use on medical marijuana: An emerging crop that has no EPA-registered plant protection agents. G.C. Miller, J. Angermann, D.M. Cook, A. Stutman
- 11:45 Concluding Remarks.

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Pesticide Dose: Effects on the Environment and Target and Non-Target Organisms

Cosponsored by ENVR

- S. O. Duke, P. Kudsk, *Organizers*
- K. R. Solomon, *Organizer, Presiding*
- S. O. Duke, *Presiding*
- 8:50 Introductory Remarks.
- 8:55 AGRO 15. Pesticide dose – a parameter with many implications. S.O. Duke
- 9:20 AGRO 16. Herbicide dose: A relative and not an absolute term. P. Kudsk
- 9:45 AGRO 17. Pesticide dose: Using conceptual models of exposure to understand risks. K.R. Solomon
- 10:10 Intermission.
- 10:30 AGRO 18. Drift, dose, and non-target organisms. J. Green, J.C. Streibig
- 10:55 AGRO 19. Variations in pesticide doses under field conditions. E.D. Velini, C.A. Carbonari, U.R. Antunias, L.A. Palladini, G.R. Tofoli, C.G. Raetano
- 11:20 AGRO 20. Use of intermittent sprayers for automatic thinning of direct seeded lettuce. S.A. Fennimore, R.F. Smith, D.K. Giles
- 11:45 Discussion.

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Feeding the World Requires Pesticides and Maximum Residue Levels

P. A. Brindle, *Organizer*

- H. B. Irrig, C. Tiu, *Organizers, Presiding*
- 8:00 Introductory Remarks.
- 8:05 AGRO 21. Brief introduction to maximum residue levels (MRLs) and challenges in harmonization. M. Miller
- 8:30 AGRO 22. Challenges in complying with multiple MRLs. K. Refsnider
- 8:55 AGRO 23. US grower priority project: Establishing import maximum residue levels (MRLs) in Taiwan and South Korea. L. Rossi
- 9:20 AGRO 24. US forage export market MRL challenges. J. Szczepanski
- 9:45 AGRO 25. Regulation of animal feed import tolerance MRLs in Japan. A. Aoki
- 10:10 Intermission.
- 10:25 AGRO 26. Conclusions and follow-up from 2014 IUPAC ACS MRL workshop. H.B. Irrig
- 10:50 AGRO 27. Harmonized risk assessments to support acceptance of another country's MRLs for imported foods. C. Fleming
- 11:15 AGRO 28. USDA's Pesticide Data Program – a residue monitoring program for foods. D.E. Haynes
- 11:40 AGRO 29. FDA pesticide residue program. C. Sack
- Hydrothermal Carbonization: Possibilities and Limits for Feedstocks, Processes and Applications**
- HTC Fundamentals and Sorption**
- Sponsored by ENVR, Cosponsored by AGRO
- National Science Foundation's Centers for Chemical Innovation**
- Sponsored by PRES, Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB
- ### SUNDAY AFTERNOON
- #### Section A
- Boston Park Plaza Hotel and Towers
Georgian Room
- #### Insecticide Action on Ion Channels: A Tribute to Prof. Toshio Narahashi
- V. L. Salgado, *Organizer*
- K. Dong, D. M. Soderlund, *Organizers, Presiding*
- 1:25 Introductory Remarks.
- 1:30 AGRO 30. Multiple nicotinic acetylcholine receptor subtypes are insecticide targets. X. Zhao, B. London, N. Rankl, V.L. Salgado
- 1:55 AGRO 31. Molecular mechanisms for diverse actions and selectivity of neonicotinoids. K. Matsuda
- 2:20 AGRO 32. Modes of action of meta-diamide insecticides and ivermectin on the rDL GABA receptor. T. Nakao
- 2:45 AGRO 33. Molecular pharmacology of homomeric UNC-49B channels from southern root-knot nematodes. Y. Ozoe, K. Nomura, T. Kita, F. Ozoe
- 3:10 Intermission.
- 3:30 AGRO 34. T345M, an additional mutation associated with insecticide resistance in the *Anopheles gambiae* GABA receptor, Rdl. J.C. Taylor-Wells, B. Brooke, I. Bermudez, A. Jones

3:55 AGRO 35. Action of pymetrozine, pyrifluquinazon, and flonicamid on chrodontal neurons requires TRPV channels. V.L. Salgado, C. Spalthoff, M. Goeptert

4:20 AGRO 36. Pymetrozine and pyrifluquinazon activate heterologously-expressed insect TRPV channels. A. Nesterov, R. Kandasamy, D. London, J. Dorsch, L. Stam, N. Rankl, V.L. Salgado

4:45 AGRO 37. Ion channel screening for insecticide discovery. C. Bradler

5:10 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Latest Trends in Environmental Fate and Exposure Assessments: Filling in Knowledge and Data Gaps Across the Commodity Groups

Cosponsored by ENVR

J. F. Ericson, G. Rattray, J. A. Robinson, M. Xiao-Huang, *Organizers*

K. Malekani, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGRO 38. Specialized exposure analysis techniques for aquatic and terrestrial animal drug. W. Hunter, H. Zahner, E. Silberhorn

1:30 AGRO 39. Geospatial technologies for characterizing veterinary medicine exposure in the watershed and placing exposure into context. J. Amos, C.M. Holmes, A.M. Ritter, I. Khanijo, M. Williams, M. Cheplick, J.A. Robinson

1:55 AGRO 40. Guidance for the consideration of unextracted residues in laboratory soil and water metabolism studies for pesticides. R.D. Jones, J. Hetrick, G. Orrick, M. Ruhman, M.T. Shamim, C. Sutton, K. White

2:20 AGRO 41. Higher-tier surface water exposure modeling approach at watershed scale of veterinary pharmaceuticals administered to beef cattle. I. Khanijo, J. Amos, A.M. Ritter, M. Cheplick, M. Williams, C.M. Holmes, J.A. Robinson

2:45 AGRO 42. Screening level environmental risk assessment (ERA) of cosmetic ingredients in the USA and beyond. I. Davies

3:10 Intermission.

3:30 AGRO 43. Modeling the soil binding affinity of positively charged organic chemicals. S. Droge

3:55 AGRO 44. Application of passive dosing to maintain constant aqueous exposures of sparingly soluble, difficult-to-test compounds. D. Letinski

4:20 AGRO 45. Simulation studies to evaluate surfactant biodegradation rates and their degradation pathways in sewer systems. J. Menzies, K. McDonough, D. McAvoy, T. Federle

4:45 AGRO 46. Critical clay content in defining sorption behavior of pesticides in soil. X. Huang

5:10 Concluding Remarks.

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Pesticide Dose: Effects on the Environment and Target and Non-Target Organisms

Cosponsored by ENVR

S. O. Duke, K. R. Solomon, *Organizers*

P. Kudsk, *Organizer, Presiding*

S. O. Duke, *Presiding*

1:25 Introductory Remarks.

1:30 AGRO 47. Catch 22: All doses select for resistance — the questions are when this may happen and how to delay evolution. J. Gressel

1:55 AGRO 48. Reduced fungicide doses in cereals: Which parameters to consider? L.N. Jorgensen

2:20 AGRO 49. Hormesis: Adaptive responses in biology and medicine. E.J. Calabrese

2:45 AGRO 50. Occurrence and significance of pesticide-induced hormesis in insects. C. Cutler, R. Guedes

3:10 Intermission.

3:55 AGRO 51. Chemical hormesis on plant pathogenic fungi and oomycetes: What we know. C. Garzon

3:30 AGRO 52. Herbicide hormesis: What do we know about the mechanisms leading to low dose growth increases? N. Cedergreen

4:20 AGRO 53. Low dose effects of glyphosate on plant reproduction in *Arabidopsis thaliana*: A biological and transcriptomics approach. F.E. Dayan, C.A. Carbonari, G. Gomes, E. Velini, D. Owens, Z. Pan, S. O. Duke

4:45 Discussion.

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Feeding the World Requires Pesticides and Maximum Residue Levels

H. B. Irrig, *Organizer*

P. A. Brindle, C. Tiu, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 AGRO 54. Canadian perspective on MRLs. P. Petelle

1:55 AGRO 55. JMPR and Codex MRLs: Roles, responsibilities, and challenges. M. Doherty

2:20 AGRO 56. Global field residue data supporting harmonized MRLs and exchangeability. C. Tiu

2:45 AGRO 57. Working toward a global regulatory program for minor uses. D. Kunkel, M.P. Braverman, W.P. Barney, J. Baron

3:10 Intermission.

3:30 AGRO 58. EU MRL regulation and import tolerance application procedures. S. Rutherford

3:55 AGRO 59. Delivering safe and effective advice on pest control in developing countries through the Plantwise programme. S. Hobbs

4:20 AGRO 60. Finding potential solutions for growers' needs in the field of pests and diseases by searching for existing solutions in other countries. F. Schuster

4:45 Discussion.

5:15 Concluding Remarks.

Section E

Boston Park Plaza Hotel and Towers
Terrace Room

Urban Agriculture: Turf, Ornamentals, Household Products, and Water-Re-Use

Cosponsored by ENVR

J. M. Clark, T. Jindal, *Organizers*

1:00 - 5:00

AGRO 61. Biological control agents for sustainable urban agriculture, safe water, and soil health. T. Jindal, A. Chauhan

AGRO 62. Lysimetric studies to access the groundwater contamination through unlined drain. T. Jindal, A. Kumar, A. Ranjan, K. Gulati, S. Thakur

AGRO 63. Microalgal agriculture: An integrated approach to remediate the wastewater for irrigation use and production of biodiesel and manure. S. Khan

AGRO 64. Physical methods in wastewater treatment. T. Jindal, J. Behari

AGRO 65. Residues of pesticide in Ghaggar River flowing through urban cotton cropping area. T. Jindal, S. Thakur, K. Gulati, A. Kumar

AGRO 66. Utilizing reduced risk pesticides and IPM strategies to mitigate golfer exposure and hazard. J.J. Doherty, J.M. Clark

AGRO 67. Attenuation of pesticide-laden runoff using vegetative filter strips. J.J. Doherty, R. Putnam, B.A. Defforio, R. Bishop, J.M. Clark

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Current Topics in Seed Treatment

Cosponsored by ANYL and ENVR

J. E. Eble, P. J. Rice, *Organizers*

1:00 - 5:00

AGRO 68. Roles of conjugated double bonds on electron-donating capacity of sorghum grains. S.M. Uchimiya

AGRO 69. Overview of seed treatment in North America, 2015. B. MacCulloch

AGRO 70. Seed enhancement evaluation. A. Patin

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Latest Trends in Environmental Fate and Exposure Assessments: Filling in Knowledge and Data Gaps Across the Commodity Groups

Cosponsored by ENVR

J. F. Ericson, K. Malekani, J. A. Robinson, M. Xiao-Huang, *Organizers*

1:00 - 5:00

AGRO 71. Achievement and measurement of soil anaerobicity during conduct of anaerobic transformation studies. M. Hall, A. Griffith, S. McLaughlin, S. Kang, K. Malekani, D. Hu

AGRO 72. Estrogen conversion in poultry litter by liquid chromatography mass spectrometry. E.J. Mullin, L.T. Yonkos, D.S. Aga

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Pesticide Dose: Effects on the Environment and Target and Non-Target Organisms

Cosponsored by ENVR

S. O. Duke, P. Kudsk, K. R. Solomon, *Organizers*

1:00 - 5:00

AGRO 73. Microtransplantation of rat brain neurolemma into *Xenopus laevis* oocytes to study the effect of environmental toxicants on endogenous voltage-sensitive ion channels. E. Murenzi, S.B. Symington, A. Taitin, M.M. Morgan, J.M. Clark

AGRO 74. Effect of glyphosate formulations on two species with different leaf surface properties. A.R. Christensen, N. Cedergreen, H. Teicher, J. Streibig

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Protection of Agricultural Productivity, Public Health and the Environment

P. J. Rice, *Organizer*

1:00 - 5:00

AGRO 75. Reduction of lignin levels in mutant sorghum lines developed for saccharification leads to increased production of insecticidal compounds in stalk pith. P. Dowd, M.A. Berhow, S. Sattler

AGRO 76. Possible glyphosate tolerance mechanism in pitted morningglory (*Ipomoea lacunosa* L.). D. Ribeiro, V. Nandula, F. Dayan, A.M. Rimando, S.O. Duke, K. Reddy, D. Shaw

AGRO 77. Withdrawn.

21st Century Chemistry Education: Formal and Informal

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Hydrothermal Carbonization: Possibilities and Limits for Feedstocks, Processes and Applications

Municipal and Agricultural Applications and Economics of HTC

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National Science Foundation's Centers for Chemical Innovation

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MONDAY MORNING

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Innovation in Metabolism, Bioavailability and Formulations Research Leading to the Discovery of Agrochemicals: Symposium Honoring Dr. Keith D. Wing, AGRO International Award for Research in Agrochemicals
Cosponsored by ORGN

B. A. Lorschach, *Organizer*

J. Green, T. C. Sparks, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 **AGRO 78.** It takes a team: Reflections on select insecticide discoveries, toxicological problem approaches, and enjoying the unexpected. K.D. Wing

9:20 **AGRO 79.** Fast, structured, adaptable approach to screen bioformulation amendments and stabilizers. C. Bartling, J. Fife, R. Jones, A. Kerr

9:45 **AGRO 80.** Are pharmaceutical enhanced solubilization technologies useful in agriculture? R. Boucher

10:10 Intermission.

10:30 **AGRO 81.** Ultrahigh resolution MS and label-free MALDI molecular imaging: A novel approach for the study of plant biosynthesis and metabolism. K.A. Kellersberger

10:55 **AGRO 82.** Visualization of small molecule distributions in plant, insect, and mammalian tissues by mass spectrometry imaging. N. Bjarnholt, C. Janfelt

11:20 **AGRO 83.** RNA interference in agriculture: Today and tomorrow. R. Heidebrecht

11:45 Concluding remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Global Research Needs: Identifying and Prioritizing Efforts to Sustain Environmental Quality
Cosponsored by ENVR and TOXI

B. W. Brooks, G. P. Cobb, D. D. Dionysiou, P. J. Rice, E. M. Ulrich, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 **AGRO 84.** Review of the practice and potential for global horizon scanning and research prioritization exercises in narrowing the environmental science-policy gap. M. Rudd, B.W. Brooks

8:55 **AGRO 85.** Formalizing the identification of high priority research needs: A case example with pharmaceuticals and personal care products. B.W. Brooks, G. Ankley, A. Boxall, M. Rudd

9:45 Discussion.

10:10 Intermission.

10:30 Discussion.

Technical program information known at press time.

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Section C

Boston Park Plaza Hotel and Towers
White Hill

Environmental Fate, Transport and Modeling of Agricultural Chemicals
Cosponsored by ENVR

S. H. Jackson, N. Peranginangin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **AGRO 86.** Environmental fate and physical-chemical properties of dicamba, 3,6-dichloro-o-anisic acid. S.H. Jackson

8:30 **AGRO 87.** Pesticides in soils: Correct kinetics and flawed parameters. D.S. Gamble

8:55 **AGRO 88.** Buffers as potential catalysts of hydrolysis and halogenation during agrochemical fate experiments in bench-scale reactors. J.D. Sivey, M. Burton, A.L. Roberts

9:20 **AGRO 89.** Evaluating unextracted pesticide residues in laboratory environmental fate studies. Y. Ding, K. Lynn, H. Wang, R. Yoder, M.J. Hastings, S. Linder

9:45 **AGRO 90.** Withdrawn.

10:10 Intermission.

10:20 **AGRO 91.** Does the incorporation of vegetative filter strip mass balance and degradation processes affect the long-term pesticide environmental exposure assessments? R. Muñoz-Carpena, G.A. Fox, O. Perez-Ovilla, A.M. Ritter

10:45 **AGRO 92.** Emerging contaminant soil fate model development for development for the USDA soil water assessment tool. L.J. Thibodeaux

11:10 **AGRO 93.** Modeling transport of a controlled release larvicide through catch basin systems. N. Pai, M. Winchell, B. Brayden, J.P. Hanzas, R. Dupree

11:35 **AGRO 94.** Evaluating ecological risk of a controlled release larvicide applied to catch basin systems that drain directly into natural waterbodies. B. Brayden, J.P. Hanzas, R. Dupree

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications
Cosponsored by ANYL and ENVR

K. Lynn, *Organizer*

L. Ritter, M. Saha, *Organizers, Presiding*

8:50 Introductory Remarks.

8:55 **AGRO 95.** Novel application of HPLC core-shell column technology: The successful separation of three small molecule conformational isomer plant metabolites of EPTC by LC-MS/MS. E.A. Schoenau, T.F. Moate, M.M. Hampton, R.B. Stobaugh

9:20 **AGRO 96.** Identification and application of matrix components for analyte protection during the GC/MS analysis of current use pesticides in snail tissues following the QuEChERS (quick, easy, cheap, effective, rugged, and safe) method. S. Morrison, J. Belden

9:45 **AGRO 97.** Ultra-trace determination of neonicotinoid insecticides in pollen, anthers, and nectar using high-throughput sample preparation and liquid chromatography with tandem mass spectrometry detection. F.A. Claussen, J. Warnick

10:10 Intermission.

10:30 **AGRO 98.** Multiresidue anticoagulant residue method using novel surrogate compounds. D.A. Goldade, S.F. Volker

10:55 **AGRO 99.** Rapid screening of herbal supplements and their extracts for pesticides utilizing a direct analysis of solid phase microextraction (SPME) fibers by DART-based ambient ionization mass spectrometry. B. Musselman, J. Lapointe, R. Goguen

11:20 **AGRO 100.** Determination of multiple rodenticides in avian tissues using a modified QuEChERS technique and LC-APCI/MS/MS detection. S.F. Volker, D.A. Goldade

11:45 Concluding Remarks.

Section E

Boston Park Plaza Hotel and Towers
Back Bay Room

Biochemical Biopesticides: Discovery and Regulation of New and Potential Products
Cosponsored by BIOL

J. R. Coats, S. O. Duke, *Organizers*

C. L. Cantrell, A. D. Gross, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 **AGRO 101.** IR-4 program for registration, efficacy testing, and development of organic products and biopesticides. M.P. Braverman, D. Kunkel, J. Baron, W.P. Barney, K.D. Coleman

8:55 **AGRO 102.** Plant/plant allelopathy for herbicide and bioherbicide discovery and development. S.O. Duke

9:20 **AGRO 103.** Insect pest-fungal spore mutualism: A potential source of new biopesticide products? J.J. Beck

9:45 **AGRO 104.** Insect control with specialized pheromone and lure application technology (SPLAT[®]). A. Mafra Neto, K. Sharma, L. Mafra, R. Borges, M. Botton, W. Urrutia, K. Spencer, J. Rico, R.O. Silva, C.R. Bernardi

10:10 Intermission.

10:30 **AGRO 105.** Challenges in applying boric acid as a toxicant for managing spotted wing drosophila. R.S. Cowles

10:55 **AGRO 106.** Development of botanical-based biopesticides and repellents against biting flies on livestock animals. J. Zhu

11:20 **AGRO 107.** Exploring the toxicity and synergism of chalcone analogs as biologically-based alternatives to control insects. A.D. Gross, N. Tabanca, R. Islam, F. Tong, A. Ali, I.A. Khan, Z.A. Kaplancikli, A. Ozdemir, J.R. Bloomquist

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Environmental Fate, Transport and Modeling of Agricultural Chemicals
Cosponsored by ENVR

S. H. Jackson, N. Peranginangin, *Organizers*

8:00 - 12:00

AGRO 113. Photolysis of herbicides absorbed to plant surfaces: Imazethapyr on corn and soybean waxes. A.M. Nienow, A. Christiansen, A. Peterson, S. Anderson, R. McLouth

AGRO 114. Uptake and accumulation of endosulfan isomers and its sulfate metabolite in lettuces grown on contaminated soil. J. Hwang, S. Jeon, S. Lee, S. Lee, J. Kim

AGRO 115. Encouraging the use of drift reduction technologies in the United States. C. Peck, F. Khan, A. Overstreet

AGRO 116. Persistence of oxadiazon residues in soil and grains in an upland rice (*Oryza sativa*) field. M. Bunquin, J. Onoya, B. Chauhan, J. Opeña, S.E. Beebout

AGRO 117. Occurrence and formation of insecticide degradation products in urban environments. J. Richards, W. Jiang, J. Gan

AGRO 118. Uptake of triclosan and triclocarban by vegetables from soils and biosolids-amended soils. Q. Fu, E. Sanganyado, Q. Ye, J. Gan

AGRO 119. MixTox SW – a software tool for mixture-toxicity exposure assessments in FOCUS surface water scenarios. D. Weber, G. Eck

AGRO 120. Residue patterns of insecticides applied on perilla leaf belonging to the minor crop in Korea. S. Jeon, J. Hwang, S. Lee, J. Kim

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF and SOCED

ACS Scholars: Rising Stars in Academe

Sponsored by PRES, Cosponsored by AGRO, CARB, CMA, COLL, ENFL, ENVR, PROF, SCHB and YCC

Memories of Henry Hill: His Legacy in Science and in Professional Service

Sponsored by HIST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES, PROF and SCHB

Sensing of Environmentally Relevant Contaminants

Sponsored by ENVR, Cosponsored by AGRO

MONDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Innovation in Metabolism, Bioavailability and Formulations Research Leading to the Discovery of Agrochemicals: Symposium Honoring Dr. Keith D. Wing, AGRO International Award for Research in Agrochemicals
Cosponsored by ORGN

J. Green, *Organizer*

B. A. Lorschach, T. C. Sparks, *Organizers, Presiding*

1:50 Introductory Remarks.

1:55 **AGRO 126.** Chance and design in pro-insecticide discovery. V.L. Salgado

2:20 **AGRO 127.** Insecticide ADME for support of early phase discovery: Combining classical and modern techniques. M.D. David

2:45 **AGRO 128.** Vssc mutations and insecticide resistance: Understanding the variations. J.G. Scott

3:10 Intermission.

3:30 **AGRO 129.** Discovery, development, and biological characteristics of cyclic keto-enol insecticides. R. Nauen, P. Luemmen, R. Fischer

3:55 **AGRO 130.** Innovations in discovery: The quest for new fungicidal crop protection solutions. B.A. Lorschach, Z.L. Benko, T.A. Boebel, N. Breaux, K. Bryan, G. Davis, J. Epp, T. Martin, K.G. Meyer, W. Owen, M. Pobanz, J.M. Ruiz, M. Sullenberger, J.D. Webster, C. Yao, D. Young

4:20 AGRO 131. Search for a systemic anthranilic diamide insecticide: The discovery of cyantraniliprole. T.P. Selby

4:45 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Endangered Species Risk Assessment for Pesticides: Advances in Methods and Process

Cosponsored by ENVR

V. Forbes, N. Golden, T. Hawkes, M. F. Leggett, N. Poletika, *Organizers*

T. Hall, C. Peck, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 AGRO 132. Development of new tools to advance the estimation of pesticide exposure and effects for listed aquatic and terrestrial species. C. Peck, C. Rossmel, K. Garber, M. Etterson

1:55 AGRO 133. Ecological risk assessment framework for endangered species assessments. S. Teed, D. Moore, M. Winchell

2:20 AGRO 134. Selection and use of data in the assessment of pesticide risk to threatened and endangered species. N. Golden, P. Shaw-Allen, K. Garber

2:45 AGRO 135. Anticipating data needs for endangered species risk assessment under the evolving "interim process" for species assessment. B. McGaughey, N. Poletika, A.C. Barefoot, T. Hall, J. Sharp, A. Frank

3:10 Intermission.

3:30 AGRO 136. Endangered Species Act Section (7) consultation in federal land management agencies. S. Bautista, W.P. Eckel

3:55 AGRO 137. Getting over the finish line: Completing pesticide consultations that comply with the ESA. C. Adkins

4:20 Discussion.

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Environmental Fate, Transport and Modeling of Agricultural Chemicals

Cosponsored by ENVR

S. H. Jackson, N. Peranganin, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 AGRO 138. How should we consider the sources of potential uncertainty inherent in the standard pesticide exposure assessment? P. Hendley, D.A. Desmarteau, J. Giddings, C.M. Holmes, A.M. Ritter

1:55 AGRO 139. Potential impact of modeling assumptions and uncertainties on drinking water concentrations predicted by PRZM-GW for crops and turf. I. Khanijo, A.M. Ritter, J. Eickhoff

2:20 AGRO 140. Comparison of SCI-GROW and PRZM-GW predicted pesticide concentrations in groundwater with NAWQA observed concentrations. T.L. Estes, M. Winchell, N. Pai

2:45 AGRO 141. Development of PRZM-GW scenarios for spring and winter wheat-growing areas. L. Padilla, M. Winchell, N. Peranganin, S. Grant

3:10 Intermission.

3:30 AGRO 142. Measuring and simulating emissions of 1,3-dichloropropene and chloropicrin after soil fumigation under field conditions. S.R. Yates, D. Ashworth, W. Zheng, J.A. Knuteson, I.J. Van Wessenbeck

3:55 AGRO 143. Modeling volatilization following pesticide application: Development of a robust pesticide emission model as a stand alone tool. S. Ghosh, S. Grant, N. Peranganin, K. Crist, R. Oldham

4:20 AGRO 144. Overview of recent refinements in assessing airborne exposures to pesticide applications: Use of co-variance methods and other field methods and modeling refinements. R. Sullivan, D.A. Sullivan

4:45 AGRO 145. Refining the dispersion modeling of airborne flux: Addressing over field nocturnal dispersion. R. Sullivan, D.A. Sullivan

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications

Cosponsored by ANYL and ENVR

M. Saha, *Organizer*

K. Lynn, L. Riter, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 AGRO 146. Use of radiolabeled material to develop, troubleshoot, and radio-validate an analytical method. S. Shaffer, C. Talken, W. Fain, M. Schofield

1:55 AGRO 147. Overcoming the analytical challenges of measuring free and total concentrations of nine pyrethroids in sediment, pore water and water column matrices using Solid Phase Micro-Extraction (SPME) and Liquid-Liquid Extraction (LLE) approaches. K. Clark, C. Chickering, J. Owen, T. Xu, P. Hendley, D.A. Koch

2:20 AGRO 148. Fast and easy method for determination of imidazolinone residues in soil by UHPLC-MS/MS. R. Zanella, M. Kemmerich, G. Bernardi, O. Prestes

2:45 AGRO 149. Development of a matrix imprinted polymer SPE and LC/MS/MS method for the analysis of pyridine herbicides in compost samples. M. Hastings

3:10 Intermission.

3:30 AGRO 150. DuPont seed treatment enterprise: Analytical strategies. P.T. Richardson

3:55 AGRO 151. Optimization of a QuEChERS based method by means of central composite design for pesticide multiresidue determination in orange juice by UHPLC-MS/MS. T.M. Rizzetti, M.L. Marlins, O. Prestes, M.B. Adaine, R. Zanella

4:20 AGRO 152. Analytical methods for residue analysis: Trends, requirements, and challenges. M. Saha

4:45 Concluding Remarks.

Section E

Boston Park Plaza Hotel and Towers
Back Bay Room

Biochemical Biopesticides: Discovery and Regulation of New and Potential Products

Cosponsored by BIOL

S. O. Duke, A. D. Gross, *Organizers*

C. L. Cantrell, J. R. Coats, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 AGRO 153. Investigation of monoterpenoids and sesquiterpenoids as natural insecticides: Comparisons of activity against mosquitoes and flies. J.R. Coats, E. Norris, A. Gross, L. Bartholomay

1:55 AGRO 154. Isolation and identification of potential biopesticidal compounds from the North American insect repelling folk remedy plant, sweetgrass, *Hierochloa odorata* (L.) P. Beauv. C.L. Cantrell, A. Ali, A.P. Jones

2:20 AGRO 155. Novel biopesticide as piperonyl butoxide-PBO substitute. K. Chauhan

2:45 AGRO 156. Mosquitocidal constituents from natural sources. K.M. Meepagala, A. Estep, J. Becnel

3:10 Intermission.

3:30 AGRO 157. Adulticidal and ovidical activity of two plant-based formulations against the Northern fowl mite, *Ornithonyssus sylviarum*. B. Bissinger, J. Owens, J. Schmidt

3:55 AGRO 158. Hop extracts: A safe alternative for honeybee diseases. F. Ahumada, J. Forte

4:20 AGRO 159. Pesticidal principles from the seeds of Terminalia mantaly H. and their effect on two pests. L.A. Nnamonu, J.V. Anyam, P.O. Onubedo

4:45 Concluding Remarks.

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications

Cosponsored by ANYL and ENVR

K. Lynn, L. Riter, M. Saha, *Organizers*

1:00 - 5:00

AGRO 108. Novel strategy for selective determination of dicamba residues in raw agricultural commodities by paired ion electrospray ionization (PIESI) mass spectrometry. H. Guo, L. Riter, C.E. Wujcik, D.W. Armstrong

AGRO 109. Effect of lanthanum on amino acid composition of soybean seedlings under supplementary UV-B radiation stress. H. Ren, L. Wang, H. Zhao, D. Li, X. Zhang, Y. Yang

AGRO 110. Isolating trace impurities for structural elucidation in a commercial fungicide formulation using preparative supercritical fluid chromatography (SFC). J.P. McCauley, M. Twohig, M. O'Leary, M. Grondine

AGRO 111. Enantioseparation and detection of triazole fungicides in wheat grain and wheat straw using ultraperformance convergence chromatography and MS/MS detection. M. Twohig, P.G. Alden, M. O'Leary

AGRO 112. Analysis of fungicide body residues in tissue via the QuEChERS (quick, easy, cheap, effective, rugged and safe) method and use of a real matrix component for analyte protection. S. Morrison, J. Belden

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Metabolites from Endophytic Microorganism to Combat Biotic Stress in Crop Plants

Cosponsored by BIOL

A. Gonzalez-Coloma, N. Kaushik, *Organizers*

1:00 - 5:00

AGRO 121. Biopesticidal potential of fungi from tropical regions of Mexico. M. Gamboa-Angulo, Heredia-Abarca, J. Cristóbal-Alejo, E. Ruiz-Sánchez, M. Andres, A. Gonzalez-Coloma

AGRO 122. Insecticidal effects of pan-tropical nodulisporic acid producing endophyte (*Hypoxylon pulicidum*) against *Spodoptera littoralis* larvae. V. Gonzalez-Menendez, N. De Pedro, B. Cautain, L. Rodriguez, M. Stadler, G. Bills, O. Genilloud, F. Vicente, A. Gonzalez-Coloma

AGRO 123. Endophyte screening from Indo-Spanish medicinal plants: Biotechnological green crop protectants. A. Gonzalez-Coloma, M. Andres, C. Diaz, C. Gimenez, R. Cabrera, N. Kaushik

AGRO 124. Fungal endophyte diversity and bioactivity in the Indian medicinal plant *Ocimum sanctum* Linn. K. Chowdhary, N. Kaushik

AGRO 125. Residues of pesticide in Hindon River flowing through urban rice cropping area. T. Jindal, S. Thakur, K. Gulati, A. Kumar, R. Lal, P. Jain

ACS Scholars: Rising Stars in Industry

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Sensing of Environmentally Relevant Contaminants

Cosponsored by ENVR, Cosponsored by AGRO

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

P. J. Rice, *Organizer*

8:00 - 10:00

72-73, 108, 112, 114, 117, 124.

See previous listings.

190-191, 194, 197-199, 201-202, 204-209, 284, 293-297, 300. See subsequent listings.

Chemical Innovation and Design (CID) Talks: The Future of Innovation Now

Sponsored by MPPG, Cosponsored by AGFD, AGRO, BIOT, MEDI, PMSE and SCHB

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TUESDAY MORNING

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Journal of Agricultural and Food Chemistry Best Paper Awards

Cosponsored by AGFD†

T. Hofmann, *Organizer*

E. M. Hotze, *Organizer, Presiding*

9:00 Award Presentation.

9:10 **AGRO 160.** Metabolism studies of environmental contaminants in plants using plant cell cultures and liquid chromatography-high resolution mass spectrometry. A. Macheries, C. Riemenschneider, B. Seiwert, T. Reemtsma

10:00 Award Presentation.

10:10 **AGRO 161.** Modeling of biological activity for improved efficacy and active compound identification of natural products used in the treatment of human diseases. N. Reese, F.J. Wyzgoski, J.C. Scheerens

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

USDA-ARS Sterling B. Hendricks Memorial Lectureship: James H. Tumlinson

Cosponsored by AGFD

S. O. Duke, C. J. Hapeman, K. Kaplan, *Organizers, Presiding*

11:30 Introductory Remarks.

11:45 **AGRO 162.** Potential for Insect herbivore pest management with chemical ecology. J.H. Tumlinson

12:35 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Endangered Species Risk Assessment for Pesticides: Advances in Methods and Process

Cosponsored by ENVR

V. Forbes, N. Golden, T. Hall, T. Hawkes, M. F. Leggett, C. Peck, *Organizers*

N. Poletika, *Organizer, Presiding*

T. Hawkes, *Presiding*

8:00 Introductory Remarks.

8:05 **AGRO 163.** Developing species maps from FESTF's aggregated species location data for EPA's assessment of pesticides and endangered species. B. McGaughey, A. Frank, D. Campana, T. Hall, D.D. Campbell

8:30 **AGRO 164.** Examining the crop footprint of organophosphate insecticides when applied to a national level endangered species pesticide risk assessment. N. Poletika, A. Frank, J. Giddings, P. Whatling, B. McGaughey

8:55 **AGRO 165.** Evaluating the potential impact of grouping CDL crop classes on the spatial extent of pesticide use sites. B. McGaughey, A. Frank, T. Hall, N. Poletika, P. Whatling, K.H. Carr, S.H. Jackson, L. Ghebremichael

9:20 **AGRO 166.** Terrestrial endangered species assessment for chlorpyrifos: Initial analyses and results. D. Moore, R.S. Teed, N. Poletika

9:45 **AGRO 167.** Validating datasets representing non-agricultural pesticide use sites for the assessment of pesticides and endangered species. B. McGaughey, T. Hall, Z. Tang, K.H. Carr, A. Frank

10:10 Intermission.

10:30 **AGRO 168.** Endangered species assessment for chlorpyrifos co-occurrence and proximity analyses: Initial results. D. Moore, R.S. Teed, N. Poletika

10:55 **AGRO 169.** Development of generic aquatic habitats for estimating pesticide exposure in threatened and endangered species. T. Hawkes, K. Myers, C. Peck

11:20 Discussion.

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis, and Ecological Effects

Cosponsored by ANYL and ENVR

D. S. Aga, J. S. Wallace, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **AGRO 170.** Transformation and fate of veterinary ionophore antibiotics in the water-soil-litter systems. C. Huang

8:55 **AGRO 171.** Fate and effect of monensin during anaerobic digestion of dairy manure. O. Arkan, W. Mulbry, C.P. Rice, S. Lansing

9:20 **AGRO 172.** Evaluation of three manure treatment systems for the removal of common veterinary antibiotics and antibiotic resistance genes. J.S. Wallace, E. Garner, A. Pruden, D.S. Aga

9:45 **AGRO 173.** Impact of manure application technologies on the fate of pirlimycin and chlortetracycline in soil. K. Xia, S. Kulesza, R. Maguire, P. Ray, K. Knowlton, J. Cushman

10:10 Intermission.

10:30 **AGRO 174.** Antibiotic interactions at the solid-water interface: Implications for understanding sorption to soils and passive sampling of natural waters. D. Vasudevan

10:55 **AGRO 175.** Development and usage of bacterial bioreporters for monitoring antibiotics used in agriculture. J. Muirine, A. Pasupulate, M. Virta

11:20 **AGRO 176.** Effects of antibiotic mixture on the metabolism of adult zebrafish. S. Kim, R.D. Sotto, C. Medriano, Y. Park

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

GMOs and the Entanglement of Intellectual Property Rights

Cosponsored by CHAL, ENVR and SCHB

A. Coates, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 **AGRO 177.** Scientific basis for GMOs. J.M. Van Emon

8:55 **AGRO 178.** GMOs and intellectual property rights: An introduction. A. Coates

9:20 **AGRO 179.** Local agencies and GMO regulation. D. Sandino

9:45 **AGRO 180.** Intellectual property rights in plants and animals — an overview. D. Kershen

10:10 Intermission.

10:30 **AGRO 181.** Intellectual property rights and applications to GMOs. J.J. Hasford

10:55 **AGRO 182.** Survey of disputes involving GMO patent rights. C.A. Burton

11:20 **AGRO 183.** Molecular breeding, gene editing technologies, and regulatory regimes — past, present, and future? D. Kershen

Section E

Boston Park Plaza Hotel and Towers
Back Bay Room

Current Advances and Challenges of Arthropod Vector Control

L. J. Jensen, D. Swale, *Organizers, Presiding*

8:50 Introductory Remarks.

8:55 **AGRO 184.** Identifying the molecular basis of insecticide resistance in mosquito vectors and agricultural pests. L. Grigoraki, J. Vontas

9:20 **AGRO 185.** Pyrethroid-resistant head lice: Updated status, lessons learned, and management in the 21st century. K.S. Yoon, K. Gellatly, S. Lee, D. Kwon, J.M. Clark

9:45 **AGRO 186.** Characterizing the physiological role of inward rectifying potassium channels in the insect nervous system. D. Swale

10:10 Intermission.

10:30 **AGRO 187.** Pyrethroid insecticides elicit olfactory response in *Drosophila melanogaster*. P. Xu, Y. Du, K.R. Chauhan, K. Dong

10:55 **AGRO 188.** Comparison of immune responses between body and head lice following bacterial challenge. J. Kim, K.S. Yoon, D.J. Previte, J.M. Clark, S. Lee

11:20 **AGRO 189.** Neural and endocrine disruption of tick reproduction: New perspectives and control approaches. R.M. Roe, D. Sonenshine

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis, and Ecological Effects

Cosponsored by ANYL and ENVR

D. S. Aga, J. S. Wallace, *Organizers*

8:00 - 12:00

AGRO 190. Uptake of three antibiotics and an anti-epileptic drug by wheat crops spray irrigated with wastewater treatment plant effluent. A. Franklin, C. Williams, D. Andrews, E. Woodward, J. Watson

AGRO 191. Analysis of pharmaceuticals in food crops grown in urine- and struvite-fertilized soil by liquid chromatography tandem mass spectrometry. R. Mullen, A. Noe-Hays, K. Nace, D.S. Aga

AGRO 192. Evaluation of benzylamine and salicylic acid as probes for pharmaceutical sorption to soils. A. Lopez, R. Goyetche, K. Carter, D. Vasudevan

AGRO 193. Structure based prediction of substituted pyridine cation exchange to soil aluminosilicates: Implications for antibiotics containing pyridine substructures. J. Sullivan, B. Stuyvesant, D. Vasudevan

AGRO 194. Quantification of ionophore antibiotics in chicken litter and identification of their degradation products during different composting procedures. J. Scariot Munaretto, D.S. Aga, R. Zanella

AGRO 195. Understanding sources of aquatic contaminants of emerging concern. P. Rice, D. Fairbairn, M. Karpuzcu, E. Kaufenberg, W. Arnold, P. Novak, W. Koskinen, B. Barber, D. Swackhamer

AGRO 196. Phytohormone levels in coconut (*Cocos nucifera* L.) water at three different stages of maturity. R.R. Singh, V. Migo, D.S. Aga

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Endangered Species Risk Assessment for Pesticides: Advances in Methods and Process

Cosponsored by ENVR

V. Forbes, N. Golden, T. Hawkes, M. F. Leggett, N. Poletika, T. Hall, C. Peck, *Organizers*

8:00 - 12:00

AGRO 203. Characterizing the range of sensitivities of aquatic and terrestrial plants to 2,4-D: A quantitative approach to selection and evaluation of data. S. McMaster, J. Staveley, J. Nusz

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES†, PROF and SCHB

Microorganism-Membrane Interactions: Towards Understanding Pathogen Removal and Membrane Biofouling

Sponsored by ENVR, Cosponsored by AGRO

Reclamation, Remediation, Restoration: Novel Approaches to Environmental Challenges

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Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

Transforming University-Industry Partnerships for an Innovative Future
Envisioning, Enabling and Executing

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

TUESDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Pollinators and Agrochemicals

Cosponsored by ENVR

M. L. Hladik, P. Reibach, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 AGRO 210. Mode of action of insecticides. V.L. Salgado

1:55 AGRO 211. Review of laboratory test procedures with the honey bee, *Apis mellifera* L., following current regulatory guidelines. M. Patnaude, J. Hoberg

2:20 AGRO 212. Survey for neonicotinoid insecticide residues in bee bread and comb wax from colonies in Washington State. A.S. Felsot, T. Lawrence, E. Culbert, V.R. Hebert, J. Santo, S. Sheppard

2:45 AGRO 213. Assessing the potential risk of chlorothalonil to honey bees using the new risk assessment guidance for the United States and Canada. J. Overmyer

3:10 Intermission.

3:30 AGRO 214. Formulation composition makes the pollinator poison. C.A. Mullin, J. Chen, J. Fine, R. Reynolds, M. Frazier

3:55 AGRO 215. Current-use pesticides in native bees collected from varying land cover areas in Colorado, USA. M.L. Hladik, M. Vandever, K.L. Smalling

4:20 AGRO 216. Risk assessment for imperiled butterflies exposed to a mosquito control pesticide on a national wildlife refuge. T. Bargar, A. Sowers, C. Anderson

4:45 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Endangered Species Risk Assessment for Pesticides: Advances in Methods and Process

Cosponsored by ENVR

V. Forbes, T. Hall, T. Hawkes, C. Peck, N. Poletika, *Organizers*

N. Golden, M. F. Leggett, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 AGRO 217. Aquatic modeling to estimate pesticide exposure to threatened and endangered species. W.P. Eckel, C. Peck, C. Laetz, G. Noguchi

1:55 AGRO 218. Aquatic endangered species assessment of chlorpyrifos: 1. Overview and risk characterization in Step 1. J. Giddings, B. McGaughey, A. Frank, M. Winchell, N. Poletika

2:20 AGRO 219. Aquatic endangered species assessment of chlorpyrifos: 2. Screening level exposure modeling, action area definition, and co-occurrence. M. Winchell, L. Padilla, J. Giddings, N. Poletika

2:45 AGRO 220. Using targeted monitoring to evaluate mitigation strategies that reduce pesticide loading to streams. K. McLain, G. Tuttle, J. Hancock, M. Bischof

3:10 Intermission.

3:30 AGRO 221. National endangered species assessment for malathion: Case study. S. Teed, R. Breton, M. Winchell, P. Whatling

3:55 AGRO 223. Protecting endangered species from pesticides with stakeholder solutions. R. Marovich

4:20 AGRO 222. Ecological risk assessment for Pacific salmon exposed to dimethoate in California. M. Whitfield Aslund, R. Breton, L. Padilla, R. Reiss, P. Whatling, M. Winchell, K. Wooding, D. Moore

4:45 Discussion.

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis, and Ecological Effects

Cosponsored by ANYL and ENVR

D. S. Aga, J. S. Wallace, *Organizers, Presiding*

1:25 Reconvening Remarks.

1:30 AGRO 224. Stereoselective biotransformation of β -blockers and antidepressants in the aquatic environment. E. Sanganyado, J. Gan

1:55 AGRO 225. Transport of tetracycline antibiotics under field conditions. M.d. Munoz, R. Autenrieth

2:20 AGRO 226. Reconnaissance study of agricultural emerging contaminants (AECs) in the South Fork watershed of the Iowa River using polar organic chemical integrative samplers (POCIS). M. Washington, M. Soupir, T. Moorman

2:45 AGRO 227. Determination of antibiotics, estrogenic hormones, and UV filters in water, sediment, and crayfish from an urban watershed. K. He, A. Timm, C. Welty, L.M. Blaney

3:10 Intermission.

3:15 AGRO 228. Effect of Irrigation Water Quality on Antibiotic Persistence in Soil. L. Dodgen

3:40 AGRO 229. Rapid screening of metabolite potential of pharmaceutical and personal care products (PPCPs) in plants using plant cell cultures. J. Gan, X. Wu

4:05 AGRO 230. Influence of soil texture on the uptake of antibiotics in wastewater irrigated lettuce. J.B. Sallach, D.D. Snow, X. Li, L. Hodges, S. Bartelt-Hunt

4:30 AGRO 231. Plant Uptake of Pharmaceuticals from Soil Treated with Urine and Struvite. L. Su

4:55 AGRO 232. Transformation of organoarsenicals in water using the UV and UV-H₂O₂ systems. A. Adak, K.P. Mangalgi, J. Lee, L.M. Blaney

5:20 Concluding Remarks.

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Immunochemistry Summit XII: Immunoassays and Other Bioanalytical Techniques

Cosponsored by ANYL, ENVR and SCHB

J. M. Van Emon, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 AGRO 233. Colorimetric microtiter plate receptor-binding assay for the detection of freshwater and marine neurotoxins targeting the nicotinic acetylcholine receptors. F.M. Rubio, L. Kamp, J. Carpino, E. Faltin, K. Loftin, J. Molgo, R. Araoz

1:55 AGRO 234. Development and application of a salivary antibody 6-plex immunoassay to determine human exposure to environmental pathogens. S. Augustine, K.J. Simmons, T.N. Eason, S. Griffin, A. Dufour, G. Fout, A. Grimm, K. Oshima, T. Wade, L. Wymer

2:20 AGRO 235. Immunoassays for environmental contaminants using single domain heavy chain antibodies (VHH). S.J. Gee, C. Bever, J. Wang, T. Xu, B.D. Hammock

2:45 AGRO 236. Recombinant antibodies that distinguish between methylated and non-methylated derivatives of phenanthrene, a major polycyclic aromatic hydrocarbon present in crude oil. Y. Sun, A.M. Bradbury, G. Ansari, D.A. Blake

3:10 Intermissions.

3:30 AGRO 237. Nanobody based immunoassay for soluble epoxide hydrolase detection using polyHRP for signal enhancement: The rediscovery of polyHRP? D. Li, Y. Cui, S.J. Gee, Y. Ying, B.D. Hammock

3:55 AGRO 238. Development of a proteomic-based technique for evaluation of natural removal of contaminants from groundwater. K. Kucharzyk, C. Bartling, L. Mullins, D. Stoecel

4:20 AGRO 239. Effects of chlorpyrifos and TCP on human kidney cells using toxicity testing and proteomics. J.M. Van Emon, D. Ash, H. Moura, F. van Breukelen, P. Pan, R. Johnson, J.R. Barr

4:45 AGRO 240. Development and testing of genetically modified crop products throughout their life cycle. L. Privalle

Section E

Boston Park Plaza Hotel and Towers
Back Bay Room

Current Advances and Challenges of Arthropod Vector Control

L. J. Jenson, D. Swale, *Organizers, Presiding*

1:50 Introductory Remarks.

1:55 AGRO 241. GPCR targets for new arthropod vector insecticides: Dopamine receptors. A. Nuss, J. Meyer, K. Ejendal, J. Conley, T. Doyle, V. Watts, C. Hill

2:20 AGRO 242. Identification of immunogenic tick saliva proteins secreted into the host during 24-48 hours after attachment. Z.M. Radulovic, L. Lewis, T. Kim, L. Porter, A. Mulenga

2:45 AGRO 243. Withdrawn.

3:10 Intermission.

3:30 AGRO 244. *Sabadilla* vs. pyrethroids: A comparison study of toxicity and characterization of insecticidal modes of action. L.J. Jenson, T.D. Anderson

3:55 AGRO 245. Novel roles of DSC1 and interactions of DSC1 with para in determining the sensitivity of pyrethroids and DDT. F.D. Rinkevich, Y. Du, J. Tolinski, A. Ueda, C. Wu, B. Zhorov, K. Dong

4:20 AGRO 246. Activity of voltage-gated potassium channel blockers and their potential as new type of insecticide to control disease vector mosquitoes. F. Tong, B. Sun, A.D. Gross, P. Lam, M. Totrov, P.R. Carlier, J.R. Bloomquist

4:45 Panel discussion an
Concluding Remarks.

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Current Advances and Challenges of Arthropod Vector Control

L. J. Jenson, D. Swale, *Organizers*

1:00 - 5:00

AGRO 197. Activation, potentiation, and antagonism of *Musca* GABA receptors by ivermectin. T. Fuse, T. Kita, F. Ozoe, Y. Ozoe

AGRO 198. Evidence of ABC transporter(s) expression in vector mosquitoes. N. Pham, T.D. Anderson

AGRO 199. Investigation into the role of PhABCC4 in ivermectin tolerance. K. Gellatly, K.S. Yoon, E. Murenzi, J.M. Clark

AGRO 200. Mutations in the inner pore and D3/D4 fenestration of cockroach sodium channel confer resistance to sodium channel-blocker insecticides. Y. Du, Y. Zhang, D. Jiang, C. Behnke, Y. Nomura, B. Zhorov, K. Dong

AGRO 201. Insecticidal activity of stilbene derivatives and their mode of action on chloride and potassium channels. B. Sun, F. Tong, R. Islam, L.J. Jenson, T.D. Anderson, J.R. Bloomquist

AGRO 202. Toxicity of the isoxazoline fluralaner to larval and adult *Aedes aegypti* mosquitoes. S. Jiang, M. Tskolani, J.R. Bloomquist

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Immunochemistry Summit XII: Immunoassays and Other Bioanalytical Techniques

Cosponsored by ANYL, ENVR and SCHB

J. M. Van Emon, *Organizer*

1:00 - 5:00

AGRO 204. Phage display based nanobodies and peptides in analysis of environmental chemicals by immunoassay. D. Li, C. Bever, J. Dong, J. Wang, Y. Cui, X. Liu, N. Vasylieva, B. Barnych, Y. Wang, K. Ahn, H. Kim, S.J. Gee, B.D. Hammock

AGRO 205. Biological validation of enzyme-linked immunosorbent assays for detection of Bt Cry proteins in the environment. V.C. Albright, R. Hellmich, J.R. Coats

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Pollinators and Agrochemicals

Cosponsored by ENVR

M. L. Hladik, P. Reibach, *Organizers*

1:00 - 5:00

AGRO 206. Nasonov pheromone actives as repellents for pollinator-pesticide exposure. N.R. Larson, L.J. Jenson, U.R. Bernier, J.R. Bloomquist, T.D. Anderson

AGRO 207. Discovery of resistance-breaking chemistries for varroa mite management. P. Vu, L.J. Jenson, J.R. Bloomquist, T.D. Anderson

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AGRO 208. Toxicodynamics of the pesticide inert *N*-methyl-2-pyrrolidone and its impacts on honeybees. J. Fine, C.A. Mullin

AGRO 209. Comparative analysis of herbicide-induced oxidative stress on honey bees. J. Williams, C.C. Brewster, R. Fell, T.D. Anderson

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

Membranes, Absorption and H₂O₂ Production

Sponsored by ENVR, Cosponsored by AGRO

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES†, PROF and SCHB

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

Transforming University-Industry Partnerships for an Innovative Future
Engineering and Education

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

WEDNESDAY MORNING

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Innovations in Agrochemical Discovery and Process Chemistry: 2015 Kenneth A Spencer Award in honor of Thomas Selby and 2015 AGRO Award for Innovation in the Chemistry of Agriculture in honor of Tom Sparks

T. K. Trullinger, *Organizer*

B. A. Lorsbach, M. Riener, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 AGRO 247. 2015 Kenneth A. Spencer Award address: A career in crop protection discovery. T.P. Selby

9:20 AGRO 248. Mesoionic insecticides: A novel class of insecticides that inhibit rather than activate nicotinic acetylcholine receptors. C.W. Holyoke, D. Cordova, W. Zhang, J.D. Barry, R.M. Leighty, R.F. Dietrich, J.J. Rauh, T.F. Pahutski, G.P. Lahm, M.T. Tong, R.M. Smith, D.R. Vincent, L.A. Christianson

9:45 AGRO 249. Synthesis and SAR studies of insecticidal pyridazin-3-yl amides, hydrazides, hydrazines, and hydrazones. M.C. Yap, A. Buysse, R. Hunter, M.H. Parker

10:10 Intermission.

10:30 AGRO 250. Synthesis and insecticidal activity of *N*-(5-aryl-1,3,4-thiadiazol-2-yl)amides. J.D. Eckelbarger, M.H. Parker, M. Yap, A. Buysse, J.M. Babcock, R. Hunter, Y. Adelfinskaya, J.G. Samaritoni, N. Garzi, T.K. Trullinger

10:55 AGRO 251. Novel class of heterocyclic sulfonamides for the control of soil nematode. G.P. Lahm, J. Desaeager, B.K. Smith, T.F. Pahutski, T. Meloro, D. Cordova, E. Benner, M. Rivera

11:20 AGRO 252. Total synthesis of indole alkaloids. N.K. Garg

12:10 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage, and Monitoring Data

Cosponsored by ENVR

M. Barrett, W. Chen, M. T. Shamim, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGRO 253. How can product usage inform pesticide exposure assessments? Examples of the use of AgroTrak® and CA Pesticide Use Reporting data. C.M. Holmes, V. Solater, P. Hendley, S.H. Jackson

8:30 AGRO 254. Use of monitoring data, toxicity identification evaluations, and usage information in the ecological risk assessment of pyrethroid insecticides. M.T. Shamim, J. Melendez, K. Sappington

8:55 AGRO 255. Evaluation of time-dependent sorption of pesticide in soil using parameters generated from lab data. J. Cheplick, R. Sur, A.M. Ritter, R. Jones, K. Jones

9:20 AGRO 256. Incomplete pesticide models for soil and water: A fate and transport - chemical kinetics disconnect. D.S. Gamble

9:45 AGRO 257. Comparison of residential pyrethroid exposure predictions based on EPA Tier 2 standard scenarios and SWMM/AGRO scenarios based on residential use survey data. M. Winchell, S.H. Jackson

10:10 Intermission.

10:30 AGRO 258. Use of soil fumigant exposure assessment system (SOFEA) outside of California. R. Reiss, I. Van Wesenbeeck, S. Cryer

10:55 AGRO 259. Factors to consider when developing screening level and more refined estimates of potential human and aquatic ecological exposures and risks resulting from chemical releases in household wastewater. P. Hendley, S.H. Jackson, A.C. Barefoot, T. Xu, A.M. Ritter, C.M. Holmes

11:20 AGRO 260. Using data to improve the efficiency of tiered assessment of pesticide exposure in groundwater. M. Barrett, R.F. Bohaty, M. Fry, A. Shelby, J. Wolf, D. Young

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Environmental Fate, Management, and Mitigation of Nitrogen in Agricultural Systems

Cosponsored by ENVR

C. J. Hapeman, *Organizer*

K. L. Armbrust, B. L. Bret, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 AGRO 261. Nutrient runoff from agricultural watersheds in southeast Indiana (USA) and development of the watershed conservation regime. T.V. Royer

8:55 AGRO 262. Can changes in conservation reduce nitrogen export from agricultural watersheds? J.L. Tank, B. Hanrahan, S. Christopher

9:20 AGRO 263. Reducing nutrient movement in manure-treated, tile-drained fields. S.K. Papiernik, G.W. Feyereisen, J.M. Baker, C.D. Wente

9:45 AGRO 264. Slow-release, non-polluting, cost-effective fertilizer system. G. McNeely, B. Green

10:10 Intermission.

10:30 AGRO 265. Limus, a novel urease inhibitor for agriculture: Enhanced effect of two thiophosphoric triamides. L. Vance, G. Pasda, A. Wissemeyer, W. Zerulla

10:55 AGRO 266. Discovery, mode of action and development of nitrapiyrin as a nitrification inhibitor. C. Voglewede, J. Troth, R. Kaan

11:20 AGRO 267. Formulation innovations for nitrapiyrin nitrification inhibitor for use with multiple fertilizer types. E. Scherder, C. Voglewede, M. Li, L. Liu, B.L. Bret

11:45 AGRO 268. Management and mitigation of nitrates from nitrogen fertilizers in California. A.S. Gunasekara, B.A. Moradi

12:10 Concluding Remark.

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds

Cosponsored by ANYL and ENVR

Y. Sapozhnikova, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 AGRO 269. Next generation sample preparation materials for selective matrix removal. D. Lucas, B.E. Richter, L. Zhao

8:55 AGRO 270. Recent dioxin survey and results in meat and poultry. M.M. O'Keefe

9:20 AGRO 271. Ambient ionization of T-2 and HT-2 toxin from food and feed matrices utilizing direct analysis in realtime (DART) coupled to mass spectrometry. M. Busman

9:45 AGRO 272. Survey of glyphosate residues in honey, corn, and soy products. F.M. Rubio, E. Guo, L. Kamp

10:10 Intermission.

10:30 AGRO 273. Halogenated flame retardants in baby food from the United States and from China and the estimated dietary intake by infants. L. Liu, A. Salamova, R.A. Hites

10:55 AGRO 274. Arsenic speciation in high matrix food products: Striving for a complete mass balance. M.B. Ellisor, W.C. Davis

11:20 AGRO 275. Analysis of two classes of persistent organic pollutants in edible oil samples. K.K. Stenerson, O. Shimelis, C. Brown

Section E

Boston Park Plaza Hotel and Towers
Back Bay Room

Pesticides and Hydrophobic Compounds in Sediment

Cosponsored by ENVR

P. Hendley, *Organizer*

J. Gan, J. Giddings, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 AGRO 276. Challenges of measuring pyrethroid adsorption coefficients in sediments using automated solid phase micro extraction (SPME) techniques. P. Hendley, T. Xu, K. Clark, C. Chickering, J. Owen

8:55 AGRO 277. Modeling compound loss from passive sampler sorbents. D. Reible, C. Thomas

9:20 AGRO 278. Investigating soot-water partition coefficients of organic compounds using frontal chromatography and polyparameter linear free energy relationship. Z. Lu, P.M. Gschwend

9:45 AGRO 279. Attenuating historically contaminated sediments by black carbon amendments: Effects of sediment types and contact time. F. Jia, J. Gan

10:10 Intermission.

10:30 AGRO 280. Equilibrium sampling of hydrophobic organic contaminants in sediment. P. Mayer, K. Mäenpää, G. Witt, S. Schaefer, S.N. Schmidt, A. Jahnke

10:55 AGRO 281. Development and application of freshwater sediment-toxicity benchmarks for currently used pesticides. L.H. Nowell, J.E. Norman, C.G. Ingersoll, P.W. Moran

11:20 AGRO 282. Comparing bioavailability measurement methods. J. Gan

11:45 AGRO 283. New interpretations of the results of HOC monitoring studies and sediment ecotoxicity studies for HOCs based on refined adsorption coefficients. P. Hendley, J. Giddings, T. Xu, T. Valenti

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Innovations in Agrochemical Discovery and Process Chemistry: 2015 Kenneth A Spencer Award in honor of Thomas Selby and 2015 AGRO Award for Innovation in the Chemistry of Agriculture in honor of Tom Sparks

B. A. Lorsbach, M. Riener, T. K. Trullinger, *Organizers*

8:00 - 12:00

AGRO 289. Larvicidal activity of prenylated stilbene analogs. J. Weng, A. Ali, A.M. Rimando

AGRO 290. Effect of lanthanum on yield and components of soybean seedlings under supplementary UV-B radiation stress. H. Ren, X. Zhang, H. Zhao, Y. Yu, L. Shuang, Y. Sun

AGRO 291. Effect of nano silicon preparation on the nutrient content of rice plant aerial parts. H. Ren, X. Zhang, W. Ding, H. Zhao, L. Wang, Y. Yang

AGRO 292. Effect of nano silicon fertilizer on rice yield and component factors. H. Ren, L. Shuang, W. Ding, Y. Sun, X. Zhang

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

AGRO 293. Renewable syntheses of agrochemicals and pharmaceuticals from biomass-derived platform chemical 5-(chloromethyl)furfural (CMF). **F. Chang**

AGRO 294. Development of a high-throughput screening system for the detection of PaOA, octopamine receptor antagonists and agonists from *Periplaneta americana*. **E. Norris, A. Gross, M. Kimber, L. Bartholomay, J.R. Coats**

AGRO 295. Development of passive samplers for measuring bioavailability of pesticides in contaminated water with performance reference compound calibration. **J. Xue, C. Liao, J. Gan**

AGRO 296. Modeling the vibrational spectroscopy of amorphous carbonaceous materials using DFT. **A. Brown, M.T. Timko, N.A. Deskins, G. Tompsett**

AGRO 297. Prospecting of oil and deoiled cakes of *Jatropha curcas* L. and *Pongamia pinnata* L. for pesticidal activity. **R. Kalra, N. Kaushik**

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by *CLINF*, Cosponsored by *AGRO, COMP, ENVR and MEDI*

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

Electrocoagulation and Electro-Fenton Processes

Sponsored by *ENVR*, Cosponsored by *AGRO*

WEDNESDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Innovations in Agrochemical Discovery and Process Chemistry: 2015 Kenneth A Spencer Award in honor of Thomas Selby and 2015 AGRO Award for Innovation in the Chemistry of Agriculture in honor of Tom Sparks

M. Riener, Organizer

B. A. Lorschach, T. K. Trullinger, Organizers, Presiding

1:25 Introductory Remarks.

1:30 AGRO 301. Studies toward understanding the SAR around the sulfoximine moiety of the sap-feeding insecticide Isoclast™. **B.M. Nugent, A. Buysse, M.R. Loso, Y. Zhu, R.B. Rogers, N. Breaux, Z.L. Benko, J.M. Babcock**

1:55 AGRO 302. Developing a scalable process to Isoclast™ — a new crop protection agent. **D.C. Bland, N.M. Irvine, T. Martin, D.E. Podhorez, S.L. Powers, J.M. Renga, R. Ross, G.A. Roth, B.D. Scherzer, T.W. Toyzan**

2:20 AGRO 303. Agrochemical process research: Searching for the holistic solution. **M. Ford**

2:45 AGRO 304. Process research of DAS-Hb1, a 6-alkylpicolinolate broadleaf herbicide. **F. Li, G. Whiteker, P.L. Johnson, J. Epp, P. Schmitzer, N.M. Irvine**

3:10 Intermission.

3:30 AGRO 305. Learning from Mother Nature: Natural products as a source of ideas and inspiration for agrochemicals. **T.C. Sparks**

4:20 AGRO 306. Discovery of naphthalene isoxazoline insecticides. **M. Xu, T. Wagerle, J.K. Long, G.P. Lahm, T.M. Stevenson, D. Cordova, J.D. Barry, R.M. Smith**

4:45 AGRO 307. Aryl heterocyclic amines (AHA) insecticides. **W.H. Dent, M. Pobanz, C. Geng, T. Letherer, K. Beavers, C. Young, T.C. Sparks, Y. Adellinskaya, R. Ross, G. Whiteker, J.M. Renga, J. Watson, R.C. Weintraub**

5:10 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage, and Monitoring Data

Cosponsored by *ENVR*

M. Barrett, W. Chen, M. T. Shamim, Organizers, Presiding

1:25 Introductory Remarks.

1:30 AGRO 308. Streamlining refined aquatic exposure estimation for agricultural uses by understanding the significance and limitations of standard Tier II assumptions. **A.M. Ritter, D.A. Desmarteau, P. Hendley**

1:55 AGRO 309. Test version of a spatial aquatic model (SAM) to estimate spatial and temporal pesticide exposures in water. **N. Thurman, M. Fry, D. Young, M. Thawley, J. Hook, J. Carleton, R. Shamblen, K. Pluntke, G. Rothman, P. Mastradone, C. Koper**

2:20 AGRO 310. Drinking water exposure assessment for chlorpyrifos in North America: Overview and conclusions. **R.F. Bohaty, J. Hetrick, D. Spatz**

2:45 AGRO 311. Higher tier aquatic exposure assessment for imidacloprid. **Z. Tang, M. Winchell, L. Padilla, D.G. Dyer**

3:10 Intermission.

3:30 AGRO 312. Higher tiered aquatic exposure assessment of a recently developed pesticide under realistic agricultural production practices improves understanding of environmental fate. **T. Xu, D.G. Dyer, D. Netzband, L.L. McConnell, O. Perez-Ovilla, E.L. Arthur, T. Hall**

3:55 AGRO 313. Improved modeling approach to evaluate pesticide product for impacts to surface waters in California. **Y. Luo**

4:20 AGRO 314. Integrating modeling and monitoring for pesticide aquatic exposure assessment. **C. Truman, W. Chen**

4:45 Concluding Remarks.

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Degradation of Halogenated Compounds in the Environment

Cosponsored by *ENVR*

K. Lee, M. Ma, K. Myung, N. M. Satchivi, Organizers, Presiding

1:50 Introductory Remarks.

1:55 AGRO 315. Microbial dechlorination of PCBs—it's not just for sediments any more. **L.A. Rodenburg, S. Capozzi**

2:20 AGRO 316. Non-chlorinated dibenzo-*p*-dioxin daughter product detected in sediment microcosms from two contaminated sites originally amended with 1,2,3,4-tetrachlorodibenzo-*p*-dioxin. **D. Fennell, H. Zhen, F. Liu, J. Liu**

2:45 AGRO 317. In situ pilot studies evaluating the efficacy of bioaugmentation for treatment of PCB-impacted sediments. **K.R. Sowers, R. Payne, U. Ghosh**

3:10 AGRO 318. Biofilm enhanced bioremediation of polychlorinated biphenyls in soil and sediment. **B.V. Kjellerup, F. Akbari, S.J. Edwards**

3:35 Intermission.

3:55 AGRO 319. Investigating anaerobic dechlorination of organochlorine pesticides. **E.A. Edwards, L. Lomheim, L. Puentes, X. Tang, L. Laquitaine, S. Gaspard**

4:20 AGRO 320. Ecology and evolution of aerobic bacteria that utilize vinyl chloride as a carbon and energy source. **X. Liu, Y. Liang, Y.O. Jin, T. Mattes**

4:45 AGRO 321. Using factor analysis to find evidence of microbial degradation in the subsurface at a historically contaminated site. **S. Capozzi, L.A. Rodenburg, V. Kruminis**

5:10 Discussion.

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds

Cosponsored by *ANYL and ENVR*

Y. Sapozhnikova, Organizer, Presiding

1:25 Introductory Remarks.

1:30 AGRO 322. Recent developments in sample preparation and GC-MS/MS analysis of environmental contaminants and pesticides in food samples. **Y. Sapozhnikova**

1:55 AGRO 323. Synthesis, spectral characterization, biological activity, and soil:water fate of brominated 17β-estradiol isomers. **H. Hakk, S. Svendsen, N. Shappell, D. Rutherford**

2:20 AGRO 324. Pesticide multiresidue analysis in straw roughage using the QuEChERS approach and HPLC/MS/MS. **L. Han, M. Feng, K. Zhu, Z. Zhang**

2:45 AGRO 325. Target and non-target screening for emerging environmental contaminants using high resolution and accurate mass LC-MS/MS. **A. Schreiber, A. Thomas, P. Winkler, N. Zhu, C. Cai, D. Cox**

3:10 Intermission.

3:30 AGRO 326. Sample preparation and cleanup for multiresidue analysis of foodstuffs and environmental samples: Simple SPE strategies for complex matrices. **M.S. Young, K. Tran**

3:55 AGRO 327. Analysis of perfluoroalkyl substances in food, drinking water, and indoor dust from New York State and the assessment of human exposure. **Q. Wu, K. Kannan**

4:20 AGRO 328. Shoot-and-Dilute gas chromatography-mass spectrometry: Polycyclic aromatic hydrocarbons screening in food using streamlined sample preparation and alternative carrier gases. **J. Kowalski, A. Rigdon, M.N. Misselwitz, J. Cochran**

Section E

Boston Park Plaza Hotel and Towers
Back Bay Room

Formulation Technologies for Improved Crop Protection

Cosponsored by *ENVR and ORGN*

T. Jindal, A. D. Malec, S. A. Sumulong, Organizers, Presiding

1:50 Introductory Remarks.

1:55 AGRO 329. Solvent free emulsifier blend for solvent free EC formulations. **J.L. Jurs**

2:20 AGRO 330. Design and development of a novel green solvent: An unsaturated alkyl amide as a surfactant-solvent hybrid. **R. Totten**

2:45 AGRO 331. Soybean oil as a “green” carrier for agrochemical formulations. **J. Groome, R. Laljudi, B. McGraw**

3:10 Intermission.

3:30 AGRO 332. Use of yeast stress-induced proteins to affect the function of surfactants and their application in agricultural formulations. **A.D. Malec, C. Podella, M. Goldfeld, J.W. Baldrige, A.H. Michalow**

3:55 AGRO 333. Understanding the applicability of in-vitro assays for assessing eye irritation and skin sensitization potential to support crop protection formulation development. **R. Acosta Amado, R.S. Settivari, S.C. Geheh, M. Corvaro**

4:20 AGRO 334. Chlorpyrifos formulations and leachability studies. **T. Jindal, K. Gulati, S. Thakur, A. Kumar**

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Degradation of Halogenated Compounds in the Environment

Cosponsored by *ENVR*

K. Lee, M. Ma, K. Myung, N. M. Satchivi, Organizers

1:00 - 5:00

AGRO 284. Anaerobic abiotic reduction of dichloroacetamide safeners in Fe(II)-amended, heterogeneous minerals systems. **A. Ricko, J.D. Sivey**

AGRO 285. Risk mitigation strategies of DDT and dieldrin residues in historical orchard soils. **C.J. Hapeman, T. Centofanti, N.A. Andrade, L. McConnell, A. Torrents, W.N. Beyer, R. Chaney, A. Nguyen, M. Anderson, J. Novak, K. Cantrell, D. Jackson**

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage, and Monitoring Data

Cosponsored by *ENVR*

M. Barrett, W. Chen, M. T. Shamim, Organizers

1:00 - 5:00

AGRO 286. Comparison of two approaches to modeling ground water exposure with EPA's PRZM-GW model. **J. Lin**

AGRO 287. Inclusion of biphasic kinetics and non-linear sorption to refine estimated regulatory groundwater concentrations of pesticides. **S. Grant, J.W. Perine, W. Chen, M. Greener**

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Formulation Technologies for Improved Crop Protection

Cosponsored by ENVR and ORGN

T. Jindal, *Organizer*

A. D. Malec, S. A. Sumulong, *Organizers*,

1:00 - 5:00

AGRO 288. Antifeedant and antifungal activity of nanobiopesticide synthesized by Eucalyptus plant extract. H. Chhipa, N. Kaushik

Section F

Boston Park Plaza Hotel and Towers
Terrace Room

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds

Cosponsored by ANYL and ENVR

Y. Sapozhnikova, *Organizer*

1:00 - 5:00

AGRO 298. Flunixin urine residues in culled dairy cows and its relevance to food safety and environmental concerns. W. Shelver, D.J. Smith, L. Tell, R. Baynes, J. Schroeder, J. Riviere

AGRO 299. Measurement of pyrethroids and their environmental degradates in fruits and vegetables using a modification of the quick easy cheap effective rugged safe (QuEChERS) method. W. Li, J. Starr, M. Morgan

AGRO 300. Effect of pH and surfactants in stereoselective fate of beta-blockers in wastewater. E. Sanganyado, J. Gan

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by CINF, Cosponsored by AGRO, COMP, ENVR and MEDI

Detection and Fate of Health-Related Microorganisms in Water

Sponsored by ENVR, Cosponsored by AGRO

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan
(Bio)electro-Oxidation

Sponsored by ENVR, Cosponsored by AGRO

Using Passive Sampling Techniques to Detect Organic Contaminants

Sponsored by ENVR, Cosponsored by AGRO and ORGN

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

WEDNESDAY EVENING

Detection and Fate of Health-Related Microorganisms in Water

Sponsored by ENVR, Cosponsored by AGRO

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

Sponsored by ENVR, Cosponsored by AGRO

Hydrothermal Carbonization: Possibilities and Limits for Feedstocks, Processes and Applications

Sponsored by ENVR, Cosponsored by AGRO

Reclamation, Remediation, Restoration: Novel Approaches to Environmental Challenges

Sponsored by ENVR, Cosponsored by AGRO

Sensing of Environmentally Relevant Contaminants

Sponsored by ENVR, Cosponsored by AGRO

Using Passive Sampling Techniques to Detect Organic Contaminants

Sponsored by ENVR, Cosponsored by AGRO and ORGN

THURSDAY MORNING

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Innovations in Agrochemical Discovery and Process Chemistry: 2015 Kenneth A Spencer Award in honor of Thomas Selby and 2015 AGRO Award for Innovation in the Chemistry of Agriculture in honor of Tom Sparks

M. Riener, *Organizer*

B. A. Lorschebach, T. K. Trullinger, *Organizers, Presiding*

8:50 Introductory Remarks.

8:55 AGRO 335. Lead generation: Revving up the engine of discovery. V.B. Hegde

9:20 AGRO 336. Fluorine chemistry at Bayer: Enabling new products. N. Lui

9:45 AGRO 337. Design and synthesis of pyridine and pyrimidine derivatives as insecticides. M. Xu, T. Briddell

10:10 Intermission.

10:30 AGRO 338. Pro-insecticidal approach toward increasing *in planta* activity. L.C. Greemer, N.C. Giampietro, F. Wessels, W. Lambert, M. Yap, G. de Boer, Y. Adelfinskaya

10:55 AGRO 339. Molecular modelling of inhibition of fatty acid biosynthesis by post-emergent herbicides. D.W. Boerth, A. Arvanites

11:20 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Biomonitoring for Pesticide Exposures

Cosponsored by ENVR

J. Driver, R. I. Krieger, J. Pleil, J. Sobus, E. M. Ulrich, *Organizers*

S. Hayes, J. N. Seiber, *Organizers, Presiding*

8:50 Introductory Remarks.

8:55 AGRO 363. Assessment of human biomonitoring data in a public health risk context: Utility of biomonitoring equivalents. S. Hays

9:20 AGRO 364. Monitoring trends in exposure to contemporary insecticides in the US population. M. Davis, L. Valentin-Blasini, A. Calafat

9:45 AGRO 365. Protein adducts in dried blood spots as exposure biomarkers in epidemiological research. W.E. Funk

10:10 Intermission.

10:30 AGRO 366. Organochlorine pesticides in follicular fluid of women undergoing assisted reproductive technologies. J. Wang, B. Huang, Q.X. Li

10:55 AGRO 367. Biomonitoring of pyrethroid exposure in Thai farmers and consumers by immunoassay. S.J. Gee, S. Thiphom, T. Prapamontol, B.D. Hammock

11:20 AGRO 368. Development of *Helisoma* Trivolvis pond snails as biological passive samplers for the biomonitoring of an agricultural fungicide in wetlands. S. Morrison, J. Belden

11:45 Concluding Remarks.

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Degradation of Halogenated Compounds in the Environment

Cosponsored by ENVR

K. Lee, M. Ma, K. Myung, N. M. Satchivi, *Organizers, Presiding*

8:50 Introductory Remarks.

8:55 AGRO 346. Corrinoid quantity and quality determine reductive dechlorination rates and extents. F. Loeffler, J. Yan

9:20 AGRO 347. Reductive dechlorination of dichlorobenzene isomers and monochlorobenzene by *Dehalobacter* spp. S. Zinder, X. Liang, J. Nelson, J. Fung, H. Fullerton

9:45 AGRO 348. Role of the genus *Dehalogenimonas* in anaerobic chlorinated alkane dehalogenation: Polychlorinated ethanes and propanes. W.M. Moe, T.A. Key, K.S. Bowman, F.A. Rainey

10:10 Intermission.

10:30 AGRO 349. Microbiology, biochemistry, and genomics of the transformation of halogenated aromatics by *Dehalococcoides* strains. L. Adrian, M. Cooper, A. Kublik, C. Yang

10:55 AGRO 350. Characterization of the activities of cis-3-chloroacrylic acid dehalogenase homologues: Analysis and implications. C.P. Whitman, J.P. Huddleston, W.H. Johnson

11:20 Discussion.

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Spray Application Technology

Cosponsored by ENVR

G. Kruger, *Organizer*

P. L. Havens, S. H. Jackson, *Organizers, Presiding*

8:50 Introductory Remarks.

8:55 AGRO 351. Complexity of spray drift research: Knowing where to look for trends that are out of the ordinary. G. Kruger, R. Henry, C.F. Creech

9:20 AGRO 352. Comparison of multiple sampling methods for evaluation of off field airborne chemical movement. S.H. Jackson, A. Hewitt

9:45 AGRO 353. Wind-controlled approach for spray drift testing. J. Fife, T. Lane

10:10 Intermission.

10:30 AGRO 354. Recommendations for uniformity in spray drift field studies. J.P. Hanzas, A. Hewitt, B.N. Toth, B. Brayden

10:55 AGRO 355. Probability of multiple applications having the same wind speed and key meteorological parameters and the resulting impact on pesticide loadings and exposure. A.M. Ritter, P. Hendley, M. Guevara

11:20 AGRO 356. Emulsion-based drift control: Influence of interfacial properties. A.L. Grzesiak, M.D. Reichert, S. Wilson, A.L. Reder, K.O. Hyde, K. Sheridan, W. Waters

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan
Photo-Assisted Processes

Sponsored by ENVR, Cosponsored by AGRO

THURSDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers
Georgian Room

Data to Decisions: Software Solutions for Modern Analytical Workflows

Cosponsored by ANYL and ENVR

L. Buchholz, L. Riter, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGRO 357. Software visualization and automation for making sense of the ever increasing amounts of mass spectral data. D.M. Cox, B. Barrett, A. Schreiber, J. Gibbons

1:30 AGRO 358. Impurity characterization of the fungicide flutriafol using liquid chromatography and time of flight MS detection to aid pesticide product registration. M. Twohig, M. O'Leary, P.G. Alden, J.P. McCauley

1:55 AGRO 359. Applying tensor decomposition model for high-dimensional toxicogenomics data analysis and interpretation. C. Gao, A. Gu

2:20 Intermission.

2:35 AGRO 360. Computer systems validation and e-data. H.H. Hardaway

3:00 AGRO 361. Straightforward, unified approach to tracking compound progression, analysis, and work-requests. B. Lynch, C. Tudge, J. Gordon, T.E. Mansley

3:25 AGRO 362. Allotrope framework: An innovative collaboration to improve data interchange, increase research efficiency, and realize the full value of your data. J.L. Van Duine

3:50 Concluding Remarks.

Section B

Boston Park Plaza Hotel and Towers
Arlington Room

Structure Elucidation in Metabolism Studies: Plant, Animal, and Soil

Cosponsored by ANYL

J. Afzal, M. A. Jalal, *Organizers, Presiding*

1:00 Introductory Remarks.

- 1:05 AGRO 340.** Challenges encountered in the structure elucidation of metabolites. **J. Afzal**
- 1:30 AGRO 341.** Trace level metabolite identification using high resolution mass spectrometry coupled to low flow separations. **J.R. Gilbert**, J. Balcer, Y. Adelfinskaya, S. Annangudi, D.G. McCaskill, P.L. Johnson, G. de Boer, M.J. Hastings
- 1:55 AGRO 342.** Identification of Indaziflam metabolites in the rat. **M.E. Krolski**, T. Nguyen
- 2:20** Intermission.
- 2:35 AGRO 343.** Fractionation and characterization of bound and unextractable pesticide residues in plants. **N. Mallipudi**, B. Lange
- 3:00 AGRO 344.** Fishing for unknown metabolites of nonradio labeled molecules “cold compounds” in samples of biological, environmental, and complex origins using high resolution time of flight mass spectrometry and METABOLYNX™. **D. Safarpour**
- 3:25 AGRO 345.** Transformation of [¹⁴C] Fluensulfone into lactose in the lactating goat. **J. LaMar**, G. Quistad

Section C

Boston Park Plaza Hotel and Towers
White Hill Room

Degradation of Halogenated Compounds in the Environment

Cosponsored by ENVR

K. Lee, M. Ma, K. Myung, N. M. Satchivi,
Organizers, Presiding

1:00 Introductory Remarks.

- 1:05 AGRO 369.** Organohalide respiration in *Sulfurospirillum multivorans*: Structure and function of the tetrachloroethene reductive dehalogenase. **T. Schubert**, C. Kunze, M. Bommer, J. Gadkari, T. Goris, H. Dobbek, G. Diekert
- 1:30 AGRO 370.** Degradation of halogenated alkaloids by the catalytic hemoglobin dehaloperoxidase from *Amphitrite ornata*. **R.A. Ghiladi**, N.L. McCombs, L. Carey
- 1:55 AGRO 371.** Challenges and new approaches to the defluorination of fluorinated aromatic compounds. **K.P. McNeill**, D. Sadowsky, C.J. Cramer

2:20 Intermission.

2:35 AGRO 372. Reductive dehalogenation is endogenous in vertebrates and other animals. **S. Rokita**

3:00 AGRO 373. Reductive dehalogenation of perchloroethene and trichloroethene in chemostat reactors and a continuous flow column. **L. Semprini**

3:25 AGRO 374. Degradation of triclosan and triclocarban and formation of degradation products in activated sludge using benchtop bioreactors. **N. Lozano**, D.L. Armstrong, C.P. Rice, M. Ramirez, A. Torrents

3:50 Discussion.

4:05 Concluding Remarks.

Section D

Boston Park Plaza Hotel and Towers
Whittier Room

Spray Application Technology

Cosponsored by ENVR

P. L. Havens, *Organizer*

S. H. Jackson, G. Kruger, *Organizers, Presiding*

1:00 Introductory Remarks.

- 1:05 AGRO 375.** Glufosinate — spray quality effects with tank mixes and nozzle selections. **K. Qin**, A. Cotie, Z. Tang, D.G. Dyer, T. Hall
- 1:30 AGRO 376.** Confirmation of the drift reduction performance of Enlist Duo® Herbicide applied with various spray nozzle designs. **P.L. Havens**, J. Schleier, G. Kruger, R. Henry
- 1:55 AGRO 377.** Influence of droplet size, application pressure, and adjuvants on the retention of dicamba spray droplets on leaves. **T.R. Butts**, C.F. Creech, R. Henry, G. Kruger

2:20 Intermission.

2:40 AGRO 378. Exposure and risk assessment for spray drift deposition of isoxaflutole on non-target plants. **R. Sur**, T. Xu, D.G. Dyer, K. Qin

3:05 AGRO 379. Novel formulation technology for reducing pesticide drift. **J. Schleier**, H. Tank, C. Voglewede, A. Chavez Green

3:30 AGRO 380. Beyond AGDRIFT — Analysis of expanded ground sprayer deposition data. **P.L. Havens**, E. Maloney, T.L. Estes, S.H. Jackson

3:55 AGRO 381. Connecting spray particle size to biology for pesticide applications. **G. Kruger**, R. Henry, C.F. Creech

ANYL

Division of Analytical Chemistry

D. Duckworth, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Analytical Chemistry in Nuclear Technology
(see *NUCL*, Sunday, Monday)

Immunoassays and Other Bioanalytical Techniques (see *AGRO*, Tuesday)

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds (see *AGRO*, Wednesday)

SOCIAL EVENTS:

ANYL Dinner (Ticketed Event),
6:00 PM: Tuesday

BUSINESS MEETINGS:

Business Meeting (Closed),
4:00 PM: Monday

SUNDAY MORNING

Section A

Renaissance Boston Waterfront
Pacific Blrm H

Beyond Quant: Re-envisioning the Foundational Course in Analytical Chemistry

C. T. Culbertson, K. Frederick, *Organizers, Presiding*

8:30 ANYL 1. Desirable features of a foundational course in analytical chemistry. **T.J. Wenzel**

9:10 ANYL 2. Producing market ready students: Quantitative Analytical Chemistry overhaul. **C.R. Dockery**, **M.C. Koether**, K.J. Linenberger, H.Z. Msimanga, W. Zhou

9:30 ANYL 3. Trading burets for cuvetts: What drives changes in quantitative analysis lab? **C.D. King**

9:50 Intermission.

10:00 ANYL 4. Beyond quant: Supporting analytical chemistry's third dimension. **D.T. Harvey**

10:20 ANYL 5. Analytical method development as a focus for the foundational analytical course. **K. Frederick**, L. Quimby, M. Roca

10:40 ANYL 6. Thinking bigger: Using student research and active-learning strategies in a two-course quantitative and instrumental analysis sequence. **E.M. White**, D.T. Miles

11:00 Discussion.

Section B

Renaissance Boston Waterfront
Pacific Blrm F

Analytical Chemistry Applications in Pharmaceutical Sciences

J. F. Castner, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 ANYL 7. Case studies in analytical chemistry best practices for pharmaceutical delivery devices designed to proactively address future regulatory landscape defined in proposed USP 661, 1663, and 1664 chapters. **A.D. Hendricker**, E.L. Carico, J.B. Dagger, D.D. Gilbert, L.B. Yu, J.D. Lennon

9:00 ANYL 8. Analytical challenges to implement and use of USP as a guidance for confirmation and identification of trace level organic extractable components. **G. Vas**

9:30 ANYL 9. Chemometric assessment of best practices for test procedures cited in USP updated chapters on extractables/leachables. **J.F. Castner**, M. Bresnick, M. Castner

10:00 Intermission.

10:15 ANYL 10. Sub-PPM detection limits in powder X-ray diffraction guided by second harmonic generation imaging. **G.J. Simpson**

10:45 ANYL 11. Development of a fast headspace GC method for determination of residual solvents in permethrin. **J. Tian**, A. Rustum

11:15 ANYL 12. Development and validation of a stability-indicating UPLC method for the assay of imidacloprid and estimation of its related compounds. **J. Tian**, A. Rustum

11:45 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Pacific Blrm H

Beyond Quant: Re-envisioning the Foundational Course in Analytical Chemistry

C. T. Culbertson, K. Frederick, *Organizers, Presiding*

2:00 ANYL 13. Quantitative analysis: Change the pedagogy not the content. **D.A. Fry**

2:20 ANYL 14. Restructuring the quantitative analysis laboratory to allow for real world applications. **K. Chichester**, I. Kimaru, L. Donahue, M.C. Koether

2:40 ANYL 15. Using reflective writing as an instrument to assess student learning in analytical chemistry. **A.E. Witter**

3:00 Intermission.

3:10 ANYL 16. Mixed bag: A hodgepodge of quantitative analysis curriculum. **C.E. Mactaylor**

3:30 ANYL 17. ANA-POGIL project: POGIL in analytical chemistry. **J. Lantz**, R.S. Cole

3:50 Discussion.

Section B

Renaissance Boston Waterfront
Pacific Blrm F

Forced Degradations in Pharmaceutical Industry

H. Yarabe, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 ANYL 18. Predictability of forced degradation studies for real world stability. **S.W. Baertschi**

1:55 ANYL 19. Industry practices for conducting forced degradation studies: AstraZeneca's approach. **S. Marden**, I. Ashworth, D. Benstead, E. Örnsvok

2:20 ANYL 20. Pharmaceutical photostability stress testing practice and case studies. **G. Sluggett**

2:45 ANYL 21. Forced degradation in an over the counter cough syrup. **D. Giamalva**, J.L. Humphrey, V. Campbell

3:10 Intermission.

3:25 ANYL 22. Leveraging the chemistry of drug degradation to support the structure elucidation process: Solid and liquid dosage form case studies. **T.C. Zelesky**

3:50 ANYL 23. Development and validation of a novel stability-indicating reversed-phase high-performance liquid chromatography method for assay of milbemycin oxime and estimation of its related compounds. **J. Huang**, A. Rustum

4:15 ANYL 24. Reduction of false positives in the peroxy radical based stress test. **P. Harmon**

4:40 Concluding Remarks.

Section C

Renaissance Boston Waterfront
Pacific Blrm G

Informatics 2.0 for the Analytical Sciences: Big Data, the Semantic Web, and Metadata

S. J. Chalk, A. J. Williams, *Organizers, Presiding*

1:30 ANYL 25. Driving needs for analytical data exchange standards and the potential impacts on the chemical sciences. **A.J. Williams**

2:00 ANYL 26. AnIML: A new analytical data standard. **S.J. Chalk**

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2:30 ANYL 27. ChAMP, the Chemical Analysis Metadata Platform: Bringing analytical chemistry to the semantic web. **S.J. Chalk, A. Williams**

3:00 ANYL 28. Before we can handle big data we need smarter data. **P. Jones, D. Vanderwall**

3:30 ANYL 29. Utilization of multiple data points and data sources in the identification of unknowns. **D. Hardy, V. Lashin, P. Russell, A. Gravel, A. Williams**

4:00 ANYL 30. Laboratory informatics environments: Why unified platforms and integration now? **G.A. McGibbon, D. Hardy, R. Sasaki**

Current Topics in Seed Treatment

Sponsored by *AGRO*, Cosponsored by *ANYL* and *ENVR*

SUNDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

General Analytical Posters

D. C. Duckworth, *Organizer*

6:00 - 8:00

ANYL 31. Determination of individual C18 and C20 long chain base GM1 Gangliosides in a heterogeneous GM1 standard: Two strategies compared. **A. Gobburi, R. Zhang, B. Willard, D. Inman, D.J. Anderson**

ANYL 32. Syntheses of lignin-derived dimers from thioacidolysis followed by Raney nickel desulfurization and their uses as GC quantitation standards. **F. Yue, F. Lu, R. Sun, J. Ralph**

ANYL 33. Determination of thermally induced isomerization of phyloquinone using electrospray ion mobility time-of-flight mass spectrometry. **P. Xiao, D. Song, H. Li**

ANYL 34. Evaluation of L-glutamide-derived supramolecular gel-forming organic phase in RP-HPLC. **H. Noguchi, T. Charoenraks, M. Takafuji, H. Ihara**

ANYL 35. Performance attributes of HPLC as it relates to the separation of biocides. **M.J. O'Leary, P.G. Alden**

ANYL 36. Evaluation of an LC-ESI-MS method for detection of sugars released after the enzymatic degradation of wood. **S. Galster, C. Farrugia, R.E. Goacher**

ANYL 37. Multilayer microfluidic paper-based analytical device using pyrolyzed paper for electrochemical detection. **E. Evans, J. Giuliani, E. Tavares da Costa, C.D. Garcia**

ANYL 38. Graphene-based sensor interface for DNA charge transfer. **L. Lu**

ANYL 39. Imaging and sampling with nanopipettes. **L.A. Baker**

ANYL 40. High-throughput microfluidic method to profile the dynamical properties of cellular reactions. **C. Vyas, A. Lam, K. Long, B. Natarajan, H. Ma**

ANYL 41. Multiplexed, in-situ detection of protein binding on plasmonic microfluidic devices. **J. He, M. Boegli, I. Bruzas, S. Unser, L. Sagle**

ANYL 42. Highly sensitive bacteria detection in large volume environmental sample by using graphene oxide coated microbeads. **C. Baek, S. Chung, J. Min**

ANYL 43. Withdrawn.

ANYL 45. Multiple reaction monitoring for targeted quantification of enzyme activities in proteome. **S. Li, P. Diego, B. Bajrami, S.K. Keshipeddy, Y.W. Lam, B. Deng, V. Farrokhi, A. McShane, R. Nemati Josheghani, A.R. Howell, X. Yao**

ANYL 46. Preparation of glucuronic acid conjugate reference materials for paralytic shellfish toxins. **P. Eangoor, A. Indrapurkar, J. Knaeck**

ANYL 47. Ultrasensitive and on-site detection of pathogens using Mag-LINA immunoassays. **S. Ahmed, A. Abbas**

ANYL 48. Qualitative and semi-quantitative analysis of glycerolipids and phospholipids in algae *scenedesmus dimorphus* by multiple-precursor and neutral-loss scanning methods. **S. Avula, J. Belovich, Y. Xu**

ANYL 49. Rapid quantification of entire phospholipid composition in hydrolyzed products of lecithin by P31-NMR. **Y. Yang, R.D. Hiserodt, J. Li**

ANYL 50. MnO₂ nanosheets based fluorescent sensing platform with organic dyes as probe with excellent analytical properties. **C. Wang, L. Mao**

ANYL 51. Ligand-RNA interaction fluorescence indicator displacement assay inspiring the discovery of Tat antagonists. **L. Qi, L. Zhang, H. Zhan, Y. Huo, J. Zhang, F. Dang, Z. Zhang**

ANYL 52. Simultaneous multiplexed cytokine analysis using semisynthetic aequorin fusion proteins. **X. Yu, D. Scott, E. Dikici, S. Daunert**

ANYL 53. Intercalation of alkynylplatinum(II) terpyridine complexes into a helical structure poly(phenylene ethynylene sulfonate) and the application in protein sensing. **S. Wang, J. Jiang, Z. Pan, K.S. Schanze**

ANYL 54. Analysis of carbohydrates in the atmosphere: Impact of Spring rain on bioaerosols in Iowa. **C. Rathnayake, J. Kettler, T. Jayaratne, E.A. Stone**

ANYL 55. Exploration of high-resolution differential ion mobility spectrometry for large proteins. **A.A. Shvartsburg**

ANYL 56. Oligomer molecular weight determination by advanced polymer chromatography system. **H. Fang, P. Cui, Q. Wu, C. Qian**

ANYL 57. Withdrawn.

ANYL 58. Understanding why semi-conductive quantum rods have high energy transfer efficiency with firefly luciferase. **L.M. Karam, K.J. Coopersmith, D.M. Fontaine, B.R. Branchini, M.M. Maye**

ANYL 59. Interactions of photosystem I with anionic peptides: A spectroscopic study. **A. Stone, A. Sunda-Meya, N. Phambu**

ANYL 60. Biocatalytic cascades for the forensic determination of personal properties based on blood markers. **J.M. Agudelo, J. Halamek, C. Huynh, E.K. Brunelle**

ANYL 61. Analysis of synthetic cathinones in oral fluid using stir bar sorptive extraction (SBSE) combined with direct analysis in real time-time of flight mass spectrometry (DART-TOFMS). **K.M. Tully, B. Musselman, J.F. Morrison**

ANYL 62. Optimization of direct analysis real time-time of flight mass spectrometry (DART-TOFMS) for the detection, characterization, and quantification of synthetic cathinones in oral fluid. **H.S. Loring, B. Musselman, J.F. Morrison**

ANYL 63. Comparing solid-sampling instrumental methods to detect the enzymatic degradation of wood. **C. Whitney, N. Zerby, R.E. Goacher**

ANYL 64. Comparative analysis of DRIFTS, ATR, and transmission FTIR sampling techniques for quantitative measurements on lignocellulose. **M. Gogna, R.E. Goacher**

ANYL 65. Ultrasensitive detection of ribosomal RNA for monitoring of cyanobacteria. **M.R. Hartman, B.P. Regmi, P. Ghatak, M.L. Richlen, D.M. Anderson, D.R. Walt**

ANYL 66. Analysis of total human urinary glycosaminoglycan disaccharides by liquid chromatography-tandem mass spectrometry. **X. Sun, L. Li, K. Overdier, L. Ammons, I. Douglas, C. Burlew, F. Zhang, E. Schmidt, L. Chi, R.J. Linhardt**

ANYL 67. Analytical methodologies to isolate and quantify free and liposomal bound doxorubicin from biological samples using LC-HRMS and LC-QQQ-MS. **P. Sisco, K. Ahlswede, J. Leakey, S. Linder**

ANYL 68. Multiclass drug and metabolite screen of 231 analytes by LC-MS/MS. **S. Lupo, F. Carroll, S. Liang, T. Kahler, P. Connolly, R. Lake, R. Freeman, C. Sprout**

ANYL 69. Withdrawn.

ANYL 70. Novel real-time, mediator-free, non-enzymatic electrochemical biosensor for glutamate detection. **Y. Yang, A. Manfredi, S. Daunert**

ANYL 71. Single-molecule multiplexed detection of proteins for early diseases detection. **T. Dinh, D. Wu, D.R. Walt**

ANYL 72. Withdrawn.

ANYL 73. Using anion-exchange chromatography coupled with high resolution accurate mass spectrometry for TCA pathway targeted metabolomics analysis. **T. Christison, J. Wang, S.S. Hu, L. Lopez, Y. Huang**

ANYL 74. Novel antibody conjugated SERS probe for distinguishing cancer cells from normal cells. **W. Qian, H. Zhao, X. Cao**

ANYL 75. Synthesis and electrochemical properties of biomass-derived nitrogen-rich carbon for electrochemical sensors. **Y. Xu, L. Lu, P. Liu, Q. Hao**

ANYL 76. Hg²⁺ detection based on on-chip extraction and fluorescence quenching of BSA-stabilized Au nanocluster. **I. Hsu, T. Shin, S. Tseng, Y. Yang, P. Chen, Y. Sun**

ANYL 77. Detection of designer drugs and relevant metabolites in raw sewage samples using high resolution mass spectrometry. **M.R. Pruy, P.R. Gardinali**

ANYL 78. Understanding the atmospheric pressure ionization of petroleum components: The effects of size, structure, and presence of heteroatoms. **A. Huba, P.R. Gardinali**

ANYL 79. Novel enzyme-modified graphene nanosheet biosensors for the detection of pesticides. **K. Morrissey, O. Kubesa, M.R. Hapel**

ANYL 80. 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, L. Hou**

ANYL 81. Efficacy of a short conditioning step for eliminating carry-over from SPME fibers. **C. McGuire, E. Harrington, A. Anderson, M. Krisch**

ANYL 82. Liquid chromatography-tandem mass spectrometry analysis of neonicotinoids in environmental water. **C. Hao, X. Zhao, L. Sui, D. Morse**

ANYL 83. New method for the determination of styrene oligomers from debris polystyrene and its application to coastline and ocean contamination. **K. Koizumi, H. Sato, A. Okabe, B. Kwon, S. Chung, D.M. Karl, H. Katsura, K. Saïdo**

ANYL 84. Solid-phase microextraction of non-steroid anti-inflammatory drugs using metal-organic framework polymer monoliths as adsorbent. **Y. Kuo, K. Wan, H. Huang**

ANYL 85. Non-invasive fecal analysis: A novel tool to assess environmental stress in aquatic and marine wildlife. **C. Rolsky, R.U. Halden**

ANYL 86. Basmati or not basmati? That is the question. **G. Cleland, A. Ladak, S. Lai, R. Sternmler, J. Burgess**

ANYL 87. LC-MS/MS analysis of pesticide residues in rice and unexpected detection of residues in an organic rice sample. **D. Shah**

ANYL 88. Novel headspace gas chromatographic method for the determination of hydrogen peroxide residues in milk. **H. Li, C. Du, M. Liu, H. Zhan**

ANYL 89. Tobacco-specific nitrosamines in the tobacco and mainstream smoke of U.S. commercial cigarettes. **S.H. Edwards, L.M. Rossiter, K.M. Taylor, M.R. Holman, Y.S. Ding, C.H. Watson**

ANYL 90. Determination of unsulfonated aromatic amines in the color additives FD&C Yellow No. 5 and FD&C Yellow No. 6 using LC-MS/MS. **N. Belai, S.R. White, B. Bowes**

ANYL 91. Colorimetric detection method for identification of fuels and post-combustion residues. **Z. Li, M. Jang, K.S. Suslick**

ANYL 92. Column performance: Comparison of the superficially porous particle (SPP) to the fully porous particle (FPP). **S. Lupo, S. Liang, F. Carroll, T. Kahler, P. Connolly, R. Lake, C. Sprout, R. Freeman**

ANYL 93. 21 Tesla Fourier transform ion cyclotron resonance mass spectrometer: A national resource for ultrahigh resolution mass analysis. **C.L. Hendrickson, J.P. Quinn, N.K. Kaiser, D.F. Smith, G.T. Blakney, T. Chen, S.C. Beu, C.R. Weisbrod, A.G. Marshall**

ANYL 94. High resolution ion mobility separations in a cyclic structure for lossless ion manipulations module with time-of-flight mass spectrometry (SLIM IMS/TOFMS). **I.K. Webb, T. Chen, S. Garimella, A. Tolmachev, R. Norheim, S. Prost, G. Anderson, Y. Ibrahim, R. Smith**

ANYL 95. Extraction technique for the characterization of cross-linked films. **S. Korf, D. Barsotti, M. Capistrano, M. Karalis, M. Lessik**

ANYL 96. Determination of the number of anion-exchange sites on a weak anion: Exchange HPLC column using frontal analysis. **A. Gobburi, K. Pedada, H. Jogiraju, D.J. Anderson**

ANYL 97. Electroless plating as a flexible tool for the creation of custom surface enhanced Raman spectroscopic (SERS) substrates. **B.I. Karawdeniya, Y. D. Y. Bandara, C. Masterson, B.D. Velleco, J. Whelan, J.R. Dwyer**

ANYL 98. Investigating the formation of polydichlorophosphazenes via NMR spectroscopy. **J.A. Stiel, C. Tessier**

ANYL 99. Electronegativity is not a sufficient criterion for assigning ¹³C chemical shifts in halogenated benzenes. **D.D. Clarke**

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

ANYL **100.** New GFC columns for low noise MALS analysis. **M. Turcotte**, T. Matsui, R. Benson

ANYL **101.** Spectroelectrochemical modulation in a photoluminescent 1,8-anthraquinone-18-crown-5 host with select metal cation guests. **D. Weatherman**, A.G. Sykes

ANYL **102.** Influence of interfacial effects by PVDF on the fluorescent properties of Rhodamine 6. **M.J. Mullen**, **M. Alhasani**, M.A. Conrad, A. Gupta, W.B. Euler

ANYL **103.** Betaine based deep eutectic solvent: A promising green solvent for the future. **S. Panda**, R.L. Gardas

ANYL **104.** Substituent effects in synchronized π - π interactions. **J. Carey**, C. Chen

ANYL **105.** Speciation of Nb(V) and Ta(V) in alkaline media. **G. Deblonde**, A. Chagnes, G. Cote, A. Moncomble, N. Delaunay, C. Coelho-Diogo, C. Bonhomme

ANYL **106.** Effect of combi-2 on the structure and phase transitions of binary membrane systems: A spectroscopic study. **B. Almarwani**, A. Sunda-Meya, N. Phambu

ANYL **107.** Study of rhodamine 6G thin films on a glass substrate. **M. Liu**, **E. Ortega**, W.B. Euler

ANYL **108.** Development and application of a cost effective luminescence imaging system with high spatiotemporal resolution. **A.S. Mathew**, C.A. DeRosa, T.P. Butler, J.N. Demas, C. Fraser

ANYL **109.** Preparative chiral SFC of acidic compounds in Discovery Chemistry: From method development to multigram quantity scale-up. **D. Wu**, S. Yip, P. Li, D.Z. Sun, A. Mathur

ANYL **110.** From Afghanistan to space: Designing a novel microfluidic assay system to diagnose and stage protein energy malnutrition. **K. Reed**, J. Tsosie, M.E. Piyasena

ANYL **111.** Paper-based optical sensor as an end-of-service-life indicator for hydrogen cyanide. **L. Greenawald**

ANYL **112.** Fluorescent probe for sulfur dioxide derivative sulfite. **K. Wang**, H. Peng, A. Draganov, B. Wang

ANYL **113.** Spatial distribution of contact pin-printed features formed on oxidized porous silicon surfaces. **S.G. Coombs**, F.V. Bright

ANYL **114.** Single molecule assay development for breast cancer detection. **S. Baig**, S. Schubert, S.R. Walter, D.R. Walt

ANYL **115.** Ruthenium-modified sensitive NO sensors: Quantifying nitric oxide in the pathobiology of cystic fibrosis. **T. Bose**, T.L. Henderson, M. Bayachou

ANYL **116.** Examining third hand smoke from illicit drugs as a potential source of recoverable trace evidence. **J.L. Bitter**, M.E. Staymates, R.A. Fletcher, J.G. Gillen

ANYL **117.** Microcylinder sensors for the extracellular microenvironment. **B. Gutierrez**, R.J. White

ANYL **118.** Multimodal oxygen imaging utilizing dual emissive polymers and a CMOS camera. **A.S. Mathew**, C.A. DeRosa, G.M. Palmer, J.N. Demas, C. Fraser

ANYL **119.** Morphological transformation of bimetallic Au-Cu rods into spheres via galvanic replacement reaction by single particle spectroscopy. **S. Thota**, S. Chen, J. Zhao

ANYL **120.** Investigating the role of polytypism in the growth of multi-shell CdSe/CdZnS quantum dots by X-ray diffraction. **K.L. Ryan**, S. Majumder, M.M. Maye

ANYL **121.** LC/MS analysis of various anionic substances using polymer-based multimode column. **M. Turcotte**, J. Sasuga, S. Sakai, R. Benson

ANYL **122.** Chemical sensing with carbon materials. **V. Kumar**

ANYL **123.** Fabrication of chemical sensors containing micropatterns of templated noncovalently crosslinked N-isopropylacrylamide copolymers. **C.J. Grenier**, **A. Timberman**, R. Yang, J. Nelson, L. Deravi, W.R. Seitz

ANYL **124.** Automated structure verification in the pharmaceutical discovery open access environment. **B.A. Becker**

ANYL **125.** Determination of isomeric halogenated aromatic compounds using gas chromatography with flame ionization detector. **C. Tsang**

ANYL **126.** Analytical and synthetic studies on substituted cathinones: Bath salt-type aminoketone designer drugs. **Y. Abiedalla**, K. Abdel-Hay, J. DeRuiter, C.R. Clark

ANYL **127.** Analytical determination of trace level alkyl sulfonate esters genotoxic impurities in drug substances by using HPLC-HILIC-CAD. **C. Tsang**

ANYL **128.** Analysis of heparin derived tetrasaccharides by 2-aminoacidone labeling ultrahigh-performance liquid chromatography-mass spectrometry. **X. Sun**, L. Li, Y. Sun, L. Chi, R.J. Linhardt

ANYL **129.** LC-MS method development and MSⁿ analysis of folic acid and Furosemide: Two FDA approved drugs. **S. Bhattacharya**, S.C. Roemer

ANYL **130.** Video rate polarization-modulation nonlinear optical microscopy for rapid analysis of pharmaceutically relevant crystals. **G.J. Simpson**

ANYL **131.** Confocal Raman spectroscopic microscopy tracks the penetration of two permeation enhancers in intact human skin ex vivo. **Q. Zhang**, Y. Pyatski, C.R. Flach, R. Mendelsohn

ANYL **132.** Quantitative HS-SPME measurements of bioactive sesquiterpene from *Lychnophora ericoides* (Vernoniaeae: Asteraceae). **N.P. Lopes**, D. Pavarini

ANYL **133.** Development of a liquid chromatography-tandem mass spectrometry (LC-MS/MS) method for quantification of subtype-selective GABA_A receptor ligands following liquid-liquid extraction (LLE) and on-line solid-phase extraction (SPE). **M.L. Guthrie**, M.M. Poe, J.M. Cook, A. Arnold

ANYL **134.** Novel method for simultaneous detection in biosolids of 11 antibiotics of common use in human health and animal husbandry. **H.Y. Done**, R.U. Halden

ANYL **135.** New voltammetry interface for teaching in undergraduate analytical chemistry courses. **D.B. Nuzzio**

MONDAY MORNING

Section A

Renaissance Boston Waterfront
Pacific Blrm H

Addressing Challenges in Spectroscopy

G. Patonay, *Organizer*

A. G. Cavinato, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 ANYL **136.** Using optical re-injection integrated cavity output spectroscopy to make simultaneous, airborne measurements of ¹³CH₄ and CH₃D isotopologues. **J.P. Wilkerson**, C. Healy, D. Sayres, J. Anderson

9:25 ANYL **137.** Automating the optimization of chromatographic selectivity using mobile phase pH for LC-UV-MS. **A.B. Dlugasch**, T. Wheat, P.R. McConville

9:45 ANYL **138.** Chromatographic mobile phases for combining detection with mass and UV spectra. **A.B. Dlugasch**, P.R. McConville

10:05 ANYL **139.** Modeling and quantitative decoupling nanoparticle near- and far-field effects on fluorophore fluorescence in solutions. **D. Zhang**

10:25 ANYL **140.** Development of a high-power pulsed laser for a two-photon LIF detection of tropospheric OH. **R. Hannun**, J.B. Smith, M.F. Witinski, J. Anderson

Section B

Renaissance Boston Waterfront
Pacific Blrm F

Advances in Analytical Separations

J. L. MacLachlan, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **141.** Chemical analysis of electronic cigarettes using solid phase micro-extraction and needle trap device coupled to gas chromatography-mass spectrometry. **V. Niri**, G. Peterson, A. Donahoe

8:25 ANYL **142.** Integrated microscale liquid chromatography: A new technique for improved sensitivity and reduced sample consumption in LC/MS peptide analysis. **E.E. Chambers**, M.E. Lame, **M.S. Young**

8:45 ANYL **143.** Determination of haloacetic acids in drinking water using 2D ion chromatography. **C. Fisher**, R. Lin, L. Lopez

9:05 ANYL **144.** Challenging separation of highly polar and ionic compounds using graphitic stationary phases in coupling with MS detection. **C. Crescenzi**, M. Rodriguez, P. Russo, A. Lapi

9:25 ANYL **145.** Fast ion chromatography-ICP-QQQ for arsenic speciation. **B.P. Jackson**

9:45 ANYL **146.** Detection of ppb levels of arsenic in beers and wines. **J.N. Driscoll**, J.L. MacLachlan

10:05 Intermission.

10:20 ANYL **147.** Development of charged surface solid-core stationary phases for optimal separations of small basic compounds and peptides. **B. Okandeji**, C. Boissel, M. Lauber, K.D. Wyndham, T. Walter, B.A. Alden, S.J. Shiner, D.P. Walsh, J.T. Cook, J.N. Fairchild

10:40 ANYL **148.** Novel HPLC-MS method for the detection of phosphorylated mono- and di-saccharides. **C. Mathon**, G. Barding, C.K. Larive

11:00 ANYL **149.** Chromatographic and electrophoretic separation of C-dots nanoparticles. **L.A. Colon**, Z. Xue, K. Tirado-González, A.C. Borges-Muñoz

11:20 ANYL **150.** Application of computer-assisted automated method development tools for HPLC method development for various pharmaceutical samples. **S. Kumar**, J. Zhuang, P. Zhang, J. Huang, A. Rustum

11:40 ANYL **151.** Exploring an achiral and chiral cross-linker by molecular imprinting using chromatographic and batch rebinding techniques. **B. Hebert**, D. Meador, D. Spivak

12:00 Concluding Remarks.

Section C

Renaissance Boston Waterfront
Pacific Blrm G

Analytical Advances in Protein-DNA Thermodynamic Analysis

C. L. Baveghems, *Organizer, Presiding*

9:55 Introductory Remarks.

10:00 ANYL **152.** Toward benign, edible solar cells: Lessons from nature. **C.V. Kumar**

10:30 ANYL **153.** Withdrawn.

11:00 Intermission.

11:15 ANYL **154.** Induced fit and the entropy of structural adaptation in the complexation of CAP and lambda-repressor with cognate DNA sequences. **D.L. Beveridge**

11:45 ANYL **155.** Dynamics of proteins on single stranded DNA. **T.M. Lohman**

12:15 Concluding Remarks.

Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications

Sponsored by AGRO, Cosponsored by ANYL and ENVR

MONDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Pacific Blrm H

Addressing Challenges in Spectroscopy

A. G. Cavinato, *Organizer*

G. Patonay, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 ANYL **156.** Coupled UV-Vis/FT-NIR spectroscopy for in-situ analysis of multiple reaction steps during polymerizations. **H. Aguirre Soto**, J.W. Stansbury

2:25 ANYL **157.** New infrared library searching system for forensic automotive paint examination. **B.K. Lavine**, M.D. Allen, A. Weakley, M. Sandercock

2:45 ANYL **158.** Spectroscopic studies of near-infrared dye properties in confined spaces. **G. Patonay**, M. Henary, E. Lewis, G. Chapman

3:05 ANYL **159.** Correlation of IR spectra with thin film structure at solid-water interfaces. **K. Hinrichs**, A. Kroning, A. Furchner

3:25 ANYL **160.** Nitrogen Raman Spectroscopy as a tool for micro-scale pore size determination for carbon nanomaterials. **P. Ray**, L. Angela D., B. John V., V. Crespi, E. Xu

3:45 Intermission.

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4:00 ANYL 161. Use of an X-ray dispersion analyzer to study sedimentation patterns: Clay minerals as an example. G. Rytwo

4:20 ANYL 162. X-ray excited luminescent chemical imaging (XELCI): Non-invasively imaging pH on the surface of implanted medical devices. J.N. Anker, F. Wang, Y. Raval, T. Zeng

4:40 ANYL 163. Rapid screening of Ti and Zn in commercial sunscreens using portable X-ray fluorescence analyzer. V. Bairi, J. Lim, I.R. Quevedo, T. Mudalige, P. Howard, S. Linder

Section B

Renaissance Boston Waterfront
Pacific Blrm F

Advances in Analytical Separations

J. L. Maclachlan, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 ANYL 164. Analysis of metals at sub ppb levels by HG-GC-PID. J.N. Driscoll, J.L. Maclachlan

2:25 ANYL 165. General static-headspace gas chromatographic method for determination of residual ethylene oxide and other impurities in polyethylene glycols. J. Huang, A. Rustum

2:45 ANYL 166. High throughput headspace sampling system. B. Van Deren, T. Scherbert

3:05 ANYL 167. Monitoring ppt levels of BTEX with a field portable GC-PID. J.N. Driscoll, J.L. Maclachlan

3:25 ANYL 168. New portable electrochemical analyzer and ion chromatograph for simultaneous in-situ analysis of marine waters and sediments. D.B. Nuzzio, M. Taillefer, J. Becker

3:45 Intermission.

4:00 ANYL 169. Investigating the molecular contribution to adaptive coloration in cephalopods. S.F. Jones-Labadie, T. Williams, C. DiBona, M.A. Griswold, L.F. Deravi

4:20 ANYL 170. Development of phage-conjugated magnetic probes for bacterial separation. J. Chen, B. Duncan, L. Wang, V.M. Rotello, S.R. Nugen

4:40 ANYL 171. In-tube microextraction: Simplest possible headspace microextraction for capillary electrophoresis. S. Cho, D.S. Chung

5:00 Closing Remarks.

Section C

Renaissance Boston Waterfront
Pacific Blrm G

Analytical Advances in Protein-DNA Thermodynamic Analysis

C. L. Baveghems, *Organizer, Presiding*

1:30 ANYL 172. DNA-recognition by RcnR/CsoR repressor proteins — contributions of conformation and wrapping to high-affinity binding. P.T. Chivers

2:00 ANYL 173. Effect of pH on complex stability: Protein-DNA vs. protein-DNA. A.V. Onufriev

2:30 ANYL 174. Structure-based mechanisms of recognition and specificity in protein-DNA interactions. Y. Li, A. Moreno, V. Birdsall, V. Deng, J. Knee, M. Hingorani, I. Mukerji

3:00 Intermission.

3:15 ANYL 175. Nanoscale hydrodynamic study of proteins under thermal agitation and electrostatic field. Y. Zhang

3:30 ANYL 176. Artificial histone complexes: Cationized glucose oxidase as a DNA digital switch. C.L. Baveghems, C.V. Kumar

3:45 ANYL 177. Innovative advances in isothermal titration calorimetry (ITC). F. Wiebke

Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications

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Undergraduate Research Posters

Analytical Chemistry

Sponsored by CHED, Cosponsored by ANYL and SOCED

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

D. C. Duckworth, *Organizer*

8:00 - 10:00

40-41, 50, 53, 55, 60-61, 65, 67-68, 70, 73, 79-80, 86, 91, 101, 103, 106, 108, 115, 121-123, 125-126, 133. See previous listings.

TUESDAY MORNING

Section A

Renaissance Boston Waterfront
Atlantic Blrm 1

Innovations in Analytical Chemistry and Their Application to National Security and Forensics (CBRNE)

Analytical and Chemometric Methods for Chemical Attribution

H. Cho, J. R. Cort, C. Fraga, *Organizers*

D. Wunschel, *Presiding*

8:30 Introductory Remarks.

8:40 ANYL 178. Accomplishments and goals of DHS S&T Chemical Forensics Program. R. Bull

9:05 ANYL 179. Analyses at the Swedish Defence Research Agency of authentic CB-samples from national and international incidents. C. Astot, S. Fredriksson, R. Norlin, J. Rattfelt Nyholm, L. Rittfeldt, R. Magnusson, C. Nilsson

9:30 ANYL 180. Sourcing of sarin and nitrogen mustard chemical agents through impurity profiling and stable isotope ratios. C. Fraga, J.J. Moran, B.P. Dockendorff, K. Bronk

9:55 Intermission.

10:20 ANYL 181. Holding studies on crude samples of Russian VX for chemical attribution signature (CAS) determination. S. Hok

10:45 ANYL 182. Investigation of the organic and inorganic chemical attribution signatures of fentanyl. A. Vu, A. DeHope, A.M. Williams

11:10 ANYL 183. Identification of chemical signatures attributable to strychnine sources using chemometric predictive modeling of a fused GC-MS, LC-MS, ICP-MS, and FTIR dataset. M.W. Gardner, A.R. Smith, C.J. Krueger, T.E. Manley, M.A. Reaves

11:35 ANYL 184. Forensic signatures for source attribution of cyanides using impurity profiling, stable isotope ratios, and chemometrics. N. Mirjanek, C. Fraga

Section B

Renaissance Boston Waterfront
Pacific Blrm F

2015 ACS Analytical Division Award Symposium

S. J. Olesik, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 ANYL 185. Interfacing analytical and organic chemistry to create sensitive, selective, and simple point-of-need assays. S.T. Phillips

9:00 ANYL 186. Transdermal hydrogen sensing for monitoring biodegradable magnesium biomedical implants. W.R. Heineman, T. Wang, D. Zhao, Z. Dong

9:30 ANYL 187. EXCEL spreadsheets as platforms to teach so many things in analytical chemistry. P.K. Dasgupta, A.F. Kadjo

10:00 ANYL 188. Infrared matrix-assisted laser desorption electrospray ionization: From fundamentals to chemical and molecular imaging. D.C. Muddiman

10:30 ANYL 189. Bioelectrochemistry: Understanding the interface between the electrode and the biological milieu. G.S. Wilson

11:00 ANYL 190. Appearances can be deceiving: Spectrochemical analysis applied to contact lens-mediated ocular surface phenomena. F.V. Bright, I.J. Horner, J.J. Hurst, N.D. Kraut, J.F. Destino, C.M. Collado, G.E. Atilla-Gokcumen

11:30 Concluding Remarks.

Section C

Renaissance Boston Waterfront
Pacific Blrm G

Advanced Analytical Techniques for Early Cancer Screening

C. Burton, *Organizer*

Y. Ma, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 ANYL 191. Phenotyping of early stage ovarian cancer by mass spectrometry imaging and untargeted metabolomics. F.M. Fernandez, D. Gaul, C. Jones, M. Monge, M.R. Paine, L.Q. Tran, J.F. McDonald

9:00 ANYL 192. Serum metabolomics for detection of early stage ovarian cancer. T.A. Szyperki, K. Odunsi, E. Garcia, D. Sukumaran, V. Karambizi, T. Zinger, A. Yilmaz, R. Hageman Blair, J. Miecznikowski, M. Heiler, J. O'Brien

9:30 ANYL 193. Metformin acts to disrupt mitochondrial-associated metabolic homeostasis in human cancer. X. Liu, E. Lengyel, I. Romero, J.W. Locasale

10:00 Intermission.

10:15 ANYL 194. Metabolite profiling of the rat gut. C.K. Larive, M. Dinges, C. Lytle

10:45 ANYL 195. Discovery and development of a blood based protein signature to guide patient treatment decisions in Prostate Cancer. From analytical evaluation to potential clinical utility. S. Pennington

11:15 ANYL 196. Urinary pteridine detection and normalization for early cancer detection. Y. Ma, C.F. Burton, H. Shi

11:45 ANYL 197. Ultrasensitive diagnostic immunoarray platform for the assessment of aggressive vs non-aggressive forms of prostate cancer.

A. Joshi, M. Sharafeldin, B.A. Otieno, C. Krause, G. Bishop, C. Dixit, J. Rusling

12:05 Concluding Remarks.

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Sponsored by CHED, Cosponsored by ANYL, BIOL, BIOT, BMGT, CORP, DAC, ENFL, PHYS and POLY

Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis, and Ecological Effects

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TUESDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 1

Innovations in Analytical Chemistry and Their Application to National Security and Forensics (CBRNE)

Sampling, Detection, and Sourcing of Chemical and Biological Threat Agents

J. R. Cort, D. Wunschel, *Organizers*

C. Fraga, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 ANYL 198. Measurement of site-specific ¹³C/¹²C stable isotope ratios from ¹³C satellite peaks in 1H NMR spectra. J.R. Cort, H. Cho, P.A. Kempler, A.E. Metaxas, J.C. Schultz

2:05 ANYL 199. COTS products for the collection of chemical threat agents. E. Durnal, K. Brady

2:30 ANYL 200. Ricin forensic profiling approach based on complex sets of biomarkers. S. Fredriksson, D. Wunschel, S. Wiklund Lindstrom, C. Nilsson, K. Wahl, C. Astot

2:55 Intermission.

3:20 ANYL 201. Mass spectrometry-based methods for the analysis of protein toxins. J.R. Barr, S. Kalb, A.E. Boyer

3:45 ANYL 202. Strategies for the detection of biological toxins in food. S.A. Khan, W.L. Stutts, A.M. Knolhoff, T.R. Croley

4:10 ANYL 203. Proteomic characterization of *B. anthracis* spore biomass produced on laboratory and soil media. D. Wunschel

4:35 ANYL 204. Influence of long-term laboratory cultivation on protein expression by environmental isolates of *Yersinia pestis*. B. Kaiser, E. Merkle, O. Leiser, A. Lin, J. Foster, D. Wagner, P. Keim, H. Kreuzer

Section B

Renaissance Boston Waterfront
Pacific Blrm F

Micro and Nanoscale Innovations in Chromatography

S. J. Olesik, *Organizer, Presiding*

2:00 ANYL 205. Self-tuning nanogels for adaptable selectivity in biomolecule separations. L.A. Holland

2:30 ANYL 206. Microfluidic devices integrating solid-phase extraction, fluorescent labeling and electrophoresis. A. Woolley, S. Kumar, M. Sonker, V. Sahara, R. Knob

- 3:00 ANYL 207.** Quantitative analysis of drug-protein interactions by micro high performance affinity chromatography. **D. Suresh, Z. Li, D.S. Hage**
- 3:30 ANYL 208.** Sustainable chromatography and mass spectrometry using nanoscale materials. **S.J. Olesik, M. Beres, M.C. Beilke**
- 4:00 ANYL 209.** Acoustofluidic cell differentiation for diagnostic applications. **M.E. Piyasena, R. Gurung, G. Gautam, S. Cox**

Section C

Renaissance Boston Waterfront
Pacific Blrm G

Advanced Analytical Techniques for Early Cancer Screening

Y. Ma, *Organizer*

C. Burton, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 ANYL 210. Inkjet-printed gold nanoparticle sensors for ultrasensitive detection of parathyroid hormone related peptide (PTHrP) in breast cancer. **B.A. Otieno, C. Krause, B. Ochietti, R. Kremer, J. Rusling**

1:40 ANYL 211. Development of serum-based single molecule assays for the early detection of cancer. **S. Schubert, S. Baig, S.R. Walter, L. Arendt, M. Palacios, D.R. Wait**

2:00 ANYL 212. Noninvasive detection of cancer biomarkers using a new sampling device for exhaled breath analysis. **P. Benedetti, E. Guerriero, C. Crescenzi**

2:20 ANYL 213. Ultrasensitive microfluidic immunoarray for serum pro-inflammatory cytokines and C-reactive protein to assess oral mucositis risk in cancer patients. **B.A. Otieno, C. Krause, G. Bishop, L. Choquette, R. Lalla, D. Peterson, J. Rusling**

2:40 ANYL 214. PHOTON for real-time sensing and imaging of rare-subsets of single cancer stem cells in heterogeneous tumor cells. **X.N. Xu, P. Cherukuri, P. Songkiatissak, S. Warren, T. Huang**

3:00 Intermission.

3:15 ANYL 215. Detection of cancer biomarkers in serum using a hybrid mechanical and optoplasmonic nanosensor. **P.M. Kosaka, V. Pini, J. Ruz, R. da Silva, M. Ujue, D. Ramos, M. Calleja, J. Tamayo**

3:35 ANYL 216. Paper based chemiluminescence immunoPAD: Rapid detection of multiple cancer biomarker proteins using magnetic beads with automated sample processing. **C.K. Tang, A. Vaze, J. Rusling**

3:55 ANYL 217. Paper/PMMA hybrid microfluidic microplate for disease biomarker detection. **S. Sanjay, M. Dou, X. Li**

4:15 ANYL 218. Withdrawn.

4:35 Concluding Remarks.

Section D

Renaissance Boston Waterfront
Pacific Blrm H

ACS Award in Analytical Chemistry: Symposium in Honor of John R. Yates III

J. R. Yates, *Organizer*

C. E. Costello, *Presiding*

1:30 Introductory Remarks.

1:35 ANYL 219. High resolution analysis of receptor tyrosine kinase signaling networks. **F.M. White**

2:10 ANYL 220. Qualitative and quantitative determinations of disease-related post-translational modifications to proteins. **C.E. Costello, J. Zaia, C. Lin, M.E. McComb**

2:45 ANYL 221. Chemoproteomic interrogation of small molecule inhibitors in vivo. **J.A. Marto**

3:20 ANYL 222. Systematic exploration of the human interactome. **E.L. Huttlin, L. Ting, R. Bruckner, F. Gebreab, M. Gygi, J. Szpyt, S. Tam, G. Zarraga, G. Colby, K. Baltier, V. Guarani, L.P. Vaites, R. Rad, B.K. Erickson, R.A. Obar, T. Harris, S. Artavanis-Tsakonas, M.E. Sowa, J.A. Paulo, J.W. Harper, S.P. Gygi**

3:55 ANYL 223. Award Address (ACS Award in Analytical Chemistry sponsored by Battelle Memorial Institute). Using mass spectrometry to understand cystic fibrosis as a protein misfolding disease. **J.R. Yates, S. Pankow, C. Bamberger**

4:40 Concluding Remarks.

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Sponsored by CHED, Cosponsored by ANYL‡, BIOT‡, BMGT‡, CORP‡, DAC‡, ENFL‡, PHYS‡ and POLY‡

Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis, and Ecological Effects

Sponsored by AGRO, Cosponsored by ANYL and ENVR

Immunochemistry Summit XII: Immunoassays and Other Bioanalytical Techniques

Sponsored by AGRO, Cosponsored by ANYL, ENVR and SCHB

WEDNESDAY MORNING

Section A

Renaissance Boston Waterfront
Atlantic Blrm 1

Innovations in Analytical Chemistry and Their Application to National Security and Forensics (CBRNE)

New Methods in Detection and Analysis

H. Cho, D. Wunschel, *Organizers*

J. R. Cort, *Organizer, Presiding*

8:30 ANYL 224. Infrared imaging and multivariate curve resolution for the forensic examination of automotive paints. **B.K. Lavine, M.D. Allen, K. Nishikida, M. Sandercock**

8:50 ANYL 225. Strontium isotope ratios of hair for human provenancing. **B. Tipple, T. Chau, L. Chesson, J. Ehleringer**

9:10 ANYL 226. Real-time, ultrasensitive detection of RDX vapors using conjugated network polymer thin films. **W. Dichtel, D. Gopalakrishnan**

9:30 ANYL 227. Effect of environmental conditions on the stability of trace explosives. **M. Najjarro, E. Sisco, J. Lawrence**

9:50 ANYL 228. DHS Chemical Forensics Program — REACTS. **K. Brady, E. Durnal**

10:10 Intermission.

10:25 ANYL 229. Monitoring ppt levels of toxic contaminants with a field portable GC-PID. **J.N. Driscoll, J.L. Maclachlan**

10:45 ANYL 230. Biomarker analysis via bioaffinity cascades in forensic analysis. **J.M. Agudelo, C. Huynh, E.K. Brunelle, J. Halamek**

11:05 ANYL 231. Pairing glycopolymers and surface-enhanced Raman spectroscopy (SERS) for the detection of toxic lectins. **V. Szlag, M. Styles, A. Campos, D. Sprouse, B. Wagh, C.L. Haynes, T.M. Reineke**

11:25 ANYL 232. Development of a spectroscopy-based smart device for the rapid detection of organic molecules of environmental, health concern and security features interest. **A. Ghauch, A. Ammouri**

Section B

Renaissance Boston Waterfront
Pacific Blrm F

Nanotechnology for Analytical Sensing and Spectroscopy Based Applications SERS and Raman Spectroscopy

R. Narayanan, *Organizer*

J. S. Shumaker-Parry, *Presiding*

9:30 ANYL 233. Nanoparticle labeling strategies as tools for the early diagnosis of infectious disease. **M.D. Porter**

10:00 ANYL 234. Identifying uranium speciation in environmental samples using Raman and SERS. **G. Lu, T. Forbes, A. Haes**

10:30 ANYL 235. Tailored silicon nitride thin-films for optical and all-electronic chemical sensing. **B.I. Karawdeniya, Y. D. Y. Bandara, J. Whelan, C. Masterson, B. Velleco, J.R. Dwyer**

11:00 ANYL 236. Solution-based SERS method for detection of trace levels of pesticides. **R. Narayanan**

11:30 ANYL 237. Weak distance dependence in Raman enhancement of raspberry-like metamolecule dimers. **Z. Qian, S. Park, Z. Fakhraai**

12:00 ANYL 238. SERS metabolic profiling: A novel multiplexing platform for infectious disease diagnosis and cancer cell identification. **Y. Chen, R. Premasiri, L. Ziegler**

Section C

Renaissance Boston Waterfront
Pacific Blrm G

Analytical Advances in Mass Spectrometry

A. A. Shvartsburg, *Organizer, Presiding*

8:40 Introductory Remarks.

8:45 ANYL 239. Ion utilization efficiency: An effective way to compare different ESI-MS interfaces. **K. Tang**

9:10 ANYL 240. Atomic force microscope tip enhanced laser ablation mass spectrometry. **K.K. Murray, S. Ghorai, C.A. Seneviratne**

9:35 ANYL 241. Novel strategy for reduction of matrix effects of anionic compounds by paired ion electrospray ionization (PIESI) mass spectrometry. **H. Guo, Z.S. Breitbach, D.W. Armstrong**

10:00 ANYL 242. Development of surface acoustic wave nebulization as an ion source. **D.R. Goodlett**

10:25 Intermission.

10:40 ANYL 243. Development of an ion cyclotron resonance mass spectrometer array. **S. Park, G. Anderson, J.D. Chavez, J.E. Bruce**

11:05 ANYL 244. Strategies for the gas-phase oxidation of polypeptide ions to [M-H]⁺, [M+H+O]⁺, and M⁺⁺ cations via ion/ion reactions. **A. Pilo, J. Bu, S.A. Mcluckey**

11:30 ANYL 245. Combining old-school and state of the art techniques to mass spectral characterization of complex mixtures. **A.C. Stenson, T.A. Brown, C.B. Henderson, B. Bythell, B. Ruddy**

11:55 ANYL 246. Monoisotopic proteomics. **R. Zubarev**

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds

Sponsored by AGRO, Cosponsored by ANYL and ENVR

WEDNESDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 1

Open Air Analytical Measurements for Forensics, Health and Homeland Security

A. Hall, B. Musselman, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 ANYL 247. "Pick your Poison": Recent developments in the analysis of natural and "unnatural" drugs of abuse by DART-MS. **R.B. Cody, R. Musah, A. Lesiak, J. Shepard**

1:55 ANYL 248. Detecting drugs and chemical agents in biological samples by paper spray mass spectrometry: Applications and new developments. **N.E. Manicke, C. Zhang, B.J. Bills, R. Potter**

2:20 ANYL 249. Isobaric drug analysis using direct analysis in real time (DART) and hydrogen/deuterium exchange. **W.D. Hoffmann, G.P. Jackson**

2:45 ANYL 250. Evaluation of direct analysis in real time-time of flight mass spectrometry (DART-TOFMS) for the analysis of synthetic cathinones in oral fluid. **J.F. Morrison, H.S. Loring, K.M. Tully, B. Musselman**

3:10 Intermission.

3:25 ANYL 251. Screening for phosphodiesterase type 5 inhibitor (PDE-5) contaminants in herbal supplements and extracts using direct analysis in real time ambient ionization system. **B. Musselman, R. Goguen, J. Lapointe**

3:50 ANYL 252. High pressure handheld mass spectrometry. **K. Gregory**

4:15 ANYL 253. Combining molecular and atomic ambient ionization technologies for complete sample characterization. **K. Evans-Nguyen, A. Windom, S. Manoliakos, T. Evans-Nguyen**

4:40 ANYL 254. Ambient mass spectrometry with macro- and microplasmas. **F.M. Fernandez, J. Keelor, M.C. Bernier, K. Benham, T.M. Orlando, P.B. Farnsworth**

5:05 Concluding Remarks.

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Section B

Renaissance Boston Waterfront
Pacific Blrm F

Nanotechnology for Analytical Sensing and Spectroscopy Based Applications

Fluorescence and Luminescence

R. Narayanan, *Organizer, Presiding*

2:00 ANYL 255. Withdrawn.

2:30 ANYL 256. Chemiluminescence reagent/catalyst dual-functionalized graphene hybrids and their analytical applications. H. Cui, D. Liu, X. Liu, X. Yu, G. Li

3:00 ANYL 257. Ratiometric fluorescence transduction of nucleic acid hybridization on a paper-based platform using a digital camera and immobilized quantum dots as donors in fluorescence resonance energy transfer. O. Noor, U.J. Krull

3:30 ANYL 258. Nanoparticle supported ratiometric fluorescent indicators for polar organics based on non-covalently cross-linked molecular imprinting technology. R. Yang, C.J. Grenier, J. Csoros, W.R. Seitz

4:00 ANYL 259. One-tube fluorescence quantification of biological targets using structure switching aptamers. H. Kallewaard, K. Plaxco

4:30 ANYL 260. Innovative ratiometric fluorescent Cu(II) indicator based on the poly(N-isopropylacrylamide) phase transition. F. Wang, R. Ding, T. Williams, W.R. Seitz, R.P. Planalp, L. Nyranshuti, J. Massing

Section C

Renaissance Boston Waterfront
Pacific Blrm G

Analytical Advances in Mass Spectrometry

A. A. Shvartsburg, *Organizer, Presiding*

1:40 ANYL 261. Emerging approaches for the purification and tandem MS characterization of disease-related biopolymers. M.E. McComb, C. Lin, J. Zaia, C.E. Costello

2:05 ANYL 262. Conservation of ion mobility derived collisional cross section (CCS) values of ions using LC and GC TOF-MS. L. Mullin, G. Cleland, M. McCullagh

2:30 ANYL 263. Enabling large-scale discovery, characterization and quantitation of neuropeptides via tandem mass spectrometry. L. Li

2:55 ANYL 264. Shotgun proteomics of *Staphylococcus aureus* protein extracts towards MALDI-TOF MS-based *S. aureus* identification. B. Wex, D.B. Awad, S. Tokajian

3:20 Intermission.

3:35 ANYL 265. Determination of hormones in fish muscle tissue using APPI-LC-MS/MS. P. Chu, S. Sklenka

4:00 ANYL 266. Quantitative proteomics for understanding post-translationally modified proteins and proteomes. B. Garcia

4:25 ANYL 267. High throughput top-down proteomics for characterizing proteoforms with post-translational modifications. S. Wu

4:50 ANYL 268. Global analysis of N-sialoglycosylated proteins on the cell surface by integrating click chemistry and MS-based proteomics. R. Wu

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds

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THURSDAY MORNING

Section A

Renaissance Boston Waterfront
Atlantic Blrm 1

Challenges in Bioanalytical Chemistry

J. Wang, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 ANYL 269. Microtechnologies to interrogate signaling in single cells. N.L. Allbritton

9:00 ANYL 270. Quantifying protein expression in single cells. S.R. Walter, S. Schubert, M. Manesse, D.R. Walt

9:20 ANYL 271. Imaging the local tensors of collagen by nonlinear optical Stokes ellipsometric microscopy. X. You, E. DeWalt, P. Schmitt, G.J. Simpson

9:40 ANYL 272. Paramagnetic NMR probe to study RNA-protein binding. L.M. Seebald, C.M. DeMott, A. Shekhtman, M. Royzen

10:00 ANYL 273. Cholesterol Regulation of Granule Exocytosis in Platelets. S.A. Finkenstaedt-Quinn, S.M. Gruba, C.L. Haynes, S. Ge

10:20 Intermission.

10:35 ANYL 274. Collection and content analysis of tear film. S. Shippy, V. Avilov, Q. Zeng

10:55 ANYL 275. Characterizing cyclooxygenase oxidation of epoxyeicosatrienoic acids (EETs) by LC-QToF-MS and LC-MS/MS: An alternative lipid signaling pathway? A. Rand, T. Cajka, B. Barnych, S. Lee, O. Fiehn, B.D. Hammock

11:15 ANYL 276. Direct cell wall imaging by Scanning Transmission X-ray Microscopy (STXM) reveals leading role for lignin-modifying enzymes on ensuaging xylanases. R.E. Goacher, D. Jeremic, R. Yan, C. Karunakaran, E. Master

11:35 ANYL 277. Comparison of RP-HPLC methods to measure adenosine amounts in mouse brain. D.D. Smith, H. Roundtree, T. Simeone, K. Simeone

11:55 Concluding Remarks.

Section B

Renaissance Boston Waterfront
Pacific Blrm F

Nanotechnology for Analytical Sensing and Spectroscopy Based Applications

Biological Applications

R. Narayanan, *Organizer*

J. R. Dwyer, *Presiding*

9:00 ANYL 278. Direct aminoglycoside coated gold nanoparticles synthesis, Characterization and antibacterial susceptibility testing. S. Tockstein, T. Modi, R. Dakshinamurthy

9:30 ANYL 279. Optical sensing using DNA-encapsulated silver clusters. J.T. Petty, M. Ganguly, O. Sergev

10:00 ANYL 280. DNA-functionalized metal oxide nanoparticles as highly sensitive and selective biosensors for arsenate and hydrogen peroxide. J. Liu, B. Liu

10:30 ANYL 281. Diazonium functionalization of nanowire mechanical resonator biosensors for improved stability. W. Zheng, S. Evoy

11:00 ANYL 282. Beyond the detection limit of PCR: Direct quantification of BCR-ABL fusion gene using AFM force mapping. Y. Lee, J. Park

11:30 ANYL 283. Multipurpose application of Sacha inchi (*Plukenetia volubilis* L.) plant: Panacea from the Andean region. B. Kumar, L.H. Cumbal, A. Debut

Section C

Renaissance Boston Waterfront
Pacific Blrm G

New Developments and Applications of Electrochemistry

D. C. Duckworth, S. H. Pratt, *Organizers*

S. A. Bryan, *Presiding*

8:25 Introductory Remarks.

8:30 ANYL 284. Up-regulation of quorum sensing molecules for early and rapid electrochemical detection of bacterial pathogens. H.J. Sismaet, T.A. Webster, E.D. Goluch

8:50 ANYL 285. Engineering bacteriophages to develop electrochemical biosensors for bacterial pathogens. S.D. Alcaine, J. Chen, D. Wang, S.R. Nugen

9:10 ANYL 286. DNA Mikado: Effects of mismatches and DNA bending upon thermal hybridization behavior on gold electrodes. G. Flechsig, K. Biala, M. Mix

9:30 ANYL 287. Gold nanoparticle chemiresistor arrays for molecular sensing. E. Chow, B. Raguse, L. Wiczorek, K. Muller, J. Cooper, L. Hubble, A. Sosa Pintos

9:50 ANYL 288. Unusually high heterogeneous electron transfer activity of carbon nanotube-supported reduced graphene oxide. X. Mao, F. Guo, E. Yan, G.C. Rutledge, T. Hatton

10:10 ANYL 289. Investigation on the electrochemistry of atom-thick graphene nanoelectrode. H. Luo

10:30 Intermission.

10:45 ANYL 290. Paper-based electroanalytical devices for in situ and cell-based biosensing. L. Sun, X. Lin, H. Gu, N. Bao

11:05 ANYL 291. Nanoscale redox titrations for the quantification of surface photocatalytic intermediates at operating water-splitting photoanodes. B.H. Simpson, X. Zhou, Z. Gossage, J. Rodriguez Lopez

11:25 ANYL 292. Browser based electrochemical instruments. D.B. Nuzzio

11:45 ANYL 293. Trace detection of manganese using cathodic stripping voltammetry with an indium tin oxide working electrode coated with a charge selective polymer film. C.A. Rusinek, A.F. Bange, I. Papautsky, W.R. Heineman

THURSDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 1

Challenges in Bioanalytical Chemistry

J. Wang, *Organizer, Presiding*

1:55 Introductory Remarks.

2:00 ANYL 294. Sensitive and selective detection of point mutations using single molecule arrays. B.P. Regmi, M.R. Hartman, D.R. Walt

2:30 ANYL 295. Withdrawn.

2:45 ANYL 296. Rapid 2D and 3D imaging by Lissajous beam-scanning microscopy. J.A. Newman, S.Z. Sullivan, R. Muir, S. Sreehari, C.A. Bouman, G.J. Simpson

3:00 ANYL 297. Butyrylcholinesterase extraction efficiency comparison between protein-G agarose spin columns and protein-G magnetic beads. A. Indapurkar, P. Eangoor, J. Knaack

3:15 ANYL 298. Chemiluminescent labels released from long spacer arm-functionalized magnetic beads: A novel strategy for enhanced detection of nucleic acids. H. Yang, N. He, Z. Li

3:30 Intermission.

3:45 ANYL 299. Reversible and selective luminescent determination of ClO₂/H₂S redox cycle in vitro and in vivo. F. Liu, S. Sun

4:00 ANYL 300. Withdrawn.

4:15 ANYL 301. Optical multiplexed diagnostic platforms for small molecule analysis based on site-encoded DNA strategies. M. Marco

4:30 ANYL 302. Flexible protein polymerization enhances immunoassay signals. C. Chen, Y. Chu, H. Lin, J. Carey

4:45 ANYL 303. Magnetic beads-based chemiluminescent assay enables ultrasensitive quantification of microRNA. Z. Li, H. Yang, N. He

5:00 Concluding Remarks.

Section B

Renaissance Boston Waterfront
Pacific Blrm F

Nanotechnology for Analytical Sensing and Spectroscopy Based Applications

Other Sensing and Spectroscopy

R. Narayanan, *Organizer*

A. Haes, *Presiding*

1:30 ANYL 304. Aluminum plasmonic antennas based on a modified nanosphere template lithography process. J.S. Shumaker-Parry, M. Swartz, M. Rodriguez, S. Blair

2:00 ANYL 305. Analytical applications of ionic liquids and GUMBOS. I.M. Warner, N. Siraj, N. Speller, I. Galpotherdeniya

2:30 ANYL 306. Non-invasive implantable system based on core-shell microcapsules for glucose sensing. X. Xie, D.G. Anderson

3:00 ANYL 307. Naked-eye detection of a single foodborne pathogen using plasmonic colorimetry. M.N. Bui, A. Abbas

3:30 ANYL 308. Rapid, nanoscale chemiresistive vapor sensors. K. Fu, B. Willis

4:00 ANYL 309. Study of ligand-induced cell signaling through the use of dissipation monitoring of the QCM-D. J.Y. Chen, M. Garcia, L.S. Penn, J. Xi

4:30 ANYL 310. Withdrawn

Data to Decisions: Software Solutions for Modern Analytical Workflows

Sponsored by AGRO, Cosponsored by ANYL and ENVR

Structure Elucidation in Metabolism Studies: Plant, Animal, and Soil

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BIOT

Division of
Biochemical
TechnologyM. Lazzara and A. Kantardjiev,
Program Chairs

SUNDAY AFTERNOON

Innovation from Discovery To
Application Plenary SessionSponsored by MPPG, Cosponsored
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MONDAY MORNING

Innovation in Health and Medicine

Sponsored by MPPG, Cosponsored
by BIOL, BIOT, MEDI and TOXI

MONDAY AFTERNOON

Undergraduate Research Posters

Biotechnology

Sponsored by CHED, Cosponsored
by BIOT and SOCED

MONDAY EVENING

Chemical Innovation and Design (CID)
Talks: The Future of Innovation NowSponsored by MPPG, Cosponsored by AGFD,
AGRO, BIOT, MEDI, PMSE and SCHB

TUESDAY MORNING

Academic Innovations for Tomorrow's
Industries: GSSPC SymposiumSponsored by CHED, Cosponsored by
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DAC‡, ENFL‡, PHYS‡ and POLY‡

TUESDAY AFTERNOON

Academic Innovations for Tomorrow's
Industries: GSSPC SymposiumSponsored by CHED, Cosponsored by
ANYL‡, BIOT‡, BMGT‡, CORP‡,
DAC‡, ENFL‡, PHYS‡ and POLY‡

BIOL

Division of Biological
Chemistry

C. Crews and V. Bandarian, Program Chairs

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 253A

Young Investigator Symposium

C. M. Crews, Organizer, Presiding

9:00 BIOL 1. Examining the molecular recognition properties of MshB deacetylase. X. Huang, M. Hernick

9:20 BIOL 2. Photostick: A method for selective isolation of target cells from culture. M. Chien, A.E. Cohen

9:40 BIOL 3. Molecular characterization of the blood brain barrier tight junctions. S. Nangia, F. Irudayanathan

10:00 BIOL 4. Computational and metabolomics methods to aid the chemical biologist. J.S. Freundlich

10:20 BIOL 5. Inhibiting loop-mediated protein-protein interactions. J. Kritzer

10:40 BIOL 6. Computational chemist's perspective on challenges in predicting structure-function relationships in catechol O-methyltransferase. H.J. Kulik

11:00 BIOL 7. Ligand gated split-small GTPases. J. Zhao, T.J. Nelson, C.I. Stains

11:20 BIOL 8. Integrated biophysical approaches to determine structures of the steroid receptor activator lncRNA ribonucleoprotein complexes. T. Leeper, J.A. Caporoso, S.M. Bilinovich, S. Christie, L. Ray, D. Morris, G.J. Buchan

11:40 BIOL 9. Mammalian genetic code expansion: For and by viruses. A. Chatterjee, R. Kelemen, Y. Zheng

Advances in Oligonucleotide
TherapeuticsSponsored by CARB, Cosponsored
by BIOL, MEDI and ORGN

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253A

Pfizer Award in Enzyme Chemistry

D. Mitchell, Organizer, Presiding

1:00 BIOL 10. Activity-based proteomics: Applications for enzyme and inhibitor discovery. B.F. Cravatt

1:45 BIOL 11. Study of unique adenylating enzymes during nonribosomal peptide biosynthesis. S. Garneau-Tsodikova

2:30 BIOL 12. Culture independent approaches for the discovery of new bacterial metabolites. S.F. Brady

3:15 BIOL 13. H-NOX domains: Versatile gas sensors from bacteria to humans. M.A. Marletta

4:00 BIOL 14. Peptide heterocyclization: The defining modification for an emerging natural product class. D. Mitchell

Advances in Oligonucleotide
TherapeuticsSponsored by CARB, Cosponsored
by BIOL, MEDI and ORGN

SUNDAY EVENING

Section A

Seaport Hotel and World Trade Center
Cityview Blrm

Current Topics in Biological Chemistry

V. Bandarian, Organizer

5:30 - 7:30

BIOL 15. Rationally designed protein domain mimics to inhibit recalcitrant protein-protein interactions. A. Modell, D. Rooklin, Y. Zhang, P. Arora

BIOL 16. Expanded genetic systems deliver DNA aptamers against hepatocellular carcinoma cells. L. Zhang

BIOL 17. Effects of mercury, a metalloestrogen, on breast cancer progression. H. Gaudet, E. Christensen, S.N. Morrow, B. Conn

BIOL 18. Spatial and temporal control of protein localization in living cells using chemical dimerizers. C. Aonbangkhen, E. Ballister, A.M. Mayo, M. Lampson, D. Chenoweth

BIOL 19. Small molecule drug conjugates targeted to cholecystokinin 2 receptor. J. Roy, C. Wayua, P. Low

BIOL 20. Curcumin binds to the pre-fibrillar aggregates of Cu/Zn superoxide dismutase (SOD1) and alters its amyloidogenic pathway resulting in reduced cytotoxicity. N.K. Bhatia, S. Deep

BIOL 21. Recombinant expression of a functional myo-inositol 1-phosphate synthase (MIPS) in *Mycobacterium smegmatis*. X. Huang, M. Hernick

BIOL 22. Identity of cofactor bound to mycothiol conjugate amidase (Mca) is influenced by expression and purification conditions. E. Kocabas, H. Liu, M. Hernick

BIOL 23. Versatility of acyl-acyl carrier protein synthetases for in vitro and in vivo labelling of the acyl carrier protein. K. Finzel, J. Beld, M.D. Burkart

BIOL 24. Sequence-independent ssDNA relieves phospholamban inhibition of SERCA in a length dependent manner. K. Soller, R. Verardi, N. Arbol, S. Robia, M. Bowser, G. Veglia

BIOL 25. Light-activated azide ligation within living animals. L. Shah, S.T. Laughlin, I.S. Carrico

BIOL 26. Photoactivatable prodrugs of kinase inhibitor vemurafenib. B. Pinchuk, R. Horbert, D. Alessi, P. Davies, C. Peifer

BIOL 27. Viscoelastic behavior of aggrecan-hyaluronic acid complexes. W. Oh, F. Horkay

BIOL 28. Withdrawn.

BIOL 29. Investigation into the effect of glutamate ligands on the metal site of the *E. coli* transcriptional regulator, RcnR. C.E. Carr, F. Musiani, S.L. Ciurli, M.J. Maroney

BIOL 30. Novel luminescence-based assay for deubiquitinases inhibitors discovery. X. Wang, W. Liu

BIOL 31. Probing the catalytic charge relay system in alanine racemase enzyme with genetically encoded histidine mimetics. V. Sharma, Y. Wang, W. Liu

BIOL 32. Anticancer potential of noval ferrocene based thioamides: Synthesis, modal studies, and cell line investigations. A. Altaf, A. Badshah, D.C. Crans, B. Lal, S. Ullah

BIOL 33. Withdrawn.

BIOL 34. Withdrawn.

BIOL 35. Arsenic based receptors for cysteine peptides. X. Liang

BIOL 36. Effects of alginate oligosaccharide mixture on the bioavailability of lysozyme as an antimicrobial agent. H. Park, R. Park, Y. Kim, J. Min

BIOL 37. Fluorescent mechanism-based probes for aerobic flavin-dependent enzyme activity. I. McCulloch, J. La Clair, M.J. Jaremenko, M.D. Burkart

BIOL 38. Redirecting small molecules for malaria: Inhibitors of enoyl-ACP reductase for *Plasmodium falciparum* (PfENR). L. Tallorin, J.D. Durrant, Q.G. Nguyen, J.A. McCammon, M.D. Burkart

BIOL 39. Structural basis for high affinity antibody recognition of an intracellular target. H. Ng

BIOL 40. Investigation of the chemical mechanism and inhibition of microsomal prostaglandin E₂ synthase 1 (MPGES1). M. Goodman, R.N. Armstrong

BIOL 41. Structure determination and RNA binding properties of SHARP. J.A. Caporoso, C. Davis, S.M. Bilinovich, L. Ray, S. Christie, S. Balaratnam, M. Anderson, S. Basu, T. Leeper

BIOL 42. Examining liposome association and small molecule inhibition of fatty acid amide hydrolase (FAAH) by hydrogen/deuterium exchange mass spectrometry. B. Kochert, A. Makriyannis, J. Engen

BIOL 43. Study of serum cytokine responses to influenza vaccine via single molecular array based assay. D. Wu, T. Dinh, D.R. Walt

BIOL 44. Role of a guanidinium cation-phosphodianion pair in the transition state stabilization of glycerol 3-phosphate dehydrogenase-catalyzed hydride transfer. A.C. Reyes, A. Koudelka, T.L. Amyes, J.P. Richard

BIOL 45. Synthesizing biologically relevant phosphoanhydrides and analogs by chemoselective coupling of phosphoramidites with phosphates. A. Hofer, G.S. Cremosnik, H. Jessen

BIOL 46. Biochemical and biophysical characterization of AzoC, a novel azoreductase from *Clostridium perfringens*. J. Morrison, G.H. John

BIOL 47. Characterization of DhpH-C, a tRNA-dependent enzyme in dehydrophos biosynthesis. E.C. Ulrich, D.J. Bougioukou, W.A. van der Donk

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- BIOL 48.** Antimicrobial and collagen-binding activities of recombinant LL37 peptide for wound healing applications. **L.D. Lozeau**, D. Kole, T. Dominko, M.W. Rolle, T.A. Camesano
- BIOL 49.** Acrylamide warheads for targeted drug design against bacterial glutaredoxins. **D. Morris**, R.B. Khattri, S. Bilinovich, T. Leeper
- BIOL 50.** Development of triptycene-based nucleic acid junction binders. **S. Barros**, D.M. Chenoweth
- BIOL 51.** Assessing the role of protein flexibility in *Helicobacter pylori* HypA nickel delivery. **P. Basak**, R. Kurian, M. Maroney
- BIOL 52.** Internal dynamics of methylcytosine binding domains in the presence of DNA. **S.M. Bilinovich**, D.C. Williams
- BIOL 53.** In vivo quantification of MMP-13 using molecular beacon to realize early, sensitive, and long-lasting arthritis diagnosis. **H. Yu**, Y. Chen, B. Vorrius, E. Darling, Q. Chen
- BIOL 54.** Withdrawn.
- BIOL 55.** Structure and aromatic substrate sequestration in the pyruvate kinase peptidyl carrier protein PtlL. **M.J. Jaremkó**, D. Lee, M.D. Burkart
- BIOL 56.** Design and development of gemcitabine-loaded liposomes for the treatment of pancreatic cancer. **C. Tsiros**
- BIOL 57.** Withdrawn.
- BIOL 58.** Two faces of Pal: Elucidating the two orientations of Pal protein in *E. coli*. **B. D'Arcy**, J. Shaw, M. Pichichero, L. Vacca Michel
- BIOL 59.** Protein-DNA interactions in malfunctioned transcription by molecular dynamic simulations. **A. Sebastian**, **J. An**, D. Xiao, J. Lu
- BIOL 60.** Supramolecular organization of cartilage extracellular matrix. **F. Horkay**, I. Horkay-Szakaly, E. Dimitriadis, P.J. Bassler
- BIOL 61.** Concepts in bioconjugate design for the development of immunological assays with heightened sensitivity and specificity. **A. Johnson**, R. Whipkey, T. Goddard, B. Parker
- BIOL 62.** Crystal contact deletion enables recoverin to crystallize with a calcium ion bound in EF-hands 2 and 3. **R.P. Kumar**, M.J. Ranaghan, A. Ganjei, D.D. Oprian
- BIOL 63.** Investigating enzymatic resistance to fosfomycin by FosB in Gram-positive bacteria. **M.E. Keithly**, M.K. Thompson, D.F. Stec, J. Harp, R.N. Armstrong
- BIOL 64.** HypA: *Helicobacter pylori*'s nickel traffic cop? **H.Q. Hu**, R.C. Johnson, D.S. Merrell, S.S. Pochapsky, T.C. Pochapsky, O. Dobrovolska, S.L. Ciurli, M.J. Maroney
- BIOL 65.** Targeting a "hot loop" in the oncogenic Skp2-Cks1 protein-protein interaction with cyclic peptide inhibitors. **K. Keenan**, S.K. Choudary, J. Kritzer
- BIOL 66.** In situ detection of hepatitis B virus genotype B with G1896A mutation using single base extension approach based on magnetic nanoparticles. **M. Xianbo**, Z. Ali, L. Taotao, T. Yongjun, H. Nongyue
- BIOL 67.** Synthesis and screening of antimicrobial peptoid combinatorial libraries against genera *Aspergillus*, *Candida*, and *Cryptococcus*. **A. Corson**, K. Fisher, K. Bicker
- BIOL 68.** Fast chelators and fluorescent sensors reveal a functional role for mobile zinc in the olfactory bulb. **J.M. Goldberg**, Y. Gao, I.G. Davison, S.J. Lippard
- BIOL 69.** Selective inhibition of MG-63 osteosarcoma cell proliferation induced by curcumin-loaded self-assembled arginine-rich-RGD nanoparticles. **K. Chang**, L. Sun, T. Webster
- BIOL 70.** Targeting cancer cells with virus-like particles for prodrug therapy. **S.N. Crooke**, A. Abid, N. Rohner, S. Thomas, M.G. Finn
- BIOL 71.** Locating the estradiol binding pocket for the G-protein coupled estrogen receptor (GPER). **A.R. Vidad**, S. Macaspac, H. Ng
- BIOL 72.** Yeast three-hybrid system for evolving a copper "clickase" enzyme. **L. Zhao**, D.F. Doyle, M.G. Finn
- BIOL 73.** Aldehyde capture ligation for synthesis of native peptide bonds. **H. Wu**, M. Raj, P. Arora
- BIOL 74.** Development of a colorimetric and fluorescent probe for continuous, real-time detection of histone deacetylase activity. **D.R. Rooker**, D. Buccella
- BIOL 75.** Photocaged diphosphoinositol pentakisphosphate: Synthesis, photochemical release, and cellular delivery. **I. Pavlovic**, D.T. Thakor, H. Jessen
- BIOL 76.** Investigation of homologous, fungal HR-PKS gene clusters, *P. oxa*. **S95** and *T. vir*. **S6**. **L. Hang**, M. Tang, Y. Tang
- BIOL 77.** Development of cysteine-targeted mass spectrometry platforms for the targeting of selenoproteins and the mitochondrial proteome: Enrichment of low abundance protein sets. **D. Bak**, E. Weerapana
- BIOL 78.** Identification, characterization, and quantitative analysis of DNA-protein cross-links induced by phosphoramidate mustard. **A. Groehler**, N.Y. Tretyakova
- BIOL 79.** Structural and functional characterization of histidine triad nucleotide binding protein 1 mutants associated with inherited peripheral neuropathy. **R. Shah**, K.M. Maize, B. Fintel, C.R. Wagner
- BIOL 80.** Heme peripheral groups interactions in proteins and the role of the dielectric constant of the medium. **J. Cerda**, A. Stockhausen, N. Wilkes, A. Langley, K. Silva
- BIOL 81.** Investigating the structure and function of PptT and PptII, phosphopantetheinyl transferases from *M. tuberculosis* and *M. ulcerans*. **C. Vickery**, N. Kosa, E. Casavant, S. duan, J. Noel, M.D. Burkart
- BIOL 82.** Soil contaminant treatment using *Corynebacterium glutamicum* coated with NH₂-functionalized silica-encapsulated Fe₃O₄ nanoparticles. **B. Kim**, T. Le, Y. Kim, J. Min
- BIOL 83.** Stimulated collagen production by complex materials of cell organelles, lysosomes with alginate oligosaccharides. **R. Park**, Y. Kim, J. Min
- BIOL 84.** Enhanced antimicrobial ability of lysosomes based on overexpression of species-recognition peptides on yeast vacuolar outer membrane. **L. Tran**, **B. Kim**, Y. Kim, J. Min
- BIOL 85.** Probing the molecular interactions of bovine gamma B crystallins using NMR spectroscopy. **K.L. Mathews**, A. Payan, D. Barnard, J. Mills, G. Thurston, L. Vacca Michel
- BIOL 86.** Elucidating the two orientations of vaccine candidate P6 from nontypeable *Haemophilus influenzae*. **B. Kisselstein**, C. Reulbach, J. Shaul, M. Pichichero, L. Vacca Michel
- BIOL 87.** Antibacterial activity of dextran-coated nanoceria at various pH values. **H. Yazici**, E. Alpaslan, t. webster
- BIOL 88.** Graphene oxide-modified titanate nanowire scaffolds: Structural, mechanical, and biological properties. **W. Dong**, **L. Hou**, H. Huang, C. Wang, X. Chen, Y. Zheng, G. Wang, R.J. Linhardt
- BIOL 89.** Effect of cholesterol on the interaction between the antimicrobial peptide jelleine-I and binary lipid mixtures. **J. De Schutter**, A. Sunda-Meya, N. Phambu
- BIOL 90.** Heterologous construction of the lasso peptide, lariatin **A. A. Adeniji-Adele**, J.W. Tomsho
- BIOL 91.** Development of small molecule inhibitors of carbohydrate acetyl transferases from human pathogens: New tools to investigate the roles of protein N-glycosylation in bacterial virulence. **J. De Schutter**, C.Y. Zamora, B. Imperiali
- BIOL 92.** Metabolic synthesis of clickable glutathione for chemoselective detection of glutathionylation. **K.T. Samarasinghe**
- BIOL 93.** Conformational changes in feleucin induced by sphingomyelin-containing model membranes. **A. Alshammari**, A. Sunda-Meya, **N. Phambu**
- BIOL 94.** Heparan sulfate signaling directs repair of pulmonary epithelium after lung injury. **M.A. Sufliya**, S. Haeger, X. Sun, E. Schmidt, R.J. Linhardt
- BIOL 95.** Computational models of the chemical evolution of complex metabolic systems. **P.M. Schwartz**, J.M. Kubala, R.S. Doyle, C. Barratt
- BIOL 96.** Biochemical and structural characterization of (4R)-limonene synthase cloned from *Citrus sinensis*. **B.R. Morehouse**, R.P. Kumar, J.O. Matos, K. Malik, D.D. Oprian
- BIOL 97.** Probing Influenza NS1A homodimerization as a target for therapeutic intervention. **D. Rushmore**, J.W. Tomsho
- BIOL 98.** Triazole-based fluorescent probes: Clickable tools for targeted ratiometric detection of Mg²⁺ in intracellular compartments. **G. Zhang**, M. Afzal, J.J. Gruskos, D. Buccella
- BIOL 99.** Unnatural amino acids with enhanced reactivity for in vivo covalent chemical capture. **C.M. Joiner**, M. Breen, A.K. Mapp
- BIOL 100.** Generic approach to purify recombinant proteins from *E. coli* using MBP and silica-binding peptides. **S. Raran-Kurussi**
- BIOL 101.** Determination of the protein-DNA interface in the metallo-regulator, RcnR. **H. Huang**, C. Bobst, I.A. Kaltashov, M.J. Maroney
- BIOL 102.** Nature of the low catalytic activity of monomeric mutants of triose-phosphate isomerase. **E.V. Contreras**, R.M. Bastida-Santoyo, M.E. Chanez-Cardenas

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 253A

Gordon Hammes Award Lecture

F. M. Rauschel, *Organizer, Presiding*

8:30 BIOL 103. Structural/functional studies of *N*-formyltransferases from pathogenic bacteria. **H. Holden**

9:15 BIOL 104. RNA goes platinum: Metals, catalysis, and drugs. **V. DeRose**, M.M. Haley, J.D. White, A.D. Moghaddam, R. Cunningham, R. Wirth, K. Plakos

10:00 BIOL 105. New oxidative pathway for enzymatic cleavage of phosphate CP bonds. **J. Seguin**, F. McSorley, L. van Staalduin, K. Pallitsch, M. Vogt, F. Hammerschmidt, Z. Jia, D.L. Zechel

10:45 BIOL 106. Finding homes for orphan enzymes. **F.M. Rauschel**

Biochemical Bioprocesses: Discovery and Regulation of New and Potential Products

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MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253A

Repligen Award for the Chemistry of Biological Processes

J. S. Blanchard, *Organizer, Presiding*

1:00 BIOL 107. Cell wall biosynthesis and its inhibition. **S. Walker**

1:50 BIOL 108. Antimicrobials to combat drug tolerance and resistance. **K. Lewis**

2:40 BIOL 109. Biological chemistry of chlamydial pathogenesis. **D.G. McCafferty**

3:30 BIOL 110. Tuberculosis: Searching for an Achilles heel. **J.S. Blanchard**

Biochemical Bioprocesses: Discovery and Regulation of New and Potential Products

Sponsored by AGRO, Cosponsored by BIOL

Metabolites from Endophytic Microorganism to Combat Biotic Stress in Crop Plants

Sponsored by AGRO, Cosponsored by BIOL

Undergraduate Research Posters

Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

V. Bandarian, C. M. Crews, *Organizers*

8:00 - 10:00

2, 9, 18, 25-26, 70, 72, 100. See previous listings.

142, 147, 157, 161, 165, 171, 188, 213, 220, 225. See subsequent listings.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 253A

Chemical Biology Approaches to Probe Ubiquitin-like Signaling

J. Schneekloth, *Organizer, Presiding*

- 8:30** BIOL **111.** Exploiting protein homeostasis for cancer therapy. R. Deshaies, J. Li
- 9:00** BIOL **112.** Small molecule antagonists of the deubiquitinase USP7 interfere with ubiquitin binding. I.E. Wertz
- 9:30** BIOL **113.** Investigating deubiquitination with DUB-specific probes. Z. Zhuang
- 10:00** BIOL **114.** Understanding how deubiquitinases catalyze isopeptide bond cleavage. E.R. Strieter, L. Anderson
- 10:30** BIOL **115.** Selective inhibition of deubiquitinating enzyme USP14. D. Finley

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

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TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253A

Innovative Platforms for Drug Discovery, Diagnostics & Target Validation

M. S. Bogoy, *Organizer, Presiding*

- 2:30** BIOL **121.** Novel mechanism of action (nMoA) compounds in therapeutics discovery. S.L. Schreiber
- 3:15** BIOL **122.** Chemoproteomics and activity-based profiling as research tools for drug discovery at Genentech. J.R. Lill
- 4:00** BIOL **123.** Integrating chemistry and evolution to enable next-generation therapeutics. D.R. Liu
- 4:45** BIOL **124.** New chemical probe technologies for diagnostic and intra-operative imaging applications. L.O. Ofori, N. Withana, M. Verdoes, J. Sorger, M.S. Bogoy

Section A

Boston Convention & Exhibition Center
Room 253A

Young Investigator Symposium

C. M. Crews, *Organizer, Presiding*

- 12:30** BIOL **116.** Discovery and improvement of covalent influenza neuraminidase inhibitors. C. Vavricka, C. Muto, M. Izumi, H. Kiyota
- 12:50** BIOL **117.** Elucidating the influences of the host's proteostasis network on HIV-1 adaptation and evolution. E.E. Nekongo, M.B. Dewal, M. Shoulders
- 1:10** BIOL **118.** Directed evolution of substrates for enzymatic generation of unnatural protein side-chains. J. Jaworski
- 1:30** BIOL **119.** Mechanistic and structural analysis of substrate recognition by prolyl 4-hydroxylase from *Bacillus anthracis*. M. Dey
- 1:50** BIOL **120.** Extended series of proximal and distal hydrogen bonds underpins RhoA catalyzed GTP hydrolysis via a strain-free transition state. R. Molt, Y. Jin, E. Pellegrini, M.W. Bowler, N.G. Richards, G. Blackburn, J.P. Waltho

TUESDAY EVENING

Section A

Westin Boston Waterfront
Galleria

Current Topics in Biological Chemistry

V. Bandarian, *Organizer*

6:00 - 8:00

- BIOL **125.** Glycosylated enzymes in the production of bioengineered heparin. J. Englaender, A.N. Shirke, R.A. Gross, M. Koffas, R.J. Linhardt
- BIOL **126.** Urate hydroperoxide as a pro-oxidant intermediate generated by urate oxidation in inflammatory and photo-induced processes. E.d. Patricio, M.V. Prates, F.M. Prado, T. Dadamos, L. Anastácio da Costa Carvalho, M. Bertotti, P. Di Mascio, A. J. Kettle, F. Carla Meotti
- BIOL **127.** Enzymology at single molecule resolution. P. Mogalsetti, M. Rojek, D.R. Walt
- BIOL **128.** Synthesis of DNA duplexes containing a covalent, but thermally reversible, interstrand cross-link at a single site. J. Gamboa Varela, K.S. Gates
- BIOL **129.** Site-specific radio-labeling of proteins for immuno-PET imaging. M. Rashidian, H. Ploegh
- BIOL **130.** Withdrawn.
- BIOL **131.** Microbial production of chondroitin sulfate. W. He, M. Koffas, R.J. Linhardt
- BIOL **132.** Semisynthetic strategy leads to alteration of the backbone amidate ligand in the NiSOD active site. J. Campecino, M.J. Maroney
- BIOL **133.** Engineering D-glucuronyl C5-epimerase for increased enzyme solubility and activity. D. Vaidyanathan, E.E. Paskaleva, G.I. Makhatazde, J.S. Dordick, R.J. Linhardt
- BIOL **134.** Investigating the role of the protein disulfide isomerase (PDI) family in cancer. T.J. Bechtel, K.S. Cole, N.J. Pace, R. Banerjee, E. Weerapana
- BIOL **135.** Changes in fruit quality and yield of tomato grown in greenhouse under deficit irrigation and reduced nitrogen application. J. Zhang
- BIOL **136.** Large scale structural rearrangement provides dual control over the catalytic and membrane binding activity of a bacterial serine hydrolase. R. Johnson, M. Smith
- BIOL **137.** FRET-based assay to screen for antagonists of hedgehog cholesterol synthesis. T. Owen, G. Ngoje, B.P. Callahan
- BIOL **138.** Chemoenzymatic synthesis of bioengineered heparin. L. Fu, M.A. Sufilita, A. Onishi, J. Englaender, B.F. Cress, F. Zhang, J.S. Dordick, R.J. Linhardt
- BIOL **139.** Fragment-based drug discovery targeting KEAP1/Nrf2 binding. M. Zhong, A. Lynch, S. Jehle, L. Luo, D. Kozakov, A. Whitty, K.N. Allen, S. Vajda
- BIOL **140.** NagD from *Yersinia pestis*, a homolog to NagD UMPase from *E. coli*. L. Dass, I. Moreno, S.F. O'Handley
- BIOL **141.** Phosphoglycolate phosphatase virulence factor from *Staphylococcus aureus*. I. Moreno, L. Dass, S.A. Ramirez, J. Hill, K. Blake, J. Thomson, S.F. O'Handley
- BIOL **142.** Development of a platform for continuous directed evolution in human cells. C. Berman, L. Papa, C.L. Moore
- BIOL **143.** Hydrocarbon stapled tryptophan and arginine-rich antimicrobial peptides may act through a membrane-disruptive mechanism. Z. Jenner, M. Gonzalez, K.A. Bruns
- BIOL **144.** Anaerobic benzoyl-CoA aromatic ring reduction by BamB-I — computational mechanistic study. M. Culka, M. Ullmann
- BIOL **145.** Phytochelatin synthase: A computational study of a papain-like enzyme involved in heavy metal detoxification. F. Gisdon, M. Ullmann
- BIOL **146.** Biochemical verification of computational prediction of a spatially extended active site for ornithine transcarbamoylase. L. Ngu, K.E. Ramos, N. DeLateur, P.J. Beuning, M. Ondrechen
- BIOL **147.** Reprogramming caspase activity by directed evolution provides alternate solutions for substrate recognition. D.J. MacPherson, M. Hill, P. Wu, O. Julien, J.A. Wells, J.A. Hardy
- BIOL **148.** Exploiting multivalency for potent bacteria labeling via iminoboronate chemistry. K. McCarthy, J. Gao
- BIOL **149.** Structure of OXA-51, the native carbapenemase of *Acinetobacter baumannii*, reveals insights into gain-of-function clinical variants. C.M. June, K. Sugg, R.A. Powers, D. Leonard
- BIOL **150.** Targetable, reaction-based small molecule-protein hybrid sensors for detecting mobile zinc. M.L. Zastrow, R.J. Radford, Z. Huang, S.J. Lippard
- BIOL **151.** Identification of the first small molecule inhibitor of DisA, a c-di-AMP synthase, from a 1000 compound library, using the coralyne assay. Y. Zheng, J. Zhou, D.A. Sayre, H.O. Sintim
- BIOL **152.** Fragment-based drug design approach to identify selective binders for orthologous proteins utilizing nuclear magnetic resonance spectroscopy. R.B. Khattri, D. Morris, C. Davis, S. Bilinovich, K. Napper, A. Defabio, T. Leeper
- BIOL **153.** Global substrate specificity of serine hydrolases in *Mycobacterium smegmatis*. B. Bassett, R. Johnson
- BIOL **154.** Simultaneous determination of AICAR and AICA-ribotide, its mono-phosphate metabolite, by LC-MS/MS. A. Brown
- BIOL **155.** Prediction and verification of the extended active site in *E. coli* DNA Polymerase III. T. Coulther, R. Parasuram, M. Ondrechen, P.J. Beuning
- BIOL **156.** Unveiling novel enzyme functions by molecular mining: A case study on methyltransferases. H. Chiu, S. Huang
- BIOL **157.** *Pyrococcus furiosus* prolyl oligopeptidase: A versatile and robust scaffold for the development of artificial metalloenzymes. K. Ellis-Guardiola, P. Srivastava, H. Yang
- BIOL **158.** Evaluation of the performance of an exponential-fed perfusion culture of *E. coli* DH5 α -NH36 for pDNA vaccines production using flow cytometry and real-time PCR. A. Garcia-Rendon, R. Munguia-Soto, A. Tejada-Mansir, A. Garibay-Escobar
- BIOL **159.** Triple-substitution clinical variant of the OXA-23 carbapenemase form *Acinetobacter baumannii* shows increased activity toward cephalosporins and aztreonam. T.M. Harper, C.M. June, R.A. Powers, D. Leonard
- BIOL **160.** Synthesis of glutathione analogs to investigate the mechanism of glutathione-dependent enzymes. O. Kempf, K. Kempf, R. Schobert, M. Ullmann, E. Bombarda
- BIOL **161.** Fabrication of multivalent protein probes for molecular analysis of label-free microRNAs. L. Jeongmin
- BIOL **162.** Re-design of calmodulin as a lead sensor. M.P. Takacs, I.V. Korendovych

BIOL **163.** Phenotypic and complementation studies of PHO13 activity in *Saccharomyces cerevisiae*. C. Kellogg, K. Blake, S.F. O'Handley, A.U. Gehret

BIOL **164.** Identification of Eg5 as a cellular substrate of HDAC1 using substrate trapping mutants. D.A. Nalawansa

BIOL **165.** Single mutations in a non-enzymatic protein give rise to various catalytic activities. T. Dunston, O. Makhlynets, O. Moroz, Y. Moroz, K. Mack, Y. Wu, P. Gosavi, J. Yoon, N. van Nuland, I.V. Korendovych

BIOL **166.** Biochemical investigation of the histone lysine methyltransferase PRDM2. E.M. Kolonko, O.E. Oluwo, S.M. Fitzpatrick, M.E. Tabatneck, N. Mansouri

BIOL **167.** Structural and energetic impact of non-natural 7-deaza-8-azaadenine and its 7-substituted derivatives on H-bond pairing potential with uracil in RNA molecules. M. Chawla, R. Credendino, R. Oliva, L. Cavallo

BIOL **168.** Structure determination of SHARP RRM1 and the binding site determination of the SHARP RRM1- SRA1 RNA ribonucleoprotein complex using NMR. C. Davis, J.A. Caporoso, S.M. Bilinovich, L. Ray, S. Balaratnam, S. Basu, T. Leeper

BIOL **169.** Synthesis and screening of a β -amino acid bisintercalator library. E. Gratton, B.L. Iverson

BIOL **170.** Small angle X-ray scattering based 3D reconstruction of ornithine transcarbamoylase suggests structural rearrangement. J. Winters, I. ngu, P.J. Beuning, M. Ondrechen, L. Makowski

BIOL **171.** Elucidation of exit tunnel-nascent peptide interaction with small molecule-peptide conjugate probes. A. Washington, S. Tapadar, A.K. Oyeler

BIOL **172.** Metabolic profiling of cuprizone-induced oligodendrocyte degeneration. A. Taraboletti

BIOL **173.** Immune response of proteins packaged to the interior of virus-like particle scaffolds. R. Demont

BIOL **174.** NMR studies of nitrogen-15 enriched cofactor interaction with Type 2 isopentenyl diphosphate:dimethylallyl diphosphate isomerase. S.S. Netti, C.D. Poulter

BIOL **175.** Structural studies of the oxetanocin biosynthetic enzyme OxaA reveal determinants for substrate binding and catalysis. J. Rabb, A. Zhong, H. Liu, C.L. Drennan

BIOL **176.** Generality of kinase-catalyzed biotinylation: A tool for kinase cell signaling pathway analysis. D. Embogama, C. Senevirathne, M. Pflum

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 177.** Crystallization of a heterocyclization domain in yersiniabactin biosynthesis. **Y. Xia, S. Mishra, D. Frueh, D.P. Dowling**
- BIOL 178.** Crystallization of a kinase involved in 5-hydroxymethyldeoxyuridine modification in phage. **C.A. Hunt, C. Guan, P. Weigle, D.P. Dowling**
- BIOL 179.** Withdrawn.
- BIOL 180.** Small molecule based antibody-recruiting agent targeting uPAR. **A. Rullo, K.J. Fitzgerald, D.A. Spiegel**
- BIOL 181.** Fluorescent chemosensors for monitoring the activity of O6-methylguanine DNA methyltransferase. **A. Beharry, E.T. Kool**
- BIOL 182.** Alternative interpretation of the "nucleation" complex in DNA primer-probe hybridization based reactions. **F. Manyanga**
- BIOL 183.** Quantifying the concentration of allysine and collagen in fibrotic tissue. **P.A. Waghorn, B. Oliveira, P. Caravan**
- BIOL 184.** Determining the relationship between structure, internalization, and delivery efficiency for protein mimics. **C.M. Backlund, T. Takeuchi, S. Futaki, G.N. Tew**
- BIOL 185.** Role of hydrogen bonding between Arg26 and Asp37 in chloroperoxidase catalysis. **E. Shersher, X. Wang**
- BIOL 186.** Hyperpolarized ¹³C NMR studies of glucose metabolism in perfused rat hearts. **B.L. Anderson, Z. Kovacs, C. Malloy, A.D. Sherry**
- BIOL 187.** Withdrawn.
- BIOL 188.** Engineering bacteriophage for the ultrasensitive detection of foodborne pathogens. **T. Hinkley, A. Jackson, S.D. Alcaine, S.R. Nugen**
- BIOL 189.** Withdrawn.
- BIOL 190.** Withdrawn.
- BIOL 191.** Synthesis and application of peptidoglycan tools to study innate immune receptor recognition and activation. **J.E. Melnyk, V. Mohanan, A.K. Schaefer, C.L. Grimes**
- BIOL 192.** Withdrawn.
- BIOL 193.** Improvement in production of gamma-aminobutyric acid from glutamate using glutamate decarboxylase separated from *Escherichia coli*. **T. Dinh, T. Kang, K. Won**
- BIOL 194.** Softer side of chemistry: Tunable, fluorescent, multicolored, stable, bioactive, bioabsorbable protein and enzyme nanoparticles (nanoproteios). **B. Stromer, C.V. Kumar**
- BIOL 195.** T-cell antigen formed from distinct metabolic pathways. **J.Y. Mak, A.J. Corbett, S.B. Eckle, R.W. Birkinshaw, L. Liu, O. Patel, J. Mahony, Z. Chen, R. Reantragoon, B. Meehan, H. Cao, N.A. Williamson, R.A. Strugnelli, D. Van Sinderen, D.P. Fairlie, L. Kjer-Nielsen, J. Rossjohn, J. McCluskey**
- BIOL 196.** Spliced X-box binding protein 1 (XBP1s) transcription factor of the unfolded protein response can regulate secreted protein N-linked glycan maturation. **M.B. Dewal, M. Shoulders**
- BIOL 197.** Nanotoxicity sensing through synthetic biology. **B. Saltepe, U. Seker**
- BIOL 198.** Pneumococcal neuraminidase substrates identified through chemoselective labeling. **J.E. McCombs, J.J. Kohler**
- BIOL 199.** Bioinformatics and quantum mechanics analysis of base-ribose stacking in functional RNAs. **M. Chawla, E. Chermak, R. Oliva, L. Cavallo**
- BIOL 200.** Use of ¹⁸F-2-fluorodeoxyglucose (FDG) to label antibody fragments for immuno-PET of pancreatic cancer. **M. Rashidian, H. Ploegh**
- BIOL 201.** In vivo biosensing via tissue-localizable near-infrared-fluorescent single-walled carbon nanotubes. **N. Iverson, P.W. Barone, L.J. Trudel, M. Shandell, S. Sen, F. Sen, V. Ivanov, E. Atolia, E. Farias, T. McNicholas, N. Reuel, N. Parry, G.N. Wogan, M. Strano**
- BIOL 202.** Novel protein array for direct detection of double-stranded DNA sequences for diagnostic applications. **M. Kim, D. Ha, A. Chakraborty, C. Ahn**
- BIOL 203.** Interaction of fluorescence dyes with CCG and GO. **S. Sun, F. Liu**
- BIOL 204.** Computational models of prebiotic chemical systems leading to the emergence of chiral symmetry breaking. **P.M. Schwartz, J.M. Kubala, B.N. Morneau, C. Barratt**
- BIOL 205.** Quantification of deubiquitinating enzyme activity in cancer cells using a protease-resistant, peptide based reporter. **A.T. Melvin**
- BIOL 206.** Aromatic amino acids: Privileged side-chains for protein-protein interaction inhibitor discovery. **W. Pomerantz, A. Urlick, C. Gee, N.K. Mishra**
- BIOL 207.** Substrate specificity of bacterial esterases. **A. White, R. Johnson, G.C. Hoops**
- BIOL 208.** Gene categorization: An algebraic topology perspective. **A.M. Kabza, D. Ho, J. Lastimosa, R. Komendarczyk**

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 253A

Eli Lilly Award in Biological Chemistry

M. Luo, *Organizer, Presiding*

9:00 BIOL 209. Next-generation bromodomain inhibitors. **J. Bradner**

9:45 BIOL 210. Chemical-proteomic strategies to investigate reactive cysteines. **E. Weerapana**

10:30 BIOL 211. Transition state and inhibitors of DNA methyltransferase DNMT1. **Q. Du, S. Gulab, A. Woolhouse, P. Tyler, V.L. Schramm**

11:15 BIOL 212. Journey of developing chemical tools to interrogate protein methyltransferases. **M. Luo**

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253A

Graduate Student & Postdoctoral Symposium

V. Bandarian, *Organizer, Presiding*

1:30 BIOL 213. PROTACs: Potent protein knockdown by hijacking E3 ubiquitin ligases. **D. Bondeson, A. Mares, I. Smith, E. Ko, S. Campos, A. Miah, K. Mulholland, N. Routly, C. Pancevac, M. Bantscheff, N. Zinn, C. Teague, M. Hobbs, C. Cox, J. Flanagan, W. den Besten, L. Kruidenier, P. Carter, J.D. Harling, I. Churcher, C.M. Crews**

1:45 BIOL 214. TYW1: A radical SAM enzyme bringing that catalyzes the biosynthesis of all wycosine derivatives. **A.P. Young, V. Bandarian**

2:00 BIOL 215. Biochemical evaluation of novel *N*-mustard analogs of *S*-adenosyl-L-methionine as probes of protein methyltransferase substrates. **S.J. Bergman, L. Comstock**

2:15 BIOL 216. Tracking distinct RNA populations using efficient and reversible covalent chemistry. **E. Duffy, M. Rutenberg-Schoenberg, C.D. Stark, M.D. Simon**

2:30 BIOL 217. Conformational restriction of the NPF motif to target EHD1 and endocytic recycling. **A. Kamens, R. Eisert, T. Corlin, J.D. Baleja, J. Kritzer**

2:45 BIOL 218. New insights into the mechanism of biological nitrogen fixation. **V. Hoeke, D.R. Dean, L.C. Seefeldt, B.M. Hoffman**

3:00 BIOL 219. Nanomechanical study of the interfacial enzymatic activity of cellulase. **W. Du, J. Xi**

3:15 BIOL 220. Modular combinatorial assembly of Type II-A CRISPR arrays for dCas9-mediated multiplex transcriptional repression in *E. coli*. **B.F. Cress, Ö.D. Toparlak, S. Guleria, M. Lebovich, J.T. Stieglitz, J. Englaender, J.A. Jones, R.J. Linhardt, M. Koffas**

3:30 BIOL 221. Chemoenzymatic synthesis of photocrosslinking O-GlcNAc peptides to capture O-GlcNAc-dependent interactions. **A.C. Rodriguez, S. Yu, B. Li, J.J. Kohler**

3:45 BIOL 222. Unraveling the importance of heme redox potentials toward controlling enzymatic activities. **A. Bhagi, Y. Lu**

4:00 BIOL 223. Structure-activity relationship studies of Gramicidin A mutants enabled by facile reductive amination. **B. Zervas, J. Gao**

4:15 BIOL 224. Toward efficient electrocatalysts for H₂ oxidation using functional mimic approach from biological reaction. **N. Kumar, S. Raugel, B. Ginovska-Pangovska, M. Dupuis, M. Helm, M. Bullock**

4:45 BIOL 225. Role of the highly-conserved intervening domain of NEMO in high-affinity binding to IKK β . **R. Shaffer, D. Petrescu, M. Finau, S.M. Cote, K.N. Allen, A. Whitty**

BMGT

Division of Business Development and Management

J. Bryant and K. Allen, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

True Stories from Entrepreneurs: BRIC Edition (see SCHB, Sunday, Monday)

Industrial Innovations in Polymer Chemistry (see POLY, Monday)

Managing Transitions (see WCC, Monday)

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry (see SCHB, Tuesday)

SOCIAL EVENTS:

WCC "Just Cocktails" networking event, 4:00 PM: Tuesday

Henry Hill reception, 5:00 PM: Tuesday

PROF- LGBT reception, 6:00 PM: Tuesday

BUSINESS MEETINGS:

BMGT Annual Open Meeting, 10:00 AM: Tuesday

MONDAY MORNING

Section A

Renaissance Boston Waterfront
Atlantic Blrm 1

The Chemistry Enterprise in 2015

Cosponsored by PRES and PROF

W. F. Carroll, *Organizer, Presiding*

J. L. Bryant, *Presiding*

8:10 Introductory Remarks.

8:15 BMGT 1. The Chemistry Enterprise in 2015: Overview and celebrity predictions. **W.F. Carroll**

8:45 BMGT 2. The Chemistry Enterprise in 2015: Energy and feedstocks then and now. **W.F. Carroll**

9:15 BMGT 3. The Chemistry Enterprise in 2015: Industry then and now. **T.M. Connolly**

9:45 BMGT 4. The Chemistry Enterprise in 2015: Science, technology, and sustainability then and now. **R. Baum**

10:15 BMGT 5. The Chemistry Enterprise in 2015: Education then and now. **B.E. Bursten**

10:45 BMGT 6. The Chemistry Enterprise in 2015: The workforce then and now. **K.C. Glasgow**

11:15 BMGT 7. The Chemistry Enterprise in 2015: Government, homeland security, and diversity then and now. **N.B. Jackson**

11:45 Concluding Remarks.

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits

Sponsored by CHED, Cosponsored by BMGT, CEI, ENVR, I&EC, MEDI, PROF, SCHB and YCC

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

MONDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 1

Leadership Skills as a Strategic Advantage: the Chemist's Competitive Edge

Cosponsored by CEPA, PRES‡, PROF and YCC

T. H. Lane, *Organizer*

C. A. Duane, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **BMGT 8.** Impact of leadership skills on corporations and organizations. L.K. Krannich

2:05 **BMGT 9.** Career Skills Cafe: Enhance your employability for success. J. Littrell

2:35 **BMGT 10.** What will get you from here to there? D. Mason

3:05 Intermission.

3:15 **BMGT 11.** Learning by doing: Leadership opportunities while you are still in the lab. R.T. Graf, J.S. Manka, T. Sulzbach

3:45 **BMGT 12.** Preparing faculty for leadership in academia: One campus program. B.A. Sawrey

4:15 **BMGT 13.** ACS commitment to creating leaders. T.H. Lane, D. Grob Schmidt

4:45 Concluding Remarks.

TUESDAY MORNING

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Sponsored by CHED, Cosponsored by ANYL‡, BIOL‡, BIOT‡, BMGT‡, CORP‡, DAC‡, ENFL‡, PHYS‡ and POLY‡

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES‡, PROF and SCHB

TUESDAY AFTERNOON

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Sponsored by CHED, Cosponsored by ANYL‡, BIOT‡, BMGT‡, CORP‡, DAC‡, ENFL‡, PHYS‡ and POLY‡

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES‡, PROF and SCHB

Women in Innovation: Business and Commerce

Sponsored by PROF, Cosponsored by BMGT, SCHB, WCC and YCC

CARB

Division of Carbohydrate Chemistry

E. Rozners, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

True Stories from Entrepreneurs: BRIC Edition (see SCHB, Sunday, Monday)

Cancer Immunotherapy: The Next Big Thing for Small Molecules (see MEDI, Monday)

Emerging Antibody Drug Conjugates: Applications of Medicinal Chemistry (see MEDI, Monday)

Biologically-Related Molecules and Processes (see ORGN, Wednesday, Thursday)

SUNDAY MORNING

Section A

Seaport Hotel and World Trade Center
Beacon Hill 2/3

Fundamental and Applied Aspects of Glyconanotechnology

R. Narain, *Organizer, Presiding*

C. Becer, *Presiding*

8:30 **CARB 1.** Precision glycopolymers and their interactions with DC-SIGN. R. Becer

9:00 **CARB 2.** Preparation of glyco-nanomaterials via RAFT living radical polymerization and application for biosensing. Y. Miura

9:30 **CARB 3.** Glycosylated gold nanoparticle biosensors: Label-free and high-throughput evaluation of glycan/lectin interactions. S. Richards, L. Otten, E. Fullam, G. Besra, M. Gibson

9:50 **CARB 4.** Heparin nanoparticles for β amyloid binding and mitigation of β amyloid associated cytotoxicity. P. Wang, X. Huang

10:10 Intermission.

10:25 **CARB 5.** Thiomaltose: A second generation maltodextrin based pathogen imaging agent. N. Murthy

10:55 **CARB 6.** Carbohydrate based systems for liver targeted cancer therapy. R. Narain

11:25 **CARB 7.** Isolation of O-linked glycan-amino acids from O-linked glycoproteins. M.A. Madson

11:45 **CARB 8.** Smart microarray platforms for understanding biochemical interactions. C.I. Biggs, M. Gibson

Section B

Seaport Hotel and World Trade Center
Waterfront 3

Advances in Oligonucleotide Therapeutics

Cosponsored by BIOL, MEDI and ORGN

M. Manoharan, *Organizer, Presiding*

D. P. Arya, *Presiding*

9:00 Introductory Remarks.

9:05 **CARB 9.** Mammalian cell nuclei: A rich source of targets for synthetic nucleic acids. D.R. Corey

9:35 **CARB 10.** Expanding chemical diversity of therapeutic oligonucleotides for treatment of neurodegenerative disorders. A. Khvorova

10:05 **CARB 11.** Recent advances in RNA Chemistry: From RNA chips to novel functional RNA structures. M.J. Damha

10:35 Intermission.

10:50 **CARB 12.** Chemical strategies for systemic delivery of RNAi drugs. M. Manoharan

11:20 **CARB 13.** Protease-triggered siRNA delivery vehicles. D. Rozema

11:50 **CARB 14.** Amide-modified RNA: Synthesis, structure, and RNA interference activity. E. Rozners, D. Mutisya, C. Selvam, P. Tanui, B. Lunstad, S.D. Kennedy, P.S. Pallan, A. Haas, D. Leake, M. Egli

National Science Foundation's Centers for Chemical Innovation

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SUNDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Beacon Hill 2/3

Fundamental and Applied Aspects of Glyconanotechnology

R. Narain, *Organizer, Presiding*

X. Huang, *Presiding*

1:35 **CARB 15.** Multiplexed biosensing with a chemical tongue: Glycosylated particles/arrays to overcome lectin promiscuity. M. Gibson, S. Richards, C.I. Biggs, L. Otten

2:05 **CARB 16.** Magnetic glyconanoparticles for disease detection. X. Huang

2:35 **CARB 17.** Peptide-conjugated glucan particles for delivery of therapeutic siRNA. J.L. Cohen, M. Aouadi, P. Vangala, M. Tencerova, S.U. Amano, Y. Shen, S.M. Nicololo, J.C. Yawe, M.P. Czech

2:55 **CARB 18.** Controllable production of nanocellulose tubes for artificial blood vessels. J. Tang, X. Li, S. Hong, L. Chen, F. Hong

3:15 Intermission.

3:30 **CARB 19.** Influence of polymer architecture and chemistry on the blood compatibility of carbohydrate based nanogels and surfaces. B.F. Lai, Y. Wang, K. Yu, M. Ahmed, R. Narain, J.N. Kizhakkedathu

4:00 **CARB 20.** Self-assembled nanoparticles consisting of temperature responsive copolymers for glyconanotechnology. Y. Kotsuchibashi, M. Ebara, R. Narain, T. Aoyagi

4:30 **CARB 21.** Probing bacterial based pathogen infections by the study of bacterial adhesion on biomimetic temperature responsive glycopolymer surfaces. Y. Wang, R. Narain, Y. Liu

4:50 **CARB 22.** Lipopeptide coated iron oxide nanoparticles as a MUC1 antigen carrier platform for anticancer vaccine. S. Sungsuwan, Z. Yin, X. Huang

5:10 **CARB 23.** Modification of rice straw with cyanuric chloride for higher yield of saccharides in hydrolysis. X. Jiang

Section B

Seaport Hotel and World Trade Center
Waterfront 3

Advances in Oligonucleotide Therapeutics

Cosponsored by BIOL, MEDI and ORGN

M. Manoharan, *Organizer, Presiding*

E. Rozners, *Presiding*

2:00 **CARB 24.** Messenger RNA as a novel therapeutic approach. M. Stanton

2:30 **CARB 25.** Insights from structure into pairing stability, nuclease resistance and RNAi activity of backbone-modified oligonucleotide analogs: Phosphorodithioate RNA, glycol nucleic acid, 5'-modified RNA and 4'-modified RNA. M. Egli, M. Manoharan, X. Yang

3:00 **CARB 26.** Hepatic targeting using monovalent N-acetylgalactosamine and its analogs improves potency of antisense oligonucleotides in mice.

T.P. Prakash, J. Yu, G.A. Kinberger, A. Low, R. Peralta, S. Murray, S. Guo, M. Katz, H. Murray, K. Schmidt, E.E. Swayze, P. Seth

3:30 Intermission.

3:45 **CARB 27.** Novel polysaccharide carrier for functional oligonucleotides: Immunocyte-targeting drug delivery system. K. Sakurai, S. Mochizuki

4:15 **CARB 28.** Rapid pH sensitive assay for miRNA binders. D.P. Arya

4:45 **CARB 29.** Pronounced effect of 2'-F-arabinose (2'-F-ANA) substitutions on the conformation and stability of I-motif structures. H. Abou Assi, R. Harkness, N. Martin-Pintado, T. Mittermaier, C. Gonzalez, M.J. Damha

5:00 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal

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National Science Foundation's Centers for Chemical Innovation

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True Stories from Entrepreneurs: BRIC Edition

Sponsored by SCHB, Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

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MONDAY MORNING

Section A

Seaport Hotel and World Trade Center
Waterfront 3

New Strategies and Applications of Aminoglycosides

Cosponsored by MEDI

C. T. Chang, *Organizer, Presiding*

9:00 CARB 30. Amphiphilic aminoglycoside adjuvants. F. Schweizer, B. Gorityala, G. Guchhait

9:40 CARB 31. Mechanistic enzymology of radical-mediated glycodiversification. H. Liu

10:20 Intermission.

10:40 CARB 32. RNA-binding molecules: Structure, function, and synthesis. S. Hanessian

11:20 CARB 33. Bacterial rRNA selective aminoglycosides. D.P. Arya

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF and SOCED

ACS Scholars: Rising Stars in Academe

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Memories of Henry Hill: His Legacy in Science and in Professional Service

Sponsored by HIST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES‡, PROF and SCHB

True Stories from Entrepreneurs: BRIC Edition

Sponsored by SCHB, Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

MONDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Waterfront 3

New Strategies and Applications of Aminoglycosides

Cosponsored by MEDI

C. T. Chang, *Organizer, Presiding*

1:30 CARB 34. Sensitization of cancer cells to anticancer drugs with aminoglycosides. G.A. O'Doherty

2:10 CARB 35. New perspectives of designer aminoglycosides: From fixing human faulty genes to controlled gene expression. T. Baasov

2:50 Intermission.

3:10 CARB 36. Aminoglycosides as antibacterial, antifungal, and anti-HIV agents. S. Garneau-Tsodikova

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

3:50 CARB 37. Amphiphilic aminoglycosides: New application for old drugs. C.T. Chang

ACS Scholars: Rising Stars in Industry

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MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

E. Rozners, *Organizer*

8:00 - 10:00

52-53, 55-57, 63-66, 68-69, 73, 76, 80, 89, 97, 101, 106-107, 110. See subsequent listings.

TUESDAY MORNING

Section A

Seaport Hotel and World Trade Center
Waterfront 3

Glycolipid Immunostimulants

Cosponsored by MEDI and ORGN

A. R. Howell, D. R. Mootoo, *Organizers*

R. W. Franck, P. Savage, *Organizers, Presiding*

8:10 Introductory Remarks.

8:15 CARB 38. Toward the development of water-soluble glycosphingolipid immunostimulants. S. Kim

8:45 CARB 39. Immunostimulatory glycolipids: Polar opposites joined at the hip. J. Gervay-Hague

9:15 CARB 40. Sphinganine-containing α -GalCers: Underappreciated iNKT cell activators? A.R. Howell

9:45 Intermission.

10:00 CARB 41. Psychosine and related glycolipids as agonists for natural killer T cells. P. Savage, S. Deng, L. Kain, A. Bendelac, L. Teyton

10:30 CARB 42. Design, synthesis, and evaluation of Th1 skewing α -GalCer analogs. S.P. Van Calenbergh

11:00 CARB 43. Aminocyclitol glycolipid mimetics are potent activators of NKT cells and immune response. A. Llebaria

11:30 CARB 44. Synthesis and Immunostimulatory activity of RCAL-56, 61, 105 and 133, the analogs of KRN7000. K. Mori, T. Tashiro, T. Shigeura, H. Watarai, M. Taniguchi

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES‡, PROF and SCHB

Transforming University-Industry Partnerships for an Innovative Future

Envisioning, Enabling and Executing

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

TUESDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Waterfront 3

Glycolipid Immunostimulants

Cosponsored by MEDI and ORGN

R. W. Franck, P. Savage, *Organizers*

A. R. Howell, D. R. Mootoo, *Organizers, Presiding*

1:30 CARB 45. Bioorthogonal synthesis and biological activity of CD1d dependent glycolipid-peptide vaccines. G.F. Painter, C. Tang, R. Anderson, B.J. Compton, A. Authier-Hall, C.M. Hayman, T. Osmond, C.R. Brooks, K.J. Farrand, O. Gasser, D.S. Larsen, R. Weinkove, I.F. Hermans

2:00 CARB 46. Withdrawn.

2:30 CARB 47. Glycolipid adjuvants and class switch in development of carbohydrate-based cancer vaccine. C. Wong

3:00 Intermission.

3:15 CARB 48. Synthesis of glycolipids based on Lewis acid promoted anomerization reactions. P.V. Murphy

3:45 CARB 49. Synthesis of fluorinated α -galactosylceramide analogs. E. Leclerc

4:15 CARB 50. Glycosyl crotylstannanes for synthesis and cytokine tuning of glycosphingolipids. A.S. Altiti, S. Bachan, L. Zhang, X. Ma, D.R. Mootoo

4:45 CARB 51. Glycolipid antigen-presentation by CD1d and mechanism of NKT cell activation. D.M. Zajonc

5:15 Concluding Remarks.

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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Transforming University-Industry Partnerships for an Innovative Future

Energizing and Education

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TUESDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

General Posters

E. Rozners, *Organizer*

7:00 - 9:00

CARB 52. Synthesis and incorporation of 5'-C-malonyl nucleotides at the 5' terminus of siRNA antisense strand: Evaluation of gene silencing activity and stability. I. Zlatev, D.J. Foster, J. Liu, K. Charisse, B. Brigham, M.A. Maier, K.R. Rajeev, M. Egli, M. Manoharan

CARB 53. Positional effect of trivalent GalNAc ligands on the gene silencing activity of siRNA conjugates. J. Nair, K. Charisse, M. Jayaraman, P. Kandasamy, C. Theile, J. Willoughby, K. Yucius, T. Nguyen, S. Milstein, V. Jadhav, M.A. Maier, K. Rajeev, M. Manoharan

CARB 54. Effect of metabolically stable (E) - and (Z) - 5'-vinylphosphonate on siRNA activity. R.G. Parmar, C. Theile, K. Charisse, V. Jadhav, I. Zlatev, M.A. Maier, K.R. Rajeev, M. Manoharan

CARB 55. Solvent-free approach to glycosyl amides: Toward the synthesis of α -N-galactosyl ceramides. D. Chenmamadhavuni, A.R. Howell

CARB 56. α -Galactosylceramide analogs: A searchable data set of cytokine induction levels. R.W. Franck

CARB 57. Cycloaddition way to O-glycosides: Vintage reactions for new tumor antigen mimetics. C. Nativi, R.W. Franck, B. Richichi

CARB 58. Synthesis, characterization and binding studies of a bipyridine based lectin mimic under physiological conditions. A.K. Addo-Mensah, M. Addo

CARB 59. Poly-amido-saccharides (PASs): Structural characterization of novel synthetic carbohydrate polymers using experimental analysis, molecular dynamic stimulations, and all-atom models. S.L. Chin, E.L. Dane, Q. Lu, L. Dominguez, J.E. Straub, M.W. Grinstaff

CARB 60. Genome mining, functional expression and inhibition of arabinogalactan biosynthesis for therapeutic treatments of *Nocardia* infection. H. Chiu, Y. Chen

CARB 61. Synthesis and immunostimulatory activity of highly purified α - and β -anomers of GalCer and GlcCer. T. Tashiro, T. Shigeura, H. Watarai, M. Taniguchi, K. Mori

CARB 62. Ultra-anisotropic swelling of oriented hydrogels of giant cyanobacterial LC exopolysaccharides. M. Okajima, T. Kaneko, R. Mishima

CARB 63. Chemical synthesis of human syndecan-3 glycopeptides bearing two heparan sulfate glycan chains. W. Yang

CARB 64. Chemical synthesis of isotopically labeled N- and O- glycopeptides for quantification of tumor associated glycopeptides. S. Ramadan, W. Yang, A. Eissa, R. Goldman, X. Huang

CARB 65. Cellulose nanofiber prepared by persulfate oxidation of bagasse pulp. C. Du, H. Li, M. Liu

CARB 66. Synthetic aminoglycosides efficiently suppress CFTR nonsense mutations and are enhanced by ivacaftor. V. Belakhov, M. Shalev, J. Schacht, D. Bedwell, S. Rowe, T. Baasov

CARB 67. Improved synthesis of CNS-active glycal-based benzylidene derivatives. E. Hanawa-Romero, I.J. Talisman, C.E. Marzabadi

CARB 68. Influence of the isothiocyano moiety on stereoselective synthesis of sialic acid glycosides and subsequent diversification. A. Mandhapat, D. Crich, R. Salla

CARB 69. Synthesis and properties of pentulose-RNA chimeric oligonucleotides. T.C. Efthymiou, R. Krishnamurthy

CARB 70. Separation of lactose, lactulose and epilactose by a new HILIC column. M. Turcotte, S. Sakai, N. Nakajima, R. Benson

CARB 71. Withdrawn.

CARB 72. Non antibacterial aminoglycoside analogs as potentiators of ineffective antibiotics against multidrug resistant *Pseudomonas aeruginosa*. B. Gorityala, D. Fernando, G. Guchhait, G. Zhanel, A. Kumar, F. Schweizer

CARB 73. Using ReSET and sialosyl iodide glycosylation to develop chemical probes to study sialic acid (Neu5Ac) biochemistry. S.S. Park, J. Gervay-Hague

CARB 74. Towards the total synthesis of (-)-Griseusin A. C. Liang, Q. Zhang, G.A. O'Doherty

CARB 75. Automated solid-phase synthesis of complex oligoxyan. **G.H. de Kruijff**, D. Schmidt, F. Schuhmacher, P.H. Seeberger, F. Pfrenkle

CARB 76. Organocatalyzed synthesis of fluorinated C-glycosides. **A.S. Altiti, S. Bachan, D.R. Mootoo**

CARB 77. Synthesis of neoglycolipids and carbohydrate-presenting liposomes for antibiotic delivery. **B. Wu, M. King, X. Chen, N. Hao, E.A. Kurt-Jones, J. Wang, R. Finberg, M. Yan**

CARB 78. De novo asymmetric synthesis of biologically important carbohydrates. **Y. Ma**

CARB 79. Novel synthetic glycopeptide conjugates as HIV vaccine candidates. **D.N. Nguyen, J.K. Bailey, J. Temme, A. Klein, I.J. Krauss**

CARB 80. SELMA selection of DNA supported carbohydrate clusters which bind to HIV antibody PGT128. **J. Temme, I.J. Krauss**

CARB 81. Characteristics of lignocellulosic fibers from hardwood pulp by laccase-catalyzed TEMPO oxidation. **H. Li, D. Zhang, M. Liu**

CARB 82. *Penicillium purpurogenum* produces a set of novel esterases when grown on sugar beet pulp. **J. Eyzaguirre, G. Oleas, R. Sepulveda, E. Callegari**

CARB 83. Polysaccharide-mediated formation of pigments from serotonin. **N. Alattas, K. Vercurysse**

CARB 84. Enhanced immunostimulation for cancer vaccine with crosslinked CpG-DNA/ β -1,3-glucan nanogel through hybridization. **N. Miyamoto, S. Mochizuki, K. Sakurai**

CARB 85. Polysaccharide-mediated formation of pigments from catecholamines. **M. Alhumaidi, K. Vercurysse**

CARB 86. Selection of glycopeptide antigens for HIV neutralizing antibodies that recognize peptide and carbohydrates. **S. Horiya, J.K. Bailey, J. Temme, I.J. Krauss**

CARB 87. Fluorinated particle-assisted rapid synthesis of oligosaccharides. **Y. Feng, J. Wu, Y. Chai**

CARB 88. Comparison of the structural features of bovine and porcine heparins. **K. St. Ange, A. Onishi, X. Sun, J.S. Dordick, R.J. Linhardt**

CARB 89. Progress towards the synthesis of *Escherichia coli* O-Antigen O111 minimum repeat. **D.L. Lloyd, C. Bennett**

CARB 90. Petasis-Ferrier approach to deoxy-sugar monosaccharides. **D. Bright, C. Bennett**

CARB 91. Synthesis of unnatural UPD-sugars toward novel heparin-family oligosaccharides. **V.L. Schultz, K. Linkens, J. Rimel, F. Zhang, R.J. Linhardt**

CARB 92. Construction of 2-deoxy thioglycoside donors using S-methyl and S-ethyl cyclopropenium iodide salts. **M. Bylsma, C. Bennett**

CARB 93. Water/air-stable iodonium thiophilic promoters for the facile construction of glycosidic linkages. **A. Chu, C. Bennett**

CARB 94. Studies towards the total synthesis of divergoldes L-N. **S. Rasapalli, U. Javed, H. Ijaz**

CARB 95. Synthesis of steroid conjugates for targeted liposomal delivery of RNA-based therapies. **H. Nguyen, V. Ferro**

CARB 96. Effects of urea, MC, and CMC on crystalline structure of bacterial cellulose. **Z. Wang, J. Xiong, J. Ye**

CARB 97. Chirality-dependent activity of Glycol Nucleic Acid (GNA) in siRNA duplexes. **M.K. Schlegel, K. Charisse, A.V. Kel'in, M. Jayaraman, D.J. Foster, S. Milstein, I. Zlatev, J. Lackey, A. Bisbe, N. Taneja, J. O'Shea, S. Shaikh, M.A. Maier, K.R. Rajeev, M. Egli, M. Manoharan**

CARB 98. First synthesis of 2-aminoacetyl-2,3-dideoxy-D-glucose. **T. Grove, Z.J. Witzczak, R. Bielski**

CARB 99. Progress towards site-specific heterogeneous glycosylation of DNA aptamers which mimic the epitope of 2G12. **B.K. Wheat, J. Temme, I.J. Krauss**

CARB 100. Development of fluorescent saccharide sensors based on a 1,2,3-triazole ring. **W. Zhai, J.S. Fossey**

CARB 101. Glycopolymers probes of carbohydrate-carbohydrate interactions: Facile synthesis via ROMP and Cu(I)-catalyzed click cycloaddition of azido-sugars. **B.W. Leeber, M. Draeger, R. Lusi, R.S. Okoth, A. Basu**

CARB 102. Second-generation mRNA display glycopeptide libraries for HIV vaccine development. **J.K. Bailey, S. Horiya, J. Temme, I.J. Krauss**

CARB 103. Targeting cancer cell metabolism using small-molecule modulators of reactive oxygen species. **F. Ndombera**

CARB 104. Perfluorophenyl azide-mediated Staudinger reaction and application in probing cell surface glycans. **M. Sundhoro, S. Jeon, N. Hao, J. Park, A. Fischer, O. Ramstrom, M. Yan**

CARB 105. Novel 4'-substituted nucleoside modifications for siRNAs. **S. Matsuda, I. Zlatev, J. Nair, K. Charisse, N. Taneja, A. Bisbe, T. Nguyen, S. Milstein, J. O'Shea, M.A. Maier, K.R. Rajeev, M. Manoharan**

CARB 106. Substrate specificity for human α -1,6-fucosyltransferase (FucT8) expressed in large scale from recombinant baculovirus infected SF9 insect cells. **A.D. Calderon Molina, L. Li, Y. Liu, X. Wang, X. Li, P.G. Wang**

CARB 107. Electrochemical assay to detect influenza viruses and measure drug susceptibility. **X. Zhang, A. N. Dhawan, J. Sweeney, Y. He, M. Vasireddi, S.S. Iyer**

CARB 108. Synthesis and positional effects of 2'-O-[2-(methylamino)-2-oxoethyl] (2'-O-NMA) modification. **S. Kuchimanchi**

CARB 109. Chemoenzymatic synthesis of a library of human milk oligosaccharides. **Z. Xiao, P.G. Wang**

CARB 110. Synthesis of novel aryl nucleosides. **W. Dong, S.A. Woski**

CARB 111. Novel chitosan-based avidin/biotin system for target-selective drug delivery. **W. Li, D. Rammelkamp, Y. Meng**

CARB 112. Supramolecular assemblies of glycosylated-nucleoside-lipids: New scaffolds for tissue engineering. **L. Latxague, M.A. Ramin, A. Ananda, O. Chassande, P. Barthelemy**

WEDNESDAY MORNING

Section A

Seaport Hotel and World Trade Center Waterfront 3

Carbohydrate Synthesis for Medicinal Chemistry and Biology

G. A. O'Doherty, *Organizer*

P. Shi, Y. Xing, *Organizers, Presiding*

9:00 CARB 113. De novo synthesis in carbohydrate medicinal chemistry. **G.A. O'Doherty**

9:30 CARB 114. Synthesis of diverse types of carrageenan octasaccharides. **C. Kinnaert, M. Clausen**

9:50 CARB 115. Synthesis and biological studies of amphiphilic kanamycins. **C.T. Chang**

10:20 CARB 116. De novo synthesis of 5a-carbasugar analogs of SL0101. **Y. Li, M. Li, G.A. O'Doherty**

10:40 Intermission.

10:55 CARB 117. Chemical synthesis of bioactive natural molecules bearing 2-deoxy sugars. **J. Zhu**

11:25 CARB 118. Efficient chemoenzymatic synthesis of an N-glycan isomer library. **P.G. Wang, L. Li, Y. Liu, C. Ma, J. Qu**

11:45 CARB 119. Investigation of anticancer entirely carbohydrate constructs Tn-PS A1 and TF-PS B. **P.R. Andraena**

WEDNESDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center Waterfront 3

Carbohydrate Synthesis for Medicinal Chemistry and Biology

G. A. O'Doherty, Y. Xing, *Organizers*

P. Shi, *Organizer, Presiding*

H. Li, *Presiding*

1:45 CARB 120. Reagent controlled approaches to deoxy-sugar oligosaccharides. **C. Bennett**

2:15 CARB 121. Synthesis of plant cell wall 1,5- α -L-oligoarabinofuranosides. **M. Daugaard, M. Clausen**

2:35 CARB 122. Synthesis and anti-oxidant activity of phenylpropanoid glycosides. **J.L. Koviach-Cote, J. Mangar, J. Brown, Z. Sabbath, E. Toroitich, A. Jones**

3:05 CARB 123. Synthetic approach towards the gilvocarcins and related C-glycoside natural products. **D. Ray, G.A. O'Doherty**

3:25 Intermission.

3:40 CARB 124. Directed evolution-based development of clustered carbohydrate HIV antigens. **I.J. Krauss**

4:10 CARB 125. Explore the structure activity relationship of resin glycoside via the de novo synthesis of both enantiomers of Batatinoside III. **X. Liu, M. Li, G.A. O'Doherty**

4:30 CARB 126. Synthesis of substrate and transition state inhibitors of *S. coelicolor* GlgEI-V279S. **S.K. Veleiti, J.J. Lindenberger, S. Thanna, D.R. Ronning, S.J. Sucheck**

THURSDAY MORNING

Section A

Seaport Hotel and World Trade Center Waterfront 3

Carbohydrate Synthesis for Medicinal Chemistry and Biology

G. A. O'Doherty, *Organizer*

H. Li, Y. Xing, *Organizers, Presiding*

9:00 CARB 127. Peptidoglycan modifications tune the stability and function of the innate immune receptor Nod2. **J.E. Melnyk, V. Mohanan, A.K. Schaefer, C.L. Grimes**

9:20 CARB 128. Development of methods for large scale production of activated sugars and biologically active oligosaccharides. **L. Aminova**

9:40 CARB 129. Cyclopropenium mediated dehydrative glycosylations of 2-deoxy sugars and its application to the construction of α -linked 2-deoxy-containing carbohydrate structures. **J.M. Nogueira, C. Bennett**

10:00 CARB 130. Preparation of O- and N-heterocycles via glycol addition reactions. **S. Eltayeb, K.N. Brogden, P.H. Dobbelaar, C.E. Marzabadi**

10:20 Intermission.

10:35 CARB 131. Synthesis of analog hexasaccharide located on the dengue virus. **A. Bhagaloo, G. Singh**

10:55 CARB 132. Convergent synthesis of thio-linked cellobiose. **F. Nami, M. Clausen**

11:15 CARB 133. Imparting functional variety to cellulose ethers via olefin cross-metathesis. **Y. Dong, K.J. Edgar**

CATL

Division of Catalysis Science and Technology

K. Ramasamy, Program Chair

OTHER SYMPOSIA OF INTEREST:

Advances in Ceria Based Catalysis: Structure, Electronic & Chemical Properties Tailored for Chemical Conversion (see ENFL, Wednesday)

Biofuels for Powering the World: Discovery to Application (see ENFL, Sunday, Monday)

International Symposium on Mesoporous Zeolites (see ENFL, Wednesday)

Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application (see ENFL, Sunday, Monday, Tuesday)

Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions (see COLL, Monday, Tuesday)

Heterogeneous Catalysis for Environmental Applications (see ENVR, Sunday, Monday, Wednesday)

BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Monday

SUNDAY MORNING

Section A

Renaissance Boston Waterfront Atlantic Blrm 3

Single Atom Catalysis

A. M. Karim, *Organizer, Presiding*

Z. Wei, *Presiding*

8:00 CATL 1. Heterogeneous catalysis at the single-atom limit: A diverse reaction landscape. **M. Flytzani-Stephanopoulos, M. Yang, C. Wang, J. Shan, J. Liu**

8:45 CATL 2. CO oxidation by Cu₂O supported Pt atoms. **A. Therrien, E.H. Sykes**

9:05 CATL 3. Anchoring single atoms for better catalysis. **J. Liu**

9:35 CATL 4. CO and NO oxidation on supported single Pt group atoms. **C.K. Narula, A.F. Lawrence, S.M. G, M.M. DeBusk**

10:05 Intermission.

10:15 CATL 5. Ceria-based surface mixed oxides: Hydrocarbon oxidation on isolated Pd- and Mn-doped ceria. **M.J. Janik**, T. Sentfle, M.D. Krcha

10:55 CATL 6. Single-site catalysis with supported metal clusters. **D. Ertler**, A. Okrut, A. Palermo, A. Solovoy, B.C. Gates, D.A. Dixon, **A.S. Katz**

11:25 CATL 7. Platinum group metal-like cobalt single atom catalysts for selective hydrogenative transformations. **T. Zhang**

Section B

Renaissance Boston Waterfront
Caspian

Role of the Outer Coordination Sphere on the Activity of Enzymes and Molecular Catalysts

B. Ginovska-Pangovska, *Organizer*
M. O'Hagan, **W. J. Shaw**, *Organizers, Presiding*

8:00 CATL 8. Catalytic mechanism of hydrogenases, beyond the active site. **C. Léger**

8:40 CATL 9. Hydroxylation of inert organic molecules by cytochrome P450/decoy system. **Y. Watanabe**

9:10 CATL 10. Biological suggestions for chemical design when moving protons. **H. Long**, **C.H. Chang**

9:40 CATL 11. New computational insights on N₂ reduction by molybdenum-containing nitrogenases. **S. Raugei**, **D. Smith**, **B.M. Hoffman**, **L.C. Seefeldt**

10:10 Intermission.

10:20 CATL 12. Role of active site amino acids and accessory iron-sulfur clusters in the catalytic activation of H₂ by [FeFe]-hydrogenase. **P.W. King**, **C. Lubner**, **D.W. Mulder**, **M. Ratzloff**, **K.A. Brown**

10:50 CATL 13. Withdrawn.

11:10 CATL 14. Connecting protein dynamic fluctuation away from the active site with catalytic function. **J. Gao**

11:40 CATL 15. Fine tuning of the catalytic efficiency and metal binding features in metalloenzymes by Outer sphere residues. **A. Vila**, **E. Giannini**, **M. Meini**, **L. González**

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Metal Organic Frameworks for Catalysis Applications

O. K. Farha, **P. K. Thallapally**, *Organizers*
M. Eddaoudi, **J. Gascon**, *Organizers, Presiding*

8:00 Intermission.

8:05 CATL 16. Chemical environment control and catalytic performance of functionalized MOFs. **O.M. Yaghi**

8:40 CATL 17. Tetravalent MOFs as catalysts: A broad field of possibilities. **D. De Vos**, **B. Bueken**, **B. Van de Voorde**

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

9:05 CATL 18. Metal-organic framework-derived nanoporous metal oxides and graphene as efficient electrocatalysts. **H. Moon**, **K. Lee**, **J. Lee**

9:30 CATL 19. Examining the stability of metal-organic frameworks under exposure to acid gases. **J.R. Schmidt**, **C. Zhang**, **J.G. McDaniel**, **K. Yu**, **K. Kiesling**

9:55 Introductory Remarks.

10:10 CATL 20. Crystalline sponge method: Application to in situ observation of chemical reactions. **M. Fujita**

10:45 CATL 21. Metal nanoparticle@metal-organic framework composites as high-performance catalysts. **Q. Xu**

11:10 CATL 22. Functional microporous polymer networks for catalysis and energy applications. **A. Thomas**

11:35 CATL 23. Control selectivity of catalysts using metal organic frameworks. **W. Huang**, **X. Li**, **T. Goh**, **C. Xiao**

Section D

Renaissance Boston Waterfront
Pacific Blrm A

Symposium Honoring Gary Haller

R. S. Weber, **Y. Yang**, *Organizers*
D. E. Resasco, **X. Wang**, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CATL 24. 2nd Generation PLA; L-lactide directly from aqueous lactic acid. **W.F. Hoelderich**

9:20 CATL 25. Selective synthesis of narrow diameter distribution carbon nanotubes. **L.D. Pfefferle**

9:50 CATL 26. Catalysts for chirality selective synthesis of single-walled carbon nanotubes. **Y. Chen**

10:20 Intermission.

10:35 CATL 27. Nanosized platinum on zirconium oxide modified carbon electrocatalyst with high durability and high performance for PEM fuel cell. **S. Lee**, **Y. Park**, **J. Kim**, **T. Kim**, **C. Pak**

11:05 CATL 28. Rules of chemical and electrochemical promotion and their application for the conversion of CO₂ to hydrocarbons. **C. Vayenas**

11:35 CATL 29. Kinetic and spectroscopic studies of catalytic mechanisms: Hydrodeoxygenation of biomass feedstocks on transition metal phosphides. **S.T. Oyama**, **A. Iino**, **J. Shin**, **P. Bui**, **A. Takagaki**, **R. Kikuchi**, **K. Bando**

12:05 Concluding Remarks.

Section E

Renaissance Boston Waterfront
Pacific Blrm B

Nano Catalysis

Y. Lei, **Y. Xu**, *Organizers, Presiding*

8:00 CATL 30. Size-selected catalysis and electrocatalysis: Correlations with physical properties. **S.L. Anderson**

8:30 CATL 31. Platinum-copper single atom alloys for selective hydrogenation and dehydrogenation reactions. **J. Liu**, **J. Shan**, **M. Yang**, **H. Li**, **T.E. Haas**, **M. Flytzani-Stephanopoulos**

9:00 CATL 32. Singly dispersed catalytic site for high activity and selectivity. **F. Tao**, **S. Zhang**, **L.T. Nguyen**

9:30 CATL 33. Adsorption and reactivity of single metal atoms studied using the Fe₃O₄(001) adatom template. **G. Parkinson**

10:00 Intermission.

10:10 CATL 34. Machine-learning enabled multimetallic electrocatalyst design for CO₂ conversion. **H. Xin**, **X. Ma**

10:40 CATL 35. DFT study on site-dependent selectivity of water-gas shift reaction on nanoscale Ni catalysts. **B. Liu**, **M. Zhou**, **T. Le**, **L. Huyhn**

11:10 CATL 36. Size and support effects in catalysis by subnanometer and nanometer size clusters. **S. Vajda**

11:40 CATL 37. Mechanistic study of CO₂ hydrogenation on Pt and Pt alloy nanoparticles. **S. Kattel**, **P. Liu**, **J.G. Chen**

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Surface Science

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Biofuels for Powering the World: Discovery to Application

Catalytic Fast Pyrolysis

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Innovative Chemistry & Electrocatalysis for Low-carbon Energy & Fuels: Discovery to Application

H₂ generation

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SUNDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

Single Atom Catalysis

A. M. Karim, *Organizer, Presiding*
Z. Wei, *Presiding*

1:00 CATL 38. Pt/Cu single atom alloys for highly selective formic acid decomposition. **M.D. Marcinkowski**, **C.J. Murphy**, **M.L. Liriano**, **N.A. Wasio**, **F.R. Lucci**, **E.H. Sykes**

1:30 CATL 39. Selective hydrogenation of butadiene by Pt/Cu at the single atom limit. **F.R. Lucci**, **J. Liu**, **M. Stephanopoulos**, **E.H. Sykes**

1:50 CATL 40. Single-atom Rh active site concentration and in-situ formation allow tuning of CO₂ reduction selectivity. **J. Matsubu**, **P. Christopher**

2:20 CATL 41. Single-atom catalysis on Rh₂O₃/SiO₂. **S. Zhang**, **L.T. Nguyen**, **J. Li**, **F. Tao**

2:50 Intermission.

3:00 CATL 42. Effect of synthesis methods on the evolution of isolated atom catalysts during propane dehydrogenation. **A. Hock**, **B. Hu**, **A. Getsoian**, **G. Zhang**, **U. Das**, **J. Bunquin**, **L.A. Curtiss**, **P.C. Stair**, **C.L. Marshall**, **J. Miller**

3:30 CATL 43. Computational studies of supported single-atom catalysts for alkane dehydrogenation. **U. Das**, **L.A. Curtiss**

4:00 CATL 44. Exploring confinement effects in zeolite catalysis. **F. Goettl**, **S. Conrad**, **P. Sauter**, **I. Hermans**

4:20 CATL 45. Multistep biomass conversion reactions catalyzed with Sn in a partially dealuminated beta framework. **J. Dijkmans**, **B.F. Sels**, **M. Dusselier**

4:40 CATL 46. Catalytic transformation of biomass-derived compounds on Lewis acid-containing zeolites. **M. Koehle**, **R.F. Lobo**

Section B

Renaissance Boston Waterfront
Caspian

Role of the Outer Coordination Sphere on the Activity of Enzymes and Molecular Catalysts

M. O'Hagan, *Organizer*

B. Ginovska-Pangovska, **W. J. Shaw**, *Organizers, Presiding*

1:00 CATL 47. Biomimetic catalytic complexes organized by DNA nanoscaffolds. **J. Fu**

1:20 CATL 48. Engineering proteins for selective catalysis. **J.C. Lewis**

1:50 CATL 49. Biohybrid catalysts constructed in a protein matrix with an artificial metal complex. **T. Hayashi**, **A. Onoda**, **K. Oohora**

2:20 Intermission.

2:30 CATL 50. Assessing the role of outer sphere modifications on catalytic structure and function of de novo protein designed metalloenzymes. **V.L. Pecoraro**, **F. Yu**, **C. Mooney**, **C. Van Stappen**, **M. Zastrow**

3:10 CATL 51. Designing functional metalloenzymes: Exploring the roles of non-covalent secondary coordination sphere interactions in conferring and fine-tuning enzymatic activities. **Y. Lu**, **P. Hosseinzadeh**, **N. Marshall**, **A. Bhagi**, **I.D. Petrik**

3:40 CATL 52. Understanding the role of non-covalent interactions during nitrite reduction in a non-heme system. **A.R. Fout**, **E.M. Matson**, **Y. Park**

4:00 CATL 53. Optimization of the performance of artificial metalloenzymes by fine-tuning of the second coordination sphere. **T.R. Ward**

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Metal Organic Frameworks for Catalysis Applications

M. Eddaoudi, **J. Gascon**, *Organizers*

O. K. Farha, **P. K. Thallapally**, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CATL 54. Atom-by-atom synthesis of catalytic inorganic clusters within mesoporous metal-organic framework materials. **J.T. Hupp**

1:40 CATL 55. Functionalization of metal-organic frameworks. **H. Hintz**, **S. Wuttke**

2:05 CATL 56. MOFs as highly selective catalytic materials. **M. Daturi**, **P. Bazin**, **G. Clet**, **A. Vimont**, **C. Serre**

2:30 CATL 57. MOFs as heterogeneous catalysts for aerobic oxidations. **M. Alvaro**

2:55 Intermission.

3:10 CATL 58. Porous CMP organo-catalysts. **A.I. Cooper**

3:45 CATL 59. Metal-organic frameworks for sustainable catalysis for water splitting. **S. Das**

4:10 CATL 60. Insight into catalytic transformations in MOF pores. **C. Doonan**

Section D

Renaissance Boston Waterfront
Pacific Blrm A

Symposium Honoring Gary Haller

X. Wang, R. S. Weber, *Organizers*

D. E. Resasco, Y. Yang, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CATL 61. Reaction pathways involving methoxy in methanol to gasoline/olefins. **G.L. Haller**

1:50 CATL 62. HMF hydrodeoxygenation studies in a continuous flow reactor. **R.J. Gorte, J. Luo, L. Arroyo-Ramirez**

2:20 CATL 63. Vanadium (V) dispersion and Al(III) or Ti(IV) anchoring effect in MCM-41 silicas investigated using optical gap Blue shift and charge transfer band Gaussian fit. **L. Bonneviot, Y. Zheng, B. Albel, G. Montagnac, P. Wu, M. He**

2:50 Intermission.

3:05 CATL 64. Conversion of carboxylic acids over zeolites. **S. Crossley**

3:35 CATL 65. Heterogeneous catalysis in complex, condensed reaction media. **R.S. Weber, R. Rousseau**

4:05 Concluding Remarks.

Section E

Renaissance Boston Waterfront
Pacific Blrm B

Nano Catalysis

Y. Lei, Y. Xu, *Organizers, Presiding*

1:00 CATL 66. Controlling catalysis on metal nanoparticles by direct photo-excitation of adsorbate-metal bonds. **M. Kale, T. Avanesian, H. Xin, P. Christopher**

1:30 CATL 67. High-energy X-ray tools for exploring catalyst formation and activity. **K.W. Chapman**

2:00 CATL 68. Exploring catalysis at APS beamline 9-BM. **T. Wu**

2:30 CATL 69. Single-molecule photoelectrocatalysis imaging in photoelectrochemical water oxidation. **P. Chen**

3:00 Intermission.

3:10 CATL 70. Model system for surface science studies of zeolites: From UHV to elevated pressures. **J.A. Boscoboinik, S. Shaikhdudinov, H. Freund**

3:40 CATL 71. Tracking surface chemistry of a catalyst during catalysis with a lab-based ambient pressure X-ray photoelectron spectrometer. **F. Tao, L.T. Nguyen**

4:00 CATL 72. Tracking phosphorus species at the surface of nanocatalysts. **S. Carenco**

4:20 CATL 73. Fe-catalyzed etching of few-layer graphene through carbon hydrogenation. **G. Cheng, I.G. Calizo, A.R. Hight Walker**

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Powder Catalysts

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Biofuels for Powering the World: Discovery to Application

Pyrolysis

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Heterogeneous Catalysis for Environmental Applications

Photocatalysis for Energy and Environment

Sponsored by ENVF, Cosponsored by CATL

Innovative Chemistry & Electrocatalysis for Low-carbon Energy & Fuels: Discovery to Application

CO₂ & Solar

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MONDAY MORNING

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

2015 ACS Catalysis Lectureship

Cosponsored by INOR

M. Helm, E. S. Wiedner, *Organizers*

S. A. Koch, *Presiding*

8:00 Introductory Remarks.

8:05 CATL 74. Mechanistic NMR studies of proton movement in [Ni(P³,N³)₂]²⁺ catalysts for H₂ production. **M.J. O Hagan, A.P. Cardenas, M. Helm, R. Bullock**

8:35 CATL 75. Electrochemistry as a mechanistic tool for investigating proton transfer reactions involving pendant proton relays. **E.S. Wiedner, M. Helm, H.J. Brown, M.T. Mock, L.A. Labios, P. Bhattacharya, M. Bullock**

9:05 CATL 76. Reaction pathways of nickel-based hydrogen-evolving catalysts. **J.L. Dempsey, B. McCarthy, E.S. Rountree**

9:35 Intermission.

9:50 CATL 77. Theoretical design of hydrogen-evolving molecular electrocatalysts. **S. Hammes-Schiffer**

10:20 CATL 78. Non-innocent ligands support water as an oxidant for alcohols: Computational studies of catalytic mechanisms. **M.B. Hall, H. Li**

10:50 CATL 79. Toward molecular electrocatalysts by computation. **M. Ho, S. Chen, N. Kumar, R. Rousseau, M. Dupuis, D.L. Dubois, R. Bullock, S. Rauegi**

Section B

Renaissance Boston Waterfront
Caspian

Role of the Outer Coordination Sphere on the Activity of Enzymes and Molecular Catalysts

W. J. Shaw, *Organizer*

B. Ginovska-Pangovska, M. O'Hagan, *Organizers, Presiding*

8:00 CATL 80. Rhodium(II) catalysis with structured peptide ligands. **Z.T. Ball**

8:30 CATL 81. Local environments matter...probing the effects of the secondary coordination sphere on metal ion reactivity. **A. Borovik**

9:00 CATL 82. Parallel synthesis of biologically inspired transition metal ligands for catalysis. **S.R. Gilbertson**

9:30 CATL 83. Ultrafast hydrogen atom abstraction inside a cationic nanocage: Role of the aqueous shell. **J. Dasgupta**

9:50 Intermission.

10:00 CATL 84. Effect of a bioinspired outer coordination sphere on molecular catalysis. **N.P. Boralugodage**

10:20 CATL 85. Outer coordination sphere proton relay enables fast oxidation of H₂ without a change in overpotential with a bioinspired iron molecular electrocatalyst. **J. Damon, N. Kumar, S. Rauegi, M. Helm**

10:40 CATL 86. Pendant proton relays and ligand non-innocence in hydrogen-evolving molecular electrocatalysts. **S. Hammes-Schiffer**

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Metal Organic Frameworks for Catalysis Applications

M. Eddaoudi, P. K. Thallapally, *Organizers*

O. K. Farha, J. Gascon, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL 87. Selective sorption and catalysis by metal-organic frameworks. **M.J. Rosseinsky**

8:40 CATL 88. Metal-organic frameworks as catalytic nanoreactors for sustainable energy applications. **V. Stavila, K. Leong, R. Parthasarathi, K. Sale, R. Davis, M. Kent, M. Allendorf**

9:05 CATL 89. Phosphine metal-organic frameworks: Versatile materials for heterogeneous metal- and organocatalysis. **M. Ranocchiar, X. Xu, F. Morel, A. Beloqui Redondo, J.A. Van Bokhoven**

9:30 CATL 90. Metal-organic frameworks as heterogeneous solid acid catalysts for fixed-bed reactions. **S. Ma**

9:55 Intermission.

10:10 CATL 91. Engineering ultrastable metal-organic frameworks for biomimetic catalysis. **H. Zhou, L. Zou**

10:45 CATL 92. POMzites: A family of zeolitic polyoxometalate frameworks from a minimal building block library. **L. Cronin**

11:10 CATL 93. Inorganometallic catalyst design. **L. Gagliardi, S.O. Odoh, O.K. Farha, J.T. Hupp, C.J. Cramer**

11:35 CATL 94. MOF-mediated synthesis of highly active and stable catalysts for C1 chemistry. **F. Kaptejin, T.A. Wezendonk, X. Sun, M. Makkee, J. Gascon**

Section D

Renaissance Boston Waterfront
Pacific Blrm A

Symposium Honoring Gary Haller

D. E. Resasco, X. Wang, *Organizers*

R. S. Weber, Y. Yang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CATL 95. Influencing catalytic rates by tailoring steric constraints. **J.A. Lercher**

9:20 CATL 96. Aromatic transformations over zeolites crystallized by charge density mismatch. **H. Abrevaya, E.P. Boldingh, D. Jan, G. Lewis, C.P. Nicholas, J. Moscoso, R. Broach**

9:50 CATL 97. Overview of isotopic tracer studies of hexane aromatization on Pt/KL catalysts. **G. Jacobs, W.D. Shafer, K. Azzam, B.H. Davis**

10:20 Intermission.

10:35 CATL 98. Is there still life in the geometric model of sulfide catalysts? **S. Soled, S. Miso, J.E. Baumgartner, C.E. Kiewer**

11:05 CATL 99. Catalyzed soot filters for diesel vehicle emission control. **Y. Li**

11:35 CATL 100. Shaping of the "milieu" for passing from fundamental studies into the definition of a technical object and finally for reaching its industrialization and utilization. **I.E. Basini**

12:05 Concluding Remarks.

Section E

Renaissance Boston Waterfront
Pacific Blrm B

Nano Catalysis

Y. Lei, Y. Xu, *Organizers, Presiding*

8:00 CATL 101. Active structure of supported Au catalysts in CO oxidation and the size effect. **W. Huang**

8:30 CATL 102. Atomically precise gold and bimetal nanoclusters for nanocatalysis. **R. Jin**

9:00 CATL 103. Supported bimetallic AuPd clusters using Au₂₅L₁₈ clusters as precursor. **K. Lee, A. Shvhare, Y. Hu, R.W. Scott**

9:20 CATL 104. Withdrawn.

9:40 CATL 105. Nanostructured gold model catalysts on thin film substrates. **W. McKee, M. Patterson, D. Huang, L. Liu, R. Kurtz, P. Sprunger, Y. Xu**

10:00 Intermission.

10:10 CATL 106. Shape-controlled noble-metal nanocrystals for catalytic applications. **Y. Xia**

10:40 CATL 107. Using nanoenvironment to control the catalytic activity of moieties immobilized on nanoparticle surface. **I. Zharov**

11:00 CATL 108. Synthesis of hybrid inorganic nanoparticles using hydrophobic polymer as rigid template and their superior activity in electrocatalysis. **Z. Huang, J. Gong, Z. Nie**

11:20 CATL 109. Comparative study of different shape of Au/CeO₂ catalysts for water-gas shift reaction. **Y. He, B. Chen, X. Liang**

11:40 CATL 110. Highly active Cr-Cu/CeO₂ catalyst for CO-O₂ and CO-NO reactions. **H. Yoshida, Y. Okabe, N. Yamashita, S. Hinokuma, M. Machida**

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Theory

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Heterogeneous Catalysis for Environmental Applications

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Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions

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MONDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

2015 ACS Catalysis Lectureship

Cosponsored by INOR

M. Helm, E. S. Wiedner, *Organizers*

M. Y. Darensbourg, *Presiding*

1:00 CATL 111. Amino acids on the outer coordination sphere of $[\text{Ni}(\text{P}^{\text{O}}_2\text{N}^{\text{R}})_2]^{2+}$ result in enhanced catalytic activity. **W.J. Shaw**, A. Dutta, A. Jain, S. Raugel, B. Ginovska-Pangovska, J.A. Roberts

1:30 CATL 112. DuBois Photocatalysis: Visible light driven H_2 generation with a phosphonated Ni bis(diphosphine) catalyst in water. **M. Gross**, C.A. Caputo, D. Wakerley, **E. Reisner**

2:00 CATL 113. Bioinspired catalytic systems and technological applications of hydrogen. **V. Artero**

2:30 CATL 114. Modified molecular Ni(II) catalysts for photocatalytic proton reduction. **M.R. Wasielewski**, M. Majewski, W. Han, B.T. Phelan

3:00 Intermission.

3:15 CATL 115. Thermodynamic considerations in the design of molecular electrocatalysts for proton and CO_2 reduction. **J.Y. Yang**, C. Tsay, B. Livesay

3:45 CATL 116. Thermochemical and mechanistic insights into the selective reduction of CO_2 to formate using iron clusters. **L.A. Berben**, A. Taheri, M.D. Rail

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

4:15 CATL 117. Using free energies for H^+ / H^+ / H^+ transfers as a guide for designing M-H based catalysts. **A.M. Appel**, J.C. Linehan, E.S. Wiedner, B.R. Galan, M.S. Jelelic, S. Peterson, C.J. Weiss, D. Miller, C. Zall, S.J. Connolly

Section B

Renaissance Boston Waterfront
Caspian

Role of the Outer Coordination Sphere on the Activity of Enzymes and Molecular Catalysts

B. Ginovska-Pangovska, *Organizer*

M. O'Hagan, W. J. Shaw, *Organizers, Presiding*

1:00 CATL 118. Molecular H_2 -evolving catalysts with proton relays: Design, mechanistic studies, and benchmarking of catalytic activity. **V. Artero**

1:30 CATL 119. Developing functional metalloenzyme mimics using model protein scaffolds. **H.S. Shafaat**, J.W. Slater, A. Manesis, H. Monaco

2:00 CATL 120. Direct comparison of the performance of a bio-inspired synthetic Ni-Catalyst and a [NiFe]-Hydrogenase covalently attached to electrodes. **O. Rüdiger**, P. Rodriguez-Macia, A. Dutta, W.W. Lubitz, W.J. Shaw

2:40 Intermission.

2:50 CATL 121. Computational studies of biomimetic hydrogen-evolving transition metal complexes. **M.J. Field**

3:20 CATL 122. Nickel superoxide dismutase: The mechanism of superoxide disproportionation effected by the enzyme and metalloprotein based NiSOD mimics. **J.M. Shearer**

3:50 CATL 123. Including acid-base equilibrium in computer simulations using constant-pH molecular dynamics. **S. Campos**, P. Magalhaes, C.A. Canvalhada, L. Filipe, M. Machuqueiro, **A.M. Baptista**

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Metal Organic Frameworks for Catalysis Applications

O. K. Farha, J. Gascon, *Organizers*

M. Eddaoudi, P. K. Thallapally, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CATL 124. Metal-organic frameworks for sustainable catalysis. **W. Lin**

1:40 CATL 125. Porphyrinic metal-organic frameworks for photoredox catalysis. **J. Zhang**

2:05 CATL 126. Imparting functionality to biocatalysts via embedding enzymes into metal-organic frameworks by a de novo approach. **C. Tsung**

2:30 CATL 127. Withdrawn.

2:55 Intermission.

3:10 CATL 128. Palladium nanoparticles encapsulated in metal-organic frameworks and their catalytic properties. **R. Cao**

3:45 CATL 129. Impact of introduction of basic sites on adsorptive and catalytic properties of fcu metal organic frameworks. **J.A. Navarro**

Section D

Renaissance Boston Waterfront
Pacific Blrm A

Symposium Honoring Gary Haller

D. E. Resasco, Y. Yang, *Organizers*

X. Wang, R. S. Weber, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CATL 130. Manipulating metal and metal oxide catalysts with their environment. **H. Kung**, M. Kung

1:50 CATL 131. Mechanistic aspects of the hydrodeoxygenation of m-cresol over supported metal catalyst. **D.E. Resasco**, Q. Tan, G. Wang, L. Nie

2:20 CATL 132. Growth, structure, and properties of pure and doped 2D silica. **E. Altman**

2:50 Intermission.

3:05 CATL 133. Atomically-dispersed supported metal catalysts for the low-temperature water-gas shift reactions. **M. Flytzani-Stephanopoulos**, M. Yang

3:35 CATL 134. Au-Pd bimetallic nanoparticle catalysts and their application in selective oxidation. **Y. Yang**

4:05 Concluding Remarks.

Section E

Renaissance Boston Waterfront
Pacific Blrm B

Nano Catalysis

Y. Lei, Y. Xu, *Organizers, Presiding*

1:00 CATL 135. Control of catalyst performance using nanometer-scale films. **J.W. Medlin**

1:30 CATL 136. Fibrous nanosilica (KCC-1) based nanocatalysts. **V. Polshettiwar**, B. Singh, R. Singh, M. Dhiman

2:00 CATL 137. Designing metal nanocatalysts for hydrogen release from liquid-phase hydrogen storage materials. **M. Yadav**, A. Singh, N. Tsumori, Q. Xu

2:20 CATL 138. Mechanism for benzyl alcohol oxidation on carbon-supported Pd nanoparticles. **A. Savara**, C. Chan-Thaw, I. Rossetti, A. Villa, L. Prati

2:40 CATL 139. Unsupported rhenium nanocrystalline catalyst for acceptorless dehydrogenation of alcohols and amines. **J. Yi**

3:00 Intermission.

3:10 CATL 140. Role of chloride in the genesis of supported nanoparticles from adsorbed platinum precursors. **J.R. Regalbuto**, J. Samad

3:40 CATL 141. Rational interpretation of catalytic performances of CoMo hydrotreating catalysts — on the role of mixed sites. **B. Guichard**, V. Costa, M. Digne, P. Raybaud

4:00 CATL 142. Catalytic performance and structure evolution of LaCoO_3 perovskite in the deoxidization of coal bed methane. **Z. Zhao**, J. Ma, Y. Guo, Y. Guo, w. Li

4:20 CATL 143. Withdrawn.

4:40 CATL 144. Controlled fabrication and enhanced photocatalytic hydrogen evolution of CdS/Au/MIL-101(Cr) heterostructure. **Y. Wang**, Y. Zhang, Z. Jiang, Y. Liu, G. Jiang, Z. Zhao, A. Duan, C. Xu

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Surface Science

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Heterogeneous Catalysis for Water and Air Treatment

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Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions

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MONDAY EVENING

Section A

Westin Boston Waterfront
Galleria

Catalysis Poster Session

K. K. Ramasamy, *Organizer*

6:30 - 8:30

CATL 145. Racemization of tertiary alcohols with heterogeneous acid catalyst. **T. Gorbé**, J.E. Backvall

CATL 146. Catalytic aerobic oxidations with iron and cobalt nanoparticles supported by graphene. **N. Bedair**, K. Ding

CATL 147. Catalytic reactivities of nickel nanoparticles supported by graphene. **S. Aleid**, K. Ding

CATL 148. Exploring the mode of action of multifunctional organocatalysts using theoretical active site models. **S. Alsancaak**, Y. Çamlisoy, N. Celebi-Olcum

CATL 149. Exploring natural proteins as catalysts for the Morita Baylis Hillman reaction. **T. Utner**, N. Celebi-Olcum

CATL 150. Competing reaction pathways in the cinchona catalyzed reactions of oxindoles with nitrosobenzene: A DFT study. **Y. Çamlisoy**, S. Alsancaak, N. Celebi-Olcum

CATL 151. Immunogenicity study of Globo H analogs with modification at the reducing or non-reducing end of the tumor antigen. **H. Lee**, C. Chen, T. Tsai, S. Li, K. Lin, Y. Cheng, C. Ren, T. Cheng, C.Y. Wu, C. Wong

CATL 152. Pyroaurite — structural characteristics and morphology as a function of cation composition. **M. Jitianu**, **G. Jonathan**, A. Patel, H. Quinones, T. Mc Clurg, A. Jitianu

CATL 153. TiO_2 and hydrotalcite composites for photocatalytic decomposition of vanillin. **M. Jitianu**, **T. Mc Clurg**, M. Baraniak, N. O'Connor, A. Jitianu

CATL 154. Self-assembly of a hybrid material for synergistic catalytic hydrogen evolution. **W. Guo**, H. Lv, Z. Chen, K.P. Sullivan, S. Lauinger, T. Lian, C.L. Hill

CATL 155. Structural and dynamical properties of water on defected BaTiO_3 surfaces: DFT and ab initio molecular dynamic simulations. **W. Sailuum**, N. Artrith, A.M. Kolpak

CATL 156. Towards hybrid catalysts involving encapsulation of transition metal complexes in metal-organic frameworks (MOFs). **Z. Li**, J.V. Morabito, R. Kyada, J.A. Byers, C. Tsung

CATL 157. Catalytic acceptorless dehydrogenation of alcohols over Ag and Pd nanoparticles immobilized on tunable hydrotalcites. **J. Bain**, A. Voutchkova

- CATL 158.** Synthesis of a TiO₂-modified unsupported Ni₂P catalyst with high HDN activity. **M. Lu, M. Li**
- CATL 159.** Porous cobalt oxide nanoparticles for electrocatalytic oxygen evolution reaction. **J. Ryu, S. Park, J. Jang, H. Kim, S. Yoo**
- CATL 160.** Hydrogen generation from hydrolysis of ammonia borane catalyzed by heterogeneous gas-phase synthesized bimetallic Pt-Ni nanoparticle. **K. Aranishi, C. Cassidy, V. Singh, M. Sowwan**
- CATL 161.** Magnetically recyclable mesoporous iron oxide supported Pd nanoparticles for catalytic nitrobenzene hydrogenation. **T. Jiang, S. Du, T. Jafari, W. Zhong, W. Song, Z. Luo, S.L. Suib**
- CATL 162.** Atomic layer-by-layer deposition of platinum on palladium octahedra for enhanced catalysts toward the oxygen reduction reaction. **X. Wang, J. Park, L. Zhang, Y. Xia**
- CATL 163.** Ruthenium-catalyzed synthesis of α -deuterated polyols for hyperpolarized imaging. **D. Sail, A. Opina, O. Vasalathy, J.B. Mitchell, M.C. Krishna, R.E. Swenson**
- CATL 164.** Catalytic deconstruction of model lignin compounds in ionic liquids. **H. Parker, T. Dutta, S. Singh, B.A. Simmons, M. Jones, C. Chuck**
- CATL 165.** Solid acid-catalyzed hydrogen transfer to breaking C_{ar}-C_{alk} bond in α,ω -diaryllkanes. **X. Yue, X. Wei, B. Sun, Y. Wang, Z. Zong**
- CATL 166.** Ruthenium catalyzed dehydrogenation and transfer hydrogenation reactions using dimethylamine borane as a hydrogen storage. **S. Tanyildizi, I.A. Morkan, S. Ozkar**
- CATL 167.** Stability of linker groups for immobilization of active single-site catalysts on hydrocalcite supports. **M. Finn, A. Azua-Barrios, A. Voutchkova-Kostal**
- CATL 168.** Effect of the propane dehydrogenation catalyst regeneration on PtSn/Al₂O₃ catalysts. **S. Kim, H. Koh, G. Kim, B. Lee, h. Lee**
- CATL 169.** Hydroxyl-functionalized microporosity organic polymer: Synthesis and high catalytic activity for chemical fixation of CO₂ to cyclic carbonates. **X. Zhang, G. Du, X. Liu, Z. Zhao, J. Liu, Y. Lu, S. Yan**
- CATL 170.** Chemo-enzymatic synthesis of ω -hydroxy fatty acids and α,ω -dicarboxylic acids from fatty acids. **H. Jang, K. Singha, J. Park, Y. Kwon**
- CATL 171.** Rationalization of the interaction between surface species and MO (MO = ZrO₂ and Al₂O₃). **Y. Choi, R. Bunama**
- CATL 172.** Ordered mesoporous carbon spheres supported Pt nanoparticles for enhanced electrocatalytic activity and durability. **L. Xu, C. Zhang, N. Shan, T. Sun, J. Chen, Y. Yan**
- CATL 173.** MoS₂ quantum dots for organic synthesis. **J. Park, F. Raza, J. Kim**
- CATL 174.** Chemistry and reactivity of hydrogen on γ -molybdenum nitride. **E.A. Mader, B.M. Wyratt, J.R. Gaudet, D. Pardue, A. Marton, S. Rudic, T. Cundari, J.M. Mayer, L.T. Thompson**
- CATL 175.** Mesoporous ceria nanoparticles: A redox-driven catalyst for the low-temperature water gas shift. **D. Vovchok, C. Guild, S.D. Senanayake, J. Llorca, W. Xu, S.L. Suib, J. Rodriguez**
- CATL 176.** In situ production of biodiesel using Lewis acid catalysts and *Lesquerella fendleri* seeds. **R. Hart, D.J. Casadonte**
- CATL 177.** Low-temperature alcohol dehydrogenation: A model reaction for biomass activation. **X. Zhang, J.M. Venegas, S.J. Desrochers, F. Zhu, M. Emmert**
- CATL 178.** Synthesis of mesoporous organosilicas containing 1,8-naphthalimides by the co-condensation method and their use as catalysts for the photodegradation of methylene blue. **B. Castanheira, F. J. Trindade, E.R. Triboni, M. Politi, S. Brochsztain**
- CATL 179.** Withdrawn.
- CATL 180.** Withdrawn.
- CATL 181.** Controlling catalyst structural dynamics to maximize electrocatalytic H₂ production rates. **A.P. Cardenas, M. Helm, R. Bullock, M. O'hagan**
- CATL 182.** Synthesis of novel (N-heterocyclic carbene) palladate complexes and their catalytic activity. **D. Guest, M. Roe, O. Navarro, B. Atualpa, V. Menezes da Silva, A. de Lima Batista**
- CATL 183.** Selective hydrogenation of biomass-derived 5-hydroxymethyl-furfural using functionalized polymer supported Ru nanoparticles catalyst. **J. Hwang, A. Dabbawala**
- CATL 184.** Rational design and synthesis of porous coordination polymers with large 1D channels and strong Lewis acid sites. **T. Kajiwara, M. Higuchi, H. Higashimura, S. Kitagawa**
- CATL 185.** Survey of nanostructured transition metal phosphide catalysts for carbon dioxide reduction. **S.A. Francis, J.C. Crompton, D. Torelli, I.M. Ferrer, R.E. Schaak, B.S. Brunshwig, N.S. Lewis**
- CATL 186.** Facile synthesis of hierarchical PS/PANI nanostructure supported Cu(II) complexes: Study of its aerobic oxidation catalytic applications and mechanic study using mobile big data appliance. **H. Wang**
- CATL 187.** CO₂ reforming of CH₄ to syngas over Ni/Nd/SBA-15 catalysts --- effects of Nd modification on catalytic performance. **H. Liu, D. He**
- CATL 188.** Synthesis characterization and photocatalytic studies of magnetic nanoparticle-silica-titania composites. **R. Serrano Garcia**
- CATL 189.** Study on the catalytic sweetening performance of cobalt sulfonated phthalocyanine synthesized with microwave method. **N. Cui, Z. Chen, H. Zhang, L. Zhu, N. Shi, D. Xia**
- CATL 190.** Condensed phase ketonization of organic acids produced by the hydrothermal liquefaction of lignocellulosic biomass. **A.R. Cooper, J.G. Frye, S. Lee, K.O. Albrecht**
- CATL 191.** Design and synthesis of mesoporous zeolites using small molecule and polymeric organosilanes. **S. Fernandez, K. Zhang, J. O'Brien, T. Pilyugina, S.L. Kobaslija**
- CATL 192.** Withdrawn.
- CATL 193.** Synthesis of BiO₂Cl₂/BiO₂Br₂/BiO₂I₂ heterojunctions: Characterization, photocatalytic activity, and degradation mechanisms. **C. Chen, C. Siao, Y. Jiang**
- CATL 194.** Oxidation energy storage of photocatalytic degradation for acid orange 7 by p-ZnO/n-TiO₂ bilayer film catalyst. **U. Sittiwong, P. Rangsunvigit, P. Ngaotrakanwivat**
- CATL 195.** Influences of alkalinity and inorganic anions on the PA degradation during CeO₂ catalytic ozonation. **W. Qun, Y. Zhichao, X. He**
- CATL 196.** Novel Ag@AgCl cubic cages modified with Cu(II) cocatalyst. **Y. Pang, C. Chen, L. Ge**
- CATL 197.** Electronic and reactive properties of defect-engineered metal-organic frameworks studied by UHV-FTIR spectroscopy. **M. Kauer, Y. Wang**
- CATL 198.** Well-defined supported aluminum hydride: A Utopian dream? **B. Werghe, A. Bendjeriou-Sedjerari, J.M. Basset**
- CATL 199.** Effect of cerium addition on the catalytic performance of CoMo sulfide catalysts in selective hydrodesulfurization of FCC gasoline. **P. Yu, M. Ke**
- CATL 200.** Adsorption/oxidation of methyl mercaptan onto modified activated carbons: Effects of oxygen functional groups and transition metals. **Q. Liu, D. Chen, M. Ke**
- CATL 201.** Quick and effective immobilization of P25 TiO₂ nanolayers on gold substrates by sub-monolayer gold electrodeposition from a TiO₂ suspension. **A.L. Baccaro, I.G. Gutz**
- CATL 202.** Au/graphene oxide/carbon nanotube flexible catalyst film: Synthesis, characterization, and its application for catalytic reduction of 4-nitrophenol. **F. Yang, C. Wang, Y. Li**
- CATL 203.** MnO_x catalysts for oxygen reductions and water oxidations. **C. Kuo, I. Mosa, J. Rusling, S.L. Suib, J. He**
- CATL 204.** Visible light mediated photoredox reactions catalyzed by PIB-bonded ruthenium bipyridine complex. **Y. Liang, D.E. Bergbreiter**
- CATL 205.** Modeling Iridium-based alloys for ethanol oxidation in fuel cell applications. **L. Mehdizadegan Namin, N.A. Deskins**
- CATL 206.** Enzymatic resolution of α,β -CHX (X = F, Cl)-ATP diastereomers by a protein kinase. **F. Ni, A. Kung, C.E. McKenna, C. Zhang**
- CATL 207.** Asymmetric "click" chemistry focusing on the copper catalyzed azide-alkyne cycloaddition. **W.D. Brittain, B. Buckley, J.S. Fossey**
- CATL 208.** Effect of Pt and Cu-Mn catalysts preparation method on the CO oxidation. **H. Lee, H. Koh, J. Jung, S. Kim, Y. Choi**
- CATL 209.** Photocatalytic properties of vanadate species as function of surface coverage. **B. Kortewille, T. Rath, J. Strunk**
- CATL 210.** Improved metathesis catalysts for propylene production: Correlating synthesis parameters with chemical and physical properties to enhance activity. **T.J. Kucharski, B.S. Hanna, M.P. Bukhovko, S. Shaikh, R.H. Abudawood, J. O'Brien, S. Fernandez, M.L. Ostraat**
- CATL 211.** Reduction reactions of nitroaromatic compounds catalyzed by silver nanoparticles. **H. Lee, J. Park, F. Raza, D. Yim, J. Kim**
- CATL 212.** Antimicrobial properties of graphitic carbon nitride (g-C₃N₄): Photocatalytic production of reactive oxygen species to reduce microbial growth. **J.H. Thurston, K. Cornell, N. Hunter**
- CATL 213.** Role of solvent in transition metal surface chemistry: A density functional theory study. **S. Iyemperumal, N.A. Deskins**
- CATL 214.** Growth of carbon nanofibers synthesized from decomposition of liquid organic waste on a Ni/Al₂O₃ catalyst: Thermodynamic and kinetic analyses. **A.S. Ismail**
- CATL 215.** Mechanism study on photocatalytic performance of electrospun TiO₂ nanofibers with different rutile fractions on degradation of phenazopyridine. **J. Liu, D.L. McCarthy, M.J. Cowen, E.A. Obuya, J.B. Decoste, W.E. Bernier, W.E. Jones**
- CATL 216.** Activation of CO₂ as a carbon source for carboxylic acid derivatives. **J. Park, K. Stowers**
- CATL 217.** CO adsorption induced inverse surface segregation of Pd on Au/Pd bimetallic surfaces and its effect on CO oxidation pathway. **H. Kim, G. Henkelman**
- CATL 218.** Fabrication and characterization of aluminum-supported Pd, Rh, and Rh-Pd nanoparticles for hydrode-bromination application. **K. Chiu**
- CATL 219.** Ring opening polymerization of *Rac*-lactide using zinc amine-bis(phenolate) complexes. **Y. Liu, C.M. Kozak**

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

K. K. Ramasamy, *Organizer*

8:00 - 10:00

- CATL 220.** Catalytic defunctionalization of amino acids to value-added amines, nitriles, or amides. **D. De Vos, L. Claes, F. De Schouwer, J. Verduyck, M. Janssen**
- CATL 221.** Catalytic oxidation of low-concentration NO over Cr-based catalysts at room temperature: Significant promotion effect of ZrO₂. **A. Wang, W. Zhan, W. Li, Y. Guo, G. Lu, Y. Guo**
- CATL 222.** Synergism of Co₃O₄ with Bi₂O₃ to strengthen the catalytic performance for soot oxidation and NOx reduction in diesel exhaust. **Z. Shang, W. Li, Y. Guo, Y. Guo**
- CATL 223.** Strategy to tune CO adsorption strength and oxygen activation simultaneously: Ultralow-temperature CO oxidation on Co₃O₄-based catalyst. **Y. Cai, G. Lu, Y. Guo, Y. Guo, W. Li**
- CATL 224.** Cascade engineered synthesis of ethyl benzyl acetoacetate over a novel multifunctional catalyst. **G.D. Yadav, S.C. Patankar**
- CATL 225.** From photocatalysis to micro/nanomotors: Light-controlled motion speed, direction, and swarming behaviors. **F. Mou, C. Chen, Y. Li, L. Kong, L. Xu, J. Guan**
- CATL 226.** Regeneration of Rh- and Pd-based automotive three way catalysts after simulated fuel shutoff. **Q. Zheng, R.J. Farrauto, M. Deeba, I. Valsamakis**
- CATL 227.** Enhanced catalytic activity for NO oxidation over A or B site doping of hexagonal phase LaCoO₃: A combined experimental and theoretical study. **H. Yin, C. Zhou, X. Liu, R. Chen, B. Shan**

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CATL 228. Mechanism of intramolecular rhodium and palladium catalyzed alkene alkoxyfunctionalizations. **M. Alghamdi**, L. Cavallo, A. Poater, I. Falivene

CATL 229. Toward efficient bio-inspired H₂ oxidation catalysts: From enzymatic function to functional mimics. **N. Kumar**, B. Ginovska-Pangovska, M. Helm, R. Bullock, W.J. Shaw, **S. Rauegi**

CATL 230. Synthesis of BiOCl / BiVO₄ composites photocatalyst with improved visible-light photocatalytic activities. **L. Song**, Y. Zheng

CATL 231. Functional group modification of mixed-linker metal-organic frameworks for ethylene oligomerization. **B. Liu**, S. Jie, Z. Bu, B. Li

CATL 232. Withdrawn.

CATL 233. Withdrawn.

CATL 234. Catalytic high pressure H₂ and CO₂ production from formic acid in the presence of Ir catalyst. **H. Kawanami**, M. Iguchi, Y. Manaka, Y. Himeda

CATL 235. Withdrawn.

TUESDAY MORNING

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

2015 ACS Catalysis Lectureship

Cosponsored by INOR

M. Helm, E. S. Wiedner, *Organizers*

T. B. Rauchfuss, *Presiding*

8:00 CATL 236. Electrocatalytic production and oxidation of H₂: Molecular catalysts that mimic the functionality of enzymes. **M. Helm**, J. Darmon, S. Rauegi

8:30 CATL 237. New oxovanadium catalysts for selective aerobic oxidation of lignin models and extracts. **R. Baker**

9:00 CATL 238. Extending the roles for the pendant base in [FeFe]-Hydrogenase active site mimics. **M.Y. Darensbourg**

9:30 CATL 239. Models for the active sites of hydrogenase enzymes: The role of the second coordination sphere. **S.A. Koch**, M. Millar, L. Gan

10:00 Intermission.

10:15 CATL 240. New dithiolates for biomimetic HER catalysis. **T.B. Rauchfuss**, W. Wang, P. Zhao, Y. Li, M. Carlson

10:45 CATL 241. Design of molecular electrocatalysts for the production and oxidation of hydrogen. **R. Bullock**, D.L. DuBois, M. Rakowski DuBois, M. Helm, M. Dupuis, S. Rauegi, J.Y. Yang, S. Hammes-Schiffer, J.A. Roberts, M. O'Hagan, W.J. Shaw, A.M. Appel, E.S. Wiedner

11:25 Concluding Remarks.

Section B

Renaissance Boston Waterfront
Caspian

Computational Catalysis

R. S. Assary, **N. Kumar**, *Organizers*, *Presiding*

8:00 CATL 242. Survival-of-the-most-transferable: Better density functionals from a combinatorial design strategy. **N. Mardirossian**, **M.P. Head-Gordon**

8:30 CATL 243. Lateral interactions, uncertainty quantification, and model discrimination in computational catalysis: A case study for the water-gas shift reaction. **A. Heyden**

9:00 CATL 244. Developing the computational framework to design effective catalysts. **P.M. Zimmerman**

9:30 CATL 245. Evaluating uncertainty in Density Functional Theory for computational catalysis. **H.J. Kulik**, E. Ioannidis

10:00 Intermission.

10:15 CATL 246. First principles analysis of metal and oxide-metal interfacial catalysis. **J. Greeley**, Z. Zhao, B. Liu, T.S. Choksi, P. Majumdar

10:45 CATL 247. Ab initio approach for prediction of oxide surface structure, stoichiometry, and electrocatalytic activity in aqueous solution. **X. Rong**, A.M. Kolpak

11:15 CATL 248. Enabling the computational design of multifaceted catalysts through structure-sensitive scaling relations. **F. Calle-Vallejo**, D. Loffreda, M.T. Koper, P. Sautet

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Catalysis by Mixed Oxides

M. Guerrero-Pérez, I. E. Wachs, *Organizers*, *Presiding*

8:30 CATL 249. Structure-reactivity relationship in mixed metal oxides. **H. Freund**

9:00 CATL 250. Support morphology effect in oxide catalysis: Vanadia clusters supported on ceria and titania nanoshapes. **Z. Wu**, V. Schwartz, S.K. Kraemer, Y. Tsai, M. Li, A. Rondinone, S.H. Overbury

9:30 CATL 251. Square pyramidal structure of oxo vanadium (V) and (IV) species over low coverage VOx/TiO₂ anatase catalysts. **L. Arnarson**, S. Rasmussen, H. Falsig, J. Lauritsen, P. Moses

10:00 Intermission.

10:15 CATL 252. Positive influence of promoters on the dispersion of metal oxide on SiO₂ support. **C.A. Carrero**, I. Hermans, J. Grant

10:45 CATL 253. Vanadium based mixed oxide nanofibers prepared by electrospun. **R. Berenguer**, **M. Guerrero-Perez**, I. Guzman, J. Fornells, J. Rodriguez-Mirasol, C. T.

11:15 CATL 254. Combined in situ molecular spectroscopic and DFT study of ethylene polymerization by supported CrO_x/SiO₂ catalysts. **A. Chakrabarti**, M. Gierada, J. Handzlik, I.E. Wachs

Section D

Renaissance Boston Waterfront
Pacific Blrm A

SABIC Young Catalysis Investigator Award: Symposium In Honor of Melanie Sanford

J. Montgomery, *Organizer*, *Presiding*

K. L. Hull, *Presiding*

8:30 CATL 255. Enantioselective redox-relay Heck reactions. **M.S. Sigman**

9:00 CATL 256. Proton-coupled electron transfer in organic synthesis and asymmetric catalysis. **R. Knowles**

10:00 Intermission.

9:30 CATL 257. Catalytic regioselective and regiodivergent functionalization of alkenes, alkynes, arenes, and allenes. **J. Montgomery**

10:15 CATL 258. Fundamental organometallic reactions to promote aerobic oxidation of hydrocarbons. **K.I. Goldberg**

10:45 CATL 259. Transition metal catalyzed C–N bond formation. **K.L. Hull**

11:15 CATL 260. Development of catalytic C–H functionalization reactions. **M.S. Sanford**

Section E

Renaissance Boston Waterfront
Pacific Blrm B

Nano Catalysis

Y. Lei, **Y. Xu**, *Organizers*, *Presiding*

8:00 CATL 261. Nanometrology of supported metal catalysts: The splendors and miseries of X-ray absorption spectroscopy. **A. Frenkel**

8:20 CATL 262. Developing bismuth-based compounds as photocatalysts for pollutants degradation. **Q. Han**

8:40 CATL 263. Novel tantalum oxyfluoride photocatalytic materials for hydrogen production. **L. Xu**, L. Deng, J. Guan

9:00 CATL 264. Unraveling the strong metal oxide-support interaction between RuO₂ and TiO₂ in superior light-driven H₂ production. **T. Nguyen Phan**, S. Luo, D. Vovchok, J. Llorca, D.E. Polyansky, E. Fujita, S.D. Senanayake, D.J. Stacchiola, J. Rodriguez

9:20 CATL 265. AuPd binary alloy nanoparticles decorated graphitic carbon nitrides for efficient photocatalytic hydrogen production. **C. Han**, L. Ge, C. Chen

9:40 CATL 266. Layered manganese oxides for formaldehyde-oxidation at room temperature: the effect of interlayer protons. **J. Wang**, D. Li, Y. Yang

10:00 Intermission.

10:10 CATL 267. Direct comparison of morphologically equivalent Co₃P and CoP nanoparticles as electrocatalysts for the hydrogen evolution reaction. **J. Callejas**, C.G. Read, J. McEnaney, E.J. Popczun, R.E. Schaak

10:30 CATL 268. Cobalt oxide nanocubes for photocatalytic water oxidation. **F. Jiao**

10:50 CATL 269. Effect of synthesis parameters on electrocatalytic performance of bimetallic iron and nickel nanoparticles for methanol oxidation. **S. Candelaria**, N. Bedford, L.F. Greenlee

11:10 CATL 270. Recent developments in nanocatalysts for fuel cell reactions. **S. Guo**

11:30 CATL 271. Nanostructured catalytic materials for hydrogenation of carbon dioxide. **H. Zeng**

Section F

Renaissance Boston Waterfront
Pacific Blrm H

In-Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles

B. Roldan-Cuenya, *Organizer*

J. A. Boscoboinik, **D. J. Stacchiola**, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CATL 272. Structure and reactivity of surfaces in vacuum and under ambient gas pressure. **M. Salmeron**

9:10 CATL 273. Caught in the act! Live observations of catalysts using high-pressure scanning probe microscopy. **I. Groot**

9:45 CATL 274. Characterization of bimetallic and carbide catalysts under reaction conditions. **J.G. Chen**

10:20 Intermission.

10:35 CATL 275. Investigation of solid/vapor, solid/liquid and liquid/vapor interfaces using photoelectron spectroscopy. **H. Bluhm**

11:10 CATL 276. Ambient pressure XPS observation of electrode surfaces during electrochemical reactions. **H. Ogasawara**

11:45 CATL 277. Structural and chemical transformations in model nanoparticle catalysts measured by ambient pressure XP. **H. Mistry**, F. Behafarid, C. Lumdee, J.A. Boscoboinik, B. Roldan-Cuenya

12:05 CATL 278. Potassium-promoted Cu₂O/Cu(111) reduction by CO. **I. Waluyo**, K. Mudiyansele, F. Xu, W. An, P. Liu, J.A. Boscoboinik, J. Rodriguez, D.J. Stacchiola

12:25 Concluding Remarks.

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Theory & Powder Catalysts

Sponsored by ENFL, Cosponsored by CATL

Innovative Chemistry & Electrocatalysis for Low-carbon Energy & Fuels: Discovery to Application

OER & HER

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Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions

Sponsored by COLL, Cosponsored by CATL

TUESDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

CO₂ Reduction and Utilization

D. Pakhare, **A. Raju**, *Organizers*, *Presiding*

1:00 CATL 279. Reforming for CO₂ utilization. **G. Kale**

1:30 CATL 280. CO₂ reforming of methane over Ni-based pyrochlore catalyst in the presence of oxygen. **N. Kumar**, J.J. Spivey

1:50 CATL 281. CO₂ conversion to syngas through the steam-biogas reforming process. **P. Roy**, K. Kim, C.S. Park, A. Raju

2:10 Intermission.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

2:25 CATL 282. CO₂ hydrogenation at extreme pressure and temperature using diamond anvil cell and FTIR spectroscopy. **M. Sangwan, T. Strobel**

2:55 CATL 283. CO₂ hydrogenation over Ru supported catalysts using electronegative and electropositive promoters. **A. Katsaounis, I. Kalaitzidou, M. Makri, D. Thelertis, C. Vayenas**

3:15 CATL 284. Catalytic conversion of CO₂ to fuel and chemicals. **Y. Sun, H. Wang, W. Wei**

3:45 CATL 285. Optimization of pyrochlore catalysts for dry reforming of methane. **F. Polo Garzon, D.A. Bruce**

Section B

Renaissance Boston Waterfront
Caspian

Computational Catalysis

R. S. Assary, N. Kumar, *Organizers, Presiding*

1:00 CATL 286. Computational studies of CO₂ reduction mechanisms on size-specific supported catalysts. **P. Zapol, C. Liu, B. Yang, S. Vajda, L.A. Curtiss**

1:30 CATL 287. O₂ and AgAu alloys: Surface structure and reactivity. **M. Montemore, E. Kaxiras, C.M. Friend, R.J. Madix**

1:50 CATL 288. Molecular-level insights into the role of water on Pt(111)-catalyzed glycerol and methanol decomposition using a combined DFT/MD model. **C.J. Bodenschatz, T. Xie, R. Getman**

2:10 CATL 289. Withdrawn.

2:30 Intermission.

2:45 CATL 290. Computational study on the selective C-O bond cleavage of lignin-derived ethers over supported Ni catalysts. **D. Mei, J. He, J.A. Lercher**

3:15 CATL 291. First-principles studies of furan upgrading by Ga/ZSM-5. **L. Cheng, L.A. Curtiss, R.S. Assary**

3:35 CATL 292. Quantum mechanical study of furan formation over transition metals-exchanged zeolites. **S. Kim, D. Robichaud, C. Mukarakate, T. Evans, L. Bu, M. Xu, B.G. Trewyn, R.S. Paton, M.R. Nimlos**

3:55 CATL 293. Understanding the active Cu₂O_x sites for methane selective oxidation to methanol in zeolite: A computational study. **Z. Zhao, L. Vilella, F. Studt**

4:15 CATL 294. Oxidation of carbon monoxide with a monovalent Zn⁺ ion embedding on zeolite: A mechanistic study. **S. Wannakao, T. Maihom, M. Probst, J. Limtrakul**

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Catalysis by Mixed Oxides

M. Guerrero-Pérez, I. E. Wachs, *Organizers, Presiding*

1:00 CATL 295. Rational design of Zn₂Zr₂O₇ catalyst for direct conversion of biomass-derived oxygenates to olefins. **Y. Wang, J. Sun**

1:30 CATL 296. Catalysts and their characteristics for the conversion of ethanol to butadiene. **B.F. Sels, W. Janssens, E.V. Makshina**

2:00 CATL 297. Toward efficient lignin valorization: Highly-selective hydrogenation and hydrogenolysis of model compounds using a copper-doped hydroxalcalite derivative. **L. Petitjean, E.S. Beach, D. Xiao, P.T. Anastas**

2:30 Intermission.

2:45 CATL 298. High-yield selective conversion of carbohydrates to methyl levulinates using mesoporous sulfated titania-based catalysts. **E. Njagi, H.C. Genuino, C. Kuo, S. Dharmarathna, A. Gudz, S.L. Suib**

3:15 CATL 299. Catalytic methyl mercaptan coupling to olefins: DFT study of the first C-C bond formation. **W. Michaels, T. Bucko, M. Makkee, J. Baltrusaitis**

3:45 CATL 300. Determining the catalyst structure and active sites of the high temperature Cr₂O₃-Fe₂O₃ water-gas shift. **M. Zhu, T. Rocha, A. Knop-Gericke, R. Schloegl, I.E. Wachs**

4:15 CATL 301. Alkali-doped manganese oxides as redox catalysts for oxidative dehydrogenation of ethane. **L. Neal, S. Yusuf, J. Sofranko, F. Li**

Section E

Renaissance Boston Waterfront
Pacific Blrm B

Nano Catalysis

Y. Lei, Y. Xu, *Organizers, Presiding*

1:00 CATL 302. Phenol degradation by heterogeneous electro-Fenton process using bi-metallic (Fe-Cu) allophane nanoclays as iron dosage. **E.G. Garrido, F. Olivares, M.S. Ureta-Zanartu**

1:20 CATL 303. MoS_x grown on graphene for highly efficient catalytic hydrogen evolution reaction. **X. Geng, T. Chen, W. Wu, W. Sun, B. Chen, Y. Al-Rikabi**

1:40 CATL 304. Metal oxides@metal-organic-frameworks as efficient electrocatalysts for oxygen reduction/evolution reactions in an alkaline electrolyte. **H. Wang, F. Yin, G. Li, B. Chen**

2:00 CATL 305. Porous carbon nitride networks with O-doping for efficient photocatalytic hydrogen evolution. **Z. Huang, J. Song, J. Zou, X. Zhang, Z. Wang, K. Li, S. Ding**

2:20 CATL 306. Graphene/TiO₂ composite electrode toward the oxygen reduction reaction. **A.M. Abdullah, H.A. Al-Kandari, S.A. Al-Kandari, A.M. Mohamed**

2:40 Intermission.

2:50 CATL 307. Transformations of 1-(2-aminophenyl)propan-2-ol to 2-methylindoline. **D. Murzin**

3:10 CATL 308. Soft-hard template approach to preparing thermally stable and highly crystalline mesoporous transition-metal oxides. **B. Liu, W. Song, Z. Luo, A. Federico, S.L. Suib, J. He**

3:30 CATL 309. One-pot encapsulation of alloyed nanoparticles using metal organic framework as crystal-line capping agent and their catalytic properties. **A.P. Young, L. Cho, C. Tsung**

3:50 CATL 310. Tailoring active sites in metal organic frameworks for selective heterogeneous catalysis. **R.J. Comito, M. Dinca, E. Metzger**

4:30 CATL 311. Oxidized Ni-W nanoparticles supported on single-walled carbon nanotubes as catalyst for ultra-deep hydrodesulfurization of gasoline. **K. Xu, C. Zhou, X. Xu, J. Kong, Y. Li**

4:50 CATL 312. Thermally stable, mixed phase (anatase/rutile) mesoporous titanium dioxide nanoparticles for visible light photocatalytic activity. **Z. Luo, A. Poyraz, C. Kuo, R. Miao, Y. Meng, S. Chen, T. Jiang, S.L. Suib**

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Powder Catalysts

Sponsored by ENFL, Cosponsored by CATL

WEDNESDAY MORNING

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

CO₂ Reduction and Utilization

D. Pakhare, A. Raju, *Organizers, Presiding*

8:30 CATL 313. Designing catalysts using an energy-based approach: Molecular catalysis for CO₂ reduction. **A.M. Appel, J.C. Linehan, E.S. Wiedner, B.R. Galan, M.S. Jeletic, S. Peterson, C.J. Weiss, D. Miller, C. Zall, S.J. Connelly**

9:00 CATL 314. Grain boundary-dependent CO₂ and CO reduction catalysis. **M. Kanan**

9:20 CATL 315. Nanoparticle active site control for CO₂ reduction. **W. Zhu, Y. Zhang, H. Zhang, A. Peterson, S. Sun**

9:40 CATL 316. Hydroxalcalite-like compounds derived highly effective Cu-based catalysts for CO₂ hydrogenation to methanol. **P. Gao, H. Wang, S. Xiao, Y. Zhang, W. Wei, Y. Sun**

10:00 Intermission.

10:15 CATL 317. Dual function materials for CO₂ capture and conversion using renewable H₂. **M.A. Arellano, M.S. Duyar, R.J. Farrauto**

10:35 CATL 318. CO₂ reduction mechanisms by (PoCoP)Ir and (PeXeP)Co pincer catalysts for production of formate and CO. **S.I. Johnson, R.J. Nielsen, D.W. Shaffer, J.Y. Yang, W.A. Goddard**

10:55 CATL 319. Computational studies of chemical and electrochemical CO₂ reduction: From metals surfaces and metal clusters to semiconductors. **C. Liu, B. Yang, P. Zapol, A. Salehi-Khojin, L.A. Curtiss**

11:15 CATL 320. One-pot catalytic conversion of microalgae to glycol in water over nickel-based catalysts. **L. Kong, L. Wang, Q. Zhao, W. Wei, Y. Sun**

Section B

Renaissance Boston Waterfront
Caspian

Computational Catalysis

R. S. Assary, N. Kumar, *Organizers, Presiding*

8:00 CATL 321. Finite size effects in submonolayer catalysts. **L. Grabow, H. Doan, Q. Yuan, S. Brankovic**

8:30 CATL 322. Toward a more accurate description of adsorption in Brønsted acid zeolites by combining static and dynamic molecular simulations. **J. Van der Mynsbrugge, K. De Wispelaere, P. Cnudde, V. Van Speybroeck**

9:00 CATL 323. Formic acid oxidation on platinum: A simple mechanistic study. **K. Schwarz, R. Sundaraman, T.P. Moffat, T. Allison**

9:20 CATL 324. Elucidating the mechanism of hydrodeoxygenation (HDO) of acetone on MoO₃. **B. Buesser, M. Shetty, Y. Roman-Leshkov, W.H. Green**

9:40 CATL 325. Catalytic reduction of ketones and aldehydes with Et₃O/B(C₆F₅)₃ frustrated Lewis pairs. **B. Ginovska-Pangovska, A.H. Hackel, D.M. Camaioni, G.K. Schenter, S. Kathmann, T. Autrey**

10:10 Intermission.

10:25 CATL 326. Dynamic stereographic map approach to substrate binding in organometallic chemistry. **L. Cavallo, I. Falivene, R. Credendino**

10:45 CATL 327. Oxidative addition of aryl chloride to mono ligated and bi-ligated linear/bent Au^I and Pd⁰ complexes. **S. Vummaleti, I. Falivene, A. Poater, L. Cavallo**

11:05 CATL 328. Computational screening of natural enzymes for Morita-Baylis-Hillman activity. **N. Celebi-Olcum**

11:25 CATL 329. Density functional modeling of an electrocatalyst for olefin purification. **R.K. Raju, M.B. Hall, E.N. Brothers**

11:45 CATL 330. Hydrophenoxylation of alkynes by cooperative gold catalysis. **A. Poater, S. Vummaleti, L. Cavallo, S.P. Nolan**

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Catalysis by Mixed Oxides

M. Guerrero-Pérez, I. E. Wachs, *Organizers, Presiding*

8:30 CATL 331. Photocatalytic hydrogen production by reducible oxides. **P. Fornasiero**

9:00 CATL 332. Operando FTIR, NAP-XPS, and XAS studies of Co³⁺O₄ and CeO₂-Co₃O₄ catalysts during preferential CO oxidation. **G. Rupprechter, L. Lukashuk, K. Föttinger**

9:30 CATL 333. Structure-reactivity relationships in V₂O₅/CeM_{1-x}O₂ (M = Zr, Ti) catalysts used for low-temperature NH₃-SCR of NO. **H. Vuong, J. Radnik, E. Kondratenko, U. Armbruster, A. Brueckner**

10:00 Intermission.

10:15 CATL 334. Catalytic combustion of vinyl chloride on LaMnO₃ perovskite oxides. **W. Li, Y. Guo**

10:45 CATL 335. Withdrawn.

11:15 CATL 336. Enhanced oxygen storage and redox properties by niobium-doped oxygen storage materials for three way automobile exhaust catalytic converters. **E. Leung, Q. Lin, K. Barmak, R.J. Farrauto**

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Section D

Renaissance Boston Waterfront
Pacific Blrm A

Catalytic Upgrading of Biomass

M. V. Olarte, S. Wettstein, *Organizers, Presiding*

8:00 CATL 337. Mechanistic study of lignin depolymerization in ionic liquids. **T. Dutta**, E. Wang, R. Parthasarathi, N. Isern, J. Sun, R. Chu, N. Tolic, J.R. Cort, B.A. Simmons, S. Singh

8:20 CATL 338. Biomass dissolution and dissociation in acidic and basic ionic liquids: A quantum chemical study. **R. Ramakrishnan Parthasarathi**, T. Dutta, J. Sun, B.A. Simmons, S. Singh

8:40 CATL 339. Catalytic conversion of biomass lignin to chemicals and fuels. **X. Zhang**

9:00 CATL 340. Metal substituted microporous and mesoporous zeolites with unique pore structures for selective biomass conversions. **B.G. Trewyn**

9:20 CATL 341. Development of reduced metal catalysts for bio-oil hydrotreating. **H. Wang**, S. Lee, D.B. Anderson, R. Taha, Z. Abdullah

9:40 CATL 342. Investigation of the HZSM-5 catalyzed co-pyrolysis of biomass and plastic: Product yield, carbon distribution and catalyst deactivation. **C. Dorado**, C.A. Mullen, A. Boateng

10:00 Intermission.

10:10 CATL 343. Transformation of 5-hydroxymethylfurfural to fine chemicals via homogeneous catalysis. **Z. Zhang**, Z. Xu, P. Yan, X. Liu, B. Chung

10:30 CATL 344. Direct catalytic conversion of cellulose to a liquid mixture of paraffins and naphthenes. **B. Op de Beek**, M. Dusselier, **B.F. Sels**

10:50 CATL 345. Investigation of the reaction kinetics of isolated Lewis acid sites in Beta zeolites for the Meerwein-Ponndorf-Verley reduction of methyl levulinate to γ -valerolactone. **H. Luo**, D. Consoli, W. Gunther, Y. Roman-Leshkov

11:10 CATL 346. Systematic study of alkali promotion of alumina supported ruthenium for levulinic acid hydrogenation to γ -valerolactone. **S. Cao**, C.T. Williams, S. Ma, J.R. Monnier, J.R. Regalbutto

11:30 CATL 347. Direct conversion of levulinic acid to 2-methyltetrahydrofuran using discrete Ru and Rh N-triphos catalysts. **P. Miller**, A. Phanopoulos, N.J. Long

Section E

Renaissance Boston Waterfront
Pacific Blrm B

In-Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles

J. A. Boscoboinik, D. J. Stacchiola, *Organizers*

B. Roldan-Cuenya, *Organizer, Presiding*

J. Rodriguez, *Presiding*

8:30 Introductory Remarks.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

8:35 CATL 348. Applications of the ReaxFF force field for identifying reactive properties for complex catalytic materials and interfaces. **A.C. Van Duin**, T. Senftle, C. Ashraf

9:10 CATL 349. Supported Pt clusters under a pressure of gas: Insights from DFT. **P. Sautet**

9:45 CATL 350. Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells. **S. Linic**, A. Holewinski

10:20 Intermission.

10:35 CATL 351. Characterizing working catalysts with correlated electron and photon probes. **E. Stach**, Y. Li, S. Zhao, D. Zakharov, R. Tappero, R.G. Nuzzo, A. Frenkel

11:10 CATL 352. Correlated imaging and spectroscopy studies of catalysts in *operando* conditions. **A. Frenkel**

11:45 CATL 353. Observations of dynamic restructuring of nanoporous gold during selective alcohol coupling reactions. **B. Zucig**, M.L. Personick, R.J. Madix, C.M. Friend

12:05 CATL 354. Study of Ir/CeO₂-TiO₂ catalysts for low temperature CO oxidation. **W. Li**, Y. Zhang, Y. Guo, X. Gong, Y. Guo

12:25 Concluding Remarks.

International Symposium on Mesoporous Zeolites

Sponsored by ENFL, Cosponsored by CATL, I&EC and INOR

WEDNESDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

CO₂ Reduction and Utilization

D. Pakhare, A. Raju, *Organizers, Presiding*

1:00 CATL 355. Effect of chloride anions on the synthesis and activity of nanoporous silver catalysts for CO₂ electroreduction. **Y. Hsieh**, S.D. Senanayake, Y. Zhang, W. Xu, D.E. Polyansky

1:25 CATL 356. Ionic liquid-enhanced electrocatalytic reduction of CO₂ with a homogeneous catalyst. **D.C. Grills**, Y. Matsubara, Y. Kuwahara

1:50 CATL 357. Ligand cooperativity in electrocatalytic CO₂ reduction by Mn(I) and Re(I) tricarbonyl complexes. **J.J. Rochford**, K. Ngo, R.P. Narayanan, B. Mahanti, M.E. McKinnon

2:15 CATL 358. Enhanced electrochemical reduction of CO₂ by galvanically replaced copper nanowires. **K.J. Carroll**, L. Su, Y. Hsiao, F. Brushett

2:35 CATL 359. Electroreduction of CO₂ over Cu and Au nanostructured catalyst. **H. Mistry**, R. Reske, F. Behafariz, A. Varela, P. Strasser, B. Roldan-Cuenya

2:55 CATL 360. Combined capture and conversion of CO₂ utilizing switchable ionic liquids. **M. Yadav**, J.C. Linehan, A.J. Karkamkar, D.J. Heldebrandt

3:15 Intermission.

3:30 CATL 361. Materials and systems for thermochemical carbon dioxide splitting as a route to solar fuels. **J.E. Miller**, I. Ermanoski, A. Ambrosini, E.B. Stechel, E.N. Coker, A.H. McDaniel

3:55 CATL 362. Development of inexpensive architectures for the photoelectrochemical conversion of carbon dioxide to fuels. **J. Rosenthal**, J.L. DiMeglio, J. Medina-Ramos

4:20 CATL 363. Probing the role of interfacial sites in photocatalytic CO₂ reduction on metal/TiO₂ nanocomposites. **C. Liu**, G. Li

4:45 CATL 364. Detection and investigation of side reactions in Re(I) based photocatalytic reduction of CO₂ — Improving the catalytic performance. **S. Meister**, R. Reithmeier, M. Tschurl, U. Heiz, B. Rieger

5:05 CATL 365. Hydrocarbon production from CO₂ and water with visible light on zero-valent iron nanoparticles. **M. Jayamma**, D.K. Ryan, M. Shen, M. Ruths, C. Wang, H. Ren, Q. Zhu

Section B

Renaissance Boston Waterfront
Caspiam

Computational Catalysis

R. S. Assary, N. Kumar, *Organizers, Presiding*

1:00 CATL 366. Understanding active sites for methane oxidation on Fe oxide surfaces from DFT calculations. **B. Liu**, J. Tang

1:30 CATL 367. Computational study of the effects of substituents on the ability of intramolecular frustrated Lewis pairs to activate hydrogen. **A.H. Hackel**, B. Ginovska, T. Autrey, G.K. Schenter, D.M. Camaioni

1:50 CATL 368. Density functional theory study of transition metal and metal alloy catalysts in energy production. **X. Wu**, X. Gong

2:10 CATL 369. Switching polymerization tasks at a single catalyst: Guidance from reaction mechanism discovery simulation. **A. Vitek**, K. Souther, A.J. McNeil, P.M. Zimmerman

2:30 CATL 370. Modeling the reactivity of the (Mo₁₃₂) Keplerate: Two case studies. **N.A. Bandeira**, C. Bo

2:50 Intermission.

3:00 CATL 371. Investigations into the interplay between adsorbed hydrogen and surface alloy structures in bimetallic hydrogen evolution catalysts. **J.E. Mueller**, C.S. Wildi, T. Jacob

3:20 CATL 372. Molecular dynamics simulations of the titania and water interface. **L. Chong**, S. Mushnoori, M. Dutt

3:40 CATL 373. Study of oxygen reduction reaction mechanism on Pt (111) by ab initio molecular dynamics calculations. **Y. He**, C. Chen, H. Yu

4:00 CATL 374. Theoretical study of aryl chain-rogwth polymerization by NHC Pd catalysts. **Y. Zhao**, A.J. McNeil, P.M. Zimmerman

4:20 CATL 375. Withdrawn.

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Catalysis by Mixed Oxides

M. Guerrero-Pérez, I. E. Wachs, *Organizers, Presiding*

1:00 CATL 376. Engineering complex, layered metal oxides: High performance nickelate oxide nanostructures for oxygen exchange and reduction. **E. Nikolla**

1:30 CATL 377. Water oxidation by Mn³⁺ in manganese oxides: Investigation of active sites. **P. Smith**, B. Deibert, G. Gardner, J. Li, G.C. Dismukes

2:00 CATL 378. Development of solid catalysts based on matrix of hexagonal-Nb₂O₅ /Anatase-TiO₂ and their application in catalytic photodegradation of organic compounds in aqueous medium with visible light. **Y.O. Asencios**, G. Fernandes da Silva

2:30 Intermission.

2:45 CATL 379. Nanoporous gold supported titania-ceria mixed oxides as high performance hydrogen production catalyst. **J. Shi**, A. Wittstock, M. Bäumer

3:15 CATL 380. Upgrading fuel performance using β -Mo²⁺C/S-ZrO₂. **F.F. Oloye**

3:45 CATL 381. Iron assisted Ag/MnO_x with enhanced formaldehyde removal efficiency. **D. Li**, J. Wang, P. Zhang

4:15 CATL 382. Adsorption of helium by Gibbs– Boltzmann mechanisms: Implications for helium density testing and Langmuir negative adsorption. **H. Lee**

Section D

Renaissance Boston Waterfront
Pacific Blrm A

Catalytic Upgrading of Biomass

M. V. Olarte, S. Wettstein, *Organizers, Presiding*

1:00 CATL 383. Small pore zeolites for biomass upgrading. **S. Wettstein**, S.M. Bruce, M.A. Carreon, J. Bond

1:20 CATL 384. Novel efficient dehydration of biomass using alternative technologies: A green avenue for furfural as molecule platform. **C. Len**, S. Le-Guenec, C. Ceballos, F. Delbecq

1:40 CATL 385. Withdrawn

2:00 CATL 386. Ring-opening and hydrogenation of furanic compounds on a ruthenium surface. **R. Bababrik**, Z. Zhao, A. Avoiian, B. Wang, D.E. Resasco

2:40 Intermission.

2:20 CATL 387. Hemicellulose arabinogalactan hydrolytic hydrogenation over bifunctional Ru catalysts. **D. Murzin**

2:50 CATL 388. First-principles investigation for hydrodeoxygenation of oxygenated aromatic compounds over Ru/TiO₂(110). **B. Baek**, L. Grabow

3:10 CATL 389. Selective Ni-catalyzed conversion of model and lignin-derived phenolic compounds to cyclohexanone-based polymer building blocks. **W. Schutyser**, S. Van den Bosch, J. Dijkmans, S. Turner, M. Meledina, G. van Tendeloo, D. Debecker, **B.F. Sels**

3:30 CATL 390. Toward understanding catalyzed transformation of lignin to fuels on a molecular level. **J.A. Lercher**

3:50 CATL 391. Reductive lignocellulose fractionation into soluble lignin-derived phenolic mono- and dimers and processable carbohydrate pulp. **S. Van den Bosch**, W. Schutyser, B.F. Sels

Section E

Renaissance Boston Waterfront
Pacific Blrm B

In-Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles

J. A. Boscoboinik, B. Roldan-Cuenya, *Organizers*

D. J. Stacchiola, *Organizer, Presiding*

I. Groot, *Presiding*

1:00 Introductory Remarks.

1:05 CATL 392. In-situ characterization of catalysts with infrared absorption spectroscopy: From UHV to solid-liquid interfaces. **F. Zaera**

1:40 CATL 393. In situ surface spectroscopy and surface microscopy of reforming and oxidation model catalysts. **G. Rupprechter**

2:15 CATL 394. Sum frequency generation spectroscopy reveals the molecular origin of catalyst poisoning in alcohol oxidation on a model supported palladium nanoparticle catalyst. **F. Geiger**

2:45 Intermission.

3:15 CATL 395. In situ studies on the behavior of metal/oxide catalysts during the water-gas shift reaction. **J. Rodriguez**, D.J. Stacchiola, S.D. Senanayake

3:50 CATL 396. In situ study of the reactivity of graphene-supported nanocluster arrays. **C. Papp**, K. Gotterbarm, F. Späth, H. Steinrueck

4:20 Concluding Remarks.

Innovative Utilization Pathways for Natural Gas

Sponsored by ENFL, Cosponsored by CATL

International Symposium on Mesoporous Zeolites

Sponsored by ENFL, Cosponsored by CATL, I&EC and INOR

WEDNESDAY EVENING

Heterogeneous Catalysis for Environmental Applications

Sponsored by ENVR, Cosponsored by CATL

THURSDAY MORNING

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

CO₂ Reduction and Utilization

D. Pakhare, A. Raju, *Organizers, Presiding*

8:30 CATL 397. Aldimine effect in bis(imino)pyridine complexes: Nonplanar nickel(II) complexes of a bis(aldimino)pyridine ligand. **B.R. Reed**, S.A. Stoian, R.P. Narayanan, J.J. Rochford, R.L. Lord, S. Groysman

9:00 CATL 398. Utilization of CO₂ for the synthesis of useful organic molecules. **A. Sathe**, A.T. Radosevich, R.M. Rioux

9:20 CATL 399. Direct homogeneous catalytic carbon dioxide hydrogenation to formic acid: The reversible formic acid – carbon dioxide/hydrogen cycle. **G. Laurency**

9:40 CATL 400. Electrochemical catalysis of CO₂ reduction by Re and Mn tricarbonyl halide azopyridine complexes. **J. Samonina-Kosicka**, R.M. Waymouth

10:00 Intermission.

10:15 CATL 401. Withdrawn.

10:35 CATL 402. Molecular promotion of CO₂ reduction and hydrogen evolution reactions: Case of pyridinium cation. **I. Chernyshova**, S. Ponnuram, D. Kanan, P. Somasundaran, C. Marianetti

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

Energy Storage Applications of Ammonia: Synthesis, Storage, Cracking and Utilization

B. David, M. Jones, *Organizers, Presiding*

8:00 CATL 403. Amide and imide mediated ammonia decomposition. **W.I. David**, M. Jones, J. Makepeace, T. Wood, H.M. Hunter

8:40 CATL 404. Ammonia decomposition over La₂O₃ supported co catalyst at 450 °C. **V. Poltavets**, H. Hajibabaei

9:00 CATL 405. Power generation from ammonia for decoupled green energy supply. **A. Valera-Medina**, D. Pugh, A. Crayford, T. Hughes, C. Beech, I. Wilkinson, B. David

9:20 CATL 406. Characterising solid-state ammonia storage materials. **M. Jones**, J. Hartley, A. Porch, B. David

9:40 CATL 407. Practical aspects of MCl₂ (M = Ni, Cu, Mg) as NH₃ stores: Structure-property relationships, stability, and cycling behavior. **J. Breternitz**, J.M. Hanlon, A. Godula-Jopek, D.H. Gregory

10:00 Intermission.

10:15 CATL 408. Comparing theory and INS experiments: The case of solid ammonia, unexpected result. **A. Ramirez-Cuesta**, Y. Cheng, L. Daemen

10:35 CATL 409. Ammonia decomposition catalysis using non-stoichiometric lithium imide. **J. Makepeace**, T. Wood, H.M. Hunter, M. Jones, W.I. David

10:55 CATL 410. Ammonia for renewable energy storage. **A. Savini**, D. Little, A.L. Odum, A. Singh, M.R. Smith, T. Hamann

11:15 CATL 411. Hydrolytic dehydrogenation of ammonia borane by multifunctional catalysis as hydrogen storage system. **A. Grau**, D.T. Johnson, N. Linares, **J. Garcia Martinez**

11:35 CATL 412. Isotopic studies of the ammonia decomposition reaction mediated by sodium amide. **T. Wood**, J. Makepeace, H.M. Hunter, M. Jones, W.I. David

THURSDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Atlantic Blrm 3

General Catalysis

A. Raju, K. K. Ramasamy, *Organizers, Presiding*

12:30 CATL 413. Withdrawn.

12:50 CATL 414. Role of temperature in converting ethanol to high molecular oxygenates over bi-functional MgO-Al₂O₃ catalyst. **K.K. Ramasamy**, C. Smith, M. Gray, H. Job, Y. Wang

1:10 CATL 415. Atomic insight into gold catalysis via scanning tunneling microscopy model study of Au(110). **F. Hiebel**, M. Montemore, B. Shong, C.M. Friend

1:30 CATL 416. Fundamental reactions and competition for active sites on gold single-crystal surfaces. **S.G. Karakalos**, Y. Xu, C.M. Friend, R.J. Madix

1:50 CATL 417. Regulation of Al distribution in the framework of ZSM-5 via post-treatment for catalytic cracking of n-butane. **J. Liu**, G. Jiang, Y. Zhang, Z. Zhao, C. Xu, Y. Wang, Q. Sun, A. Duan, J. Liu, Y. Wei

2:10 Intermission.

2:20 CATL 418. Efficient catalytic cracking of n-octane on nanosheets of ZSM-5 zeolite. **X. Xiao**, G. Jiang, Z. Zhao, C. Xu, Y. Wang, A. Duan, J. Liu, Y. Wei

2:40 CATL 419. Mesostructured zeolites as superior catalysts for diffusion-limited reactions: Bridging the gap between zeolites and MCM-4. **A. Grau**, N. Linares, **J. Garcia Martinez**, K. Li, J. Valla

3:00 CATL 420. Highly active Ni₂P/beta catalysts in hydrocracking of polyaromatic hydrocarbons into BTX. **Y. Kim**, Y. Lee

3:20 CATL 421. 1D modeling of transport and sulfur interactions for methane steam and dry reforming on Ni/YSZ. **W.S. Jablonski**, S. Villano, A.M. Dean

3:40 CATL 422. Co-Ni bimetallic catalyst on syngas hydrogenation. **M. Gray**, K.K. Ramasamy, H. Job, Y. Wang

Section B

Renaissance Boston Waterfront
Caspian

General Catalysis

Heterogeneous

A. J. Karkamkar, M. Yadav, *Organizers, Presiding*

12:30 CATL 423. Effect of yttria content on YSZ oxygen conductivity and YSZ interaction with alumina as a reforming catalyst co-support. **E. Achouri**, N. Braidy, N. Abatzoglou, J. Chaouki

12:50 CATL 424. High-efficient removal of nitrogen oxides by catalysis techniques over specially structured catalysts. **X. Tang**, F. Gao, H. Yi, S. Zhao, Q. Yu

1:10 CATL 425. Toward rational design of supports for single-site catalysts: Probing electronic support interactions of palladium catalysts on tunable mixed metal oxides. **A. Voutchkova**, D.E. Ramaker, S.R. Daly, N. Wu, J. Bright, N. An, A. Azua-Barrios, M. Finn

1:30 CATL 426. Design of silica-based metal complex catalysts for activation of CH₄ and CO₂. **A.J. Karkamkar**, M. Yadav

1:50 CATL 427. Efficient and stable atwer oxidation catalysts: A superhydrophobic approach. **B. Chen**, N. Morlanes, K. Takanabe, V.O. Rodionov

2:10 Intermission.

2:20 CATL 428. Facile fabrication of ZSM-5 nanosheet and their behaviour in the catalytic conversion of methanol to propylene. **Y. Shang**, Y. Xu, Y. Min, Y. Song, X. Zhao, Y. Gong

2:40 CATL 429. Low-temperature removal of carbonyl sulfide over mixed oxides derived from M/Al (M=Zn, Ni) hydroxalate-like compound. **H. Yi**, S. Zhao, X. Tang, F. Gao, Q. Yu

3:00 CATL 430. Supported PdFe nanoparticles for the water gas shift reaction. **L. Arroyo-Ramirez**, V. Doan-Nguyen, H. Yun, C.B. Murray, R.J. Gorte

3:20 CATL 431. Nanoconfinement synthesized MOF derived preparations of CeO₂ tubes supported CuO catalysts. **Y. Feng**, J. Jiang, M. Zhang

Section C

Renaissance Boston Waterfront
Atlantic Blrm 2

General Catalysis

Other

R. Ramakrishnan Parthasarathi, H. Shou, *Organizers, Presiding*

12:30 CATL 432. Withdrawn.

12:50 CATL 433. Investigation of the electron transfer kinetics on a Fe-based metal organic framework catalyst in nonaqueous electrolytes for Li-air batteries. **G. Yilmaz**, E. Bayram, S. Mukerjee

1:10 CATL 434. Exploring Hoveyda-Grubbs-type catalysts via silica-supported systems. **J. Lim**, J. Cheong, S. Lee, S. Lee

1:30 CATL 435. Heterogenization of homogenous catalytic reaction with boron nitride supported molybdate ionic liquid. **W. Zhu**, B. Dai, P. Wu, H. Li, S. Dai

1:50 CATL 436. Seeded approach for controllable synthesis of EU-1/ZSM-48 co-crystalline zeolites with long crystallization stability period. **Y. Zhang**, L. Xing, L. Zhang, L. Sun, H. Wang, Y. Gong

2:10 Intermission.

2:20 CATL 437. Synthesis of double-doped C/N/Cr₂O₃ visible-light photocatalyst from metal organic frameworks (MOFs) for partial oxidation of cyclohexane with molecular oxygen. **H. Wang**, Y. Zhang, L. Zhang, L. Ge

2:40 CATL 438. Modification of carbon aerogels as support Fe-Mo phase for stability enhancement in refractories hydrocarbon hydrotreating reactions. **A. Barbosa Lopez**, W. Licona, A. Alvarez

3:00 CATL 439. Direct asymmetric Michael-type reactions with bifunctional organocatalysts. **C. Gianelli**, S.J. Connon

3:20 CATL 440. Withdrawn.

Section D

Renaissance Boston Waterfront
Pacific Blrm H

Catalytic Upgrading of Biomass

M. V. Olarte, S. Wettstein, *Organizers, Presiding*

1:00 CATL 441. Exploring the mildest conditions for the catalytic conversion of biomass via hydrogenation and hydrogenolysis. **R. Gagne**, L. Petitjean, E.S. Beach, P.T. Anastas, **D. Xiao**

1:20 CATL 442. Hydrodeoxygenation of furan on oxygen vacancy sites of MoO₃(O10): A DFT investigation. **S. Kasiraju**, L. Grabow

1:40 CATL 443. One-pot visible-light mediated photocatalytic hydrolysis and oxidation of cellobiose to gluconic acid and lower chain carbohydrates. **L. Da Via**, T.E. Davies, N. Greeves, J.A. Lopez-Sanchez

2:00 CATL 444. Selective condensation of pinenes to high energy density dimers using silica alumina aerogel catalysts. **J. Jung**, J. Choi, J. Ha, D. Suh, J. Choi, K. Lee

2:40 Intermission.

2:20 CATL 445. Direct hydrogenation of biomass-derived butyric acid to n-butanol over a ruthenium-tin bimetallic catalyst. **D. Hong**, P.P. Upare, D. Hwang, Y. Hwang, J. Chang

2:50 CATL 446. Sustainable production of acrylic acid from renewable resources from lactic acid. **C. Wang**, D. Theng, K. Tang, A. Borgna

3:10 CATL 447. Glycerol hydrogenolysis to propanediols over Pd-Re catalyst – influence of different Pd precursors. **Y. Li**, L. Ma, **D. He**

3:30 CATL 448. Electrochemical hydrogenation using non-precious nanoparticle catalysts. **K.J. Carroll**, T. Burger, I. Langenegger, S. Chavez, S.T. Hunt, Y. Roman-Leshkov, F. Brushett

3:50 CATL 449. Upgrading fatty oils to higher value products using alumina catalyzed ketonization. **S.I. Hommeltoft**

- 4:10 CATL 450.** Effects of $\text{SiO}_2/\text{AlPO}_3$ ratio of ZSM-5 on the unsymmetric hydrocracking of biodiesel to bio-aviation kerosene. X. Luo, Y. Zhou, Q. Wei
- 4:30 CATL 451.** New Diels-Alder based strategy for renewable aromatics from biobased furanics. S. Thiagarajan, H.C. Genuino, J. Van der Waal, E. Dejong, J. Van Havenen, B. Weckhuysen, P. Bruijninx, D. Van Es

Section E

Renaissance Boston Waterfront
Pacific Blrm B

In-Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles

D. J. Stacchiola, *Organizer*

J. A. Boscoboinik, B. Roldan-Cuenya, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CATL 452. Transition metal nanoparticles on metal oxide nanoparticles (TMnp/MOnp) as model catalysts: Ptnp/Fe²O₃np. J.C. Hemminger

1:40 CATL 453. In situ XAFS studies on improving catalyst stability and selectivity via ALD overcoating. H. Zhang, C. Canlas, A.J. Kropf, C.L. Marshall

2:10 CATL 454. ALD-grown Pd nanoparticles supported on TiO₂- and SrO-terminated SrTiO₃ nanocuboids. B. Chen, C. George, L. Hu, Y. Lin, L. Crosby, X. Hu, P.C. Stair, L. Marks, K.R. Poeppelmeier, N.M. Schweitzer, R.P. Van Duyne, M.J. Bedzyk

2:30 Intermission.

3:00 CATL 455. Withdrawn.

3:30 CATL 456. Size-selected vanadium oxide clusters on TiO₂(110)-(1×1) and their role in oxidative dehydrogenation of methanol: Every atom counts. S.K. Buratto, H. Neilson, J. Buffon, J. Robins

4:00 CATL 457. In-situ studies of redox-mediated reconstruction of Cu(111) during CO oxidation. F. Xu, K. Mudiyansele, A. Baber, M.G. White, D.J. Stacchiola

4:20 Concluding Remarks.

Section F

Renaissance Boston Waterfront
Pacific Blrm A

General Catalysis

Other

P. Bhattacharya, N. Kumar, *Organizers, Presiding*

12:30 CATL 458. In-situ metamorphosis of cobalt phosphide (CoP) nanoparticles toward efficient and robust oxygen evolution catalyst. J. Ryu, J. Jang, H. Kim, S. Yoo

12:50 CATL 459. Comparative DFT study on the performance of homogeneous, heterogeneous, and hybrid Ir-based catalysts for water oxidation. M. Garcia-Melchor, L. Vilella, N. Lopez, J.K. Norskov, A. Vojvodic

1:10 CATL 460. Withdrawn.

1:30 CATL 461. Synthesis of the uniform covering micro- and mesoporous composite material Y/ASA. Y. Yin, S. Cui, B. Liu

1:50 CATL 462. Photocatalytic degradation of phenolic compounds on TiO₂-supported graphene oxide and reduced graphene oxide composites. H.A. Al-Kandari, A.M. Abdullah, S.A. Al-Kandari, A.M. Mohamed

2:10 Intermission.

2:20 CATL 463. Optimization and development of cost effective synthetic methodology for fuel cell electrocatalysts. B. Lal, A. Altaf, A. Badshah

2:40 CATL 464. Trace explosives detection using zinc oxide nanowires. Z. Caron, D. Mallin, M. Champlin, O. Gregory

3:00 CATL 465. Preparation of palladium-poly pyrrole-montmorillonite nanocomposite and its application as a catalyst for oxygen reduction reaction. C. Senarathna, R. Rajapakse

3:20 CATL 466. Phosphine ligand evolution: Design, application, and opportunities in palladium-catalyzed cross-coupling reactions. H. Jong, Y. Lim, Y. Yang, F. Yong, W. Wu, X. Chew, C. Johannes, T. Daniel, S. Chia, E. Robins, A. Ma

CELL

Division of Cellulose and Renewable Materials

C. Frazier, *Program Chair*

TUESDAY MORNING

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES+, PROF and SCHB

TUESDAY AFTERNOON

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES+, PROF and SCHB

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CHED

Division of Chemical Education

I. Levy, I. Black and B. Rios-McKee, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Wikipedia and Chemistry: Collaborations in Science and Education (see *CINF, Sunday*)

Opportunities for US/Cuba Collaboration in Chemistry, Chemical Engineering and Chemistry Education (see *IAC, Sunday*)

21st Century Chemistry Education: Formal and Informal (see *PRES, Sunday, Monday*)

Chemistry and the International System of Weights and Measures. (see *CCQM, Wednesday*)

SOCIAL EVENTS:

High School-College Interface Luncheon (Tickets Required), 12:00 PM: Sunday

Division Reception, 5:30 PM: Sunday

Green Chemistry Commitment Luncheon, 12:00 PM: Monday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 253C

High School Program

Cosponsored by SOCED

Financially supported by ACS Education
K. Anderson, *Organizer*

S. B. Mitchell, *Organizer, Presiding*

8:00 Registration.

8:30 Introductory Remarks.

8:35 CHED 1. Probing neurons and sequencing DNA: my adventures in simple pH chemistry. A.E. Cohen

9:15 CHED 2. Work safely and have fun, too! E.M. Howson

9:35 CHED 3. Green chemistry: The science of solutions. K. Anderson

10:05 Intermission.

10:15 CHED 4. Inspiring the next generation of innovators. A. Lambert, E. Hines, K. Anderson

10:45 CHED 5. Periodic table: Highlights from the history of an icon. C.J. Giunta

11:05 CHED 6. From discovery to practical application: Molecular spectroscopy in the high school chemistry curriculum. D. McGraw

11:25 CHED 7. Using chemical education research. D. Cullen

11:55 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 253B

Toxicology and Environmental Impact in the Chemistry Curriculum: Science and Strategies for Educators – State of the Art Symposium

Cosponsored by CEI

I. J. Levy, J. C. Warner, *Organizers*

A. S. Cannon, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CHED 8. Opportunities to incorporate toxicology into the chemistry curriculum: Report from the field. N.D. Anastas

9:40 CHED 9. Toxicology of “low doses”: Understanding endocrine disrupting chemicals. L. Vandenberg

10:40 Intermission.

11:00 CHED 10. Designing safer chemicals: Environmental attributes in chemical design. R.S. Boethling

12:00 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 207

Undergraduate Research Papers

Cosponsored by SOCED

C. V. Gauthier, J. V. Ruppel, N. Snyder, *Organizers*

J. R. Miecznikowski, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 11. Inquiries in physical sciences: A bottom-up approach for incorporating next generation science standards (NGSS) in K-8 physical science education. T. Gupta, H. Mechels

8:45 CHED 12. Improving undergraduate chemistry experience through a Guided-Inquiry (GI) based chemistry curriculum. T. Gupta, A. Mehta, T.D. Jangula

8:55 CHED 13. Understanding students' misconceptions of acid-base chemistry. T. Mead, M.T. Dianovsky

9:05 Intermission.

9:15 CHED 14. Gold nanoparticles grafted by aryls from diazonium salts. W. Adams, O. Tytler, J. Park, K. Kim, Y. Pajouhafsar, A. Mohamed, H. Abdou

9:25 CHED 15. Towards carbon-based nanotechnology: A novel supramolecular nanodiode from a self-assembled cyclic β-peptide nanotube host and a metallic single-walled carbon nanotube guest. M. Cartamil, N. Nieves, M.F. Alvarado, A. Castro-Llanos, S. Muñoz

9:35 CHED 16. Toward carbon-based nanotechnology: Molecular nanotopography and electrical conductivity of zigzag and armchair carbon and boron nitride nanotubes from self-consistent field Hartree-Fock 3-21G electrostatic potential maps. A. Abrahantes, V. Padilla, S. Muñoz

9:45 CHED 17. Toward carbon-based nanotechnology: Molecular nanotopography and electrical conductivity of armchair and zigzag single-walled carbon nanotubes from self-consistent field Hartree-Fock 3-21G electrostatic potential maps. H. Suchinsky, D. Villagomez, S. Muñoz

9:55 Intermission.

10:05 CHED 18. Synthesis and characterization of new thermoplastic elastomers with tunable upper service temperatures containing polybenzofulvene. T. White, W. Wang, N. Kang, J.W. Mays

10:15 CHED 19. Utilizing a ring expansion strategy for synthesis of medium peptide ring. S. Hamedzadeh, K. Ha, C. Hall, A. Katritzky

10:25 CHED 20. Metal content in wild gathered fungi in western Pennsylvania: Evidence for biological remediation? K.A. Wozniak, C. Leghart, S. Nix, R.M. Hall, D.A. Reynolds

10:35 CHED 21. Investigating the effects of chemicals in planarian survival, regeneration, and asexual reproduction. J. Valls, L. Mata, P. Valverde

10:45 Concluding Remarks.

Section D

Boston Convention & Exhibition Center
Room 208

General Papers

S. A. Fleming, *Organizer*

B. Findley, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 22. Adding context for teaching kinetics, quantum mechanics, and spectroscopy in physical chemistry. E.M. Marzluff, M.A. Crawford

8:55 CHED 23. Chemically intuitive procedure for drawing Lewis structures. Y. Zhu

9:15 CHED 24. Student misconceptions about conversions. R.H. Langley, C. Davis, M. Cervantes

9:35 Intermission.

9:45 CHED 25. Evidence-based argument and Primo Levi's *The Periodic Table*: An inorganic term project. J. Heising

10:05 CHED 26. Evans' challenging problems in organic chemistry: An interactive app for learning on the go. N. Sievertsen, E.M. Carreira, D.A. Evans

10:25 CHED 27. Using crystal structure data to teach fundamental concepts in inorganic chemistry. A.L. Fernandez

10:45 CHED 28. Solvatofluorochromism and changes in dipole moment. B. Findley, S. Conroy, G. Hamilton

11:05 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253C

Education for Sustainable Development and Innovative Technologies Across Culture

Cosponsored by CEI

R. M. Kelly, *Organizer*

P. G. Mahaffy, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 29. Malta Conferences: Crosscultural educational collaborations toward a sustainable future in the Middle East. M.Z. Hoffman, Z.M. Lerman

1:55 CHED 30. Environmental concentration in CSBSJU's chemistry major. A.A. Peterson, C.M. Strollo

2:15 CHED 31. Integrating sustainability into the undergraduate curriculum at UC Berkeley. A.M. Baranger, M.C. Douskey, M. Robak, G. Kerstiens, L. Armstrong

2:35 Intermission.

2:45 CHED 32. Uncovering chemical thinking in students' real-life decision making. H. Sevan, G. Banks, M. Clinchot, S. Cullipher, R. Huie, J. Lambert, R. Lewis, C. Ngai, G.A. Szeinberg, V. Talanquer, M. Weinrich

3:05 CHED 33. Transduction: An innovative interdisciplinary experiment exploring environmental health through a "signals/interactive media/human interface" framework. C. Fraser

3:25 CHED 34. Choosing the best climate change models: Key features and future opportunities. D.B. King, J.E. Lewis, K. Anderson, D.E. Latch, S. Suthimer, G.H. Webster, C.H. Middlecamp, R.S. Moog

3:45 Intermission.

3:55 CHED 35. Sustainability as a thread in chemical education. A.D. Jorgensen

4:15 CHED 36. Teaching sustainable development in the chemistry classroom: The implications of surfactant tensions for enacting a feminist chemistry curriculum. J. Bhattacharya

4:35 CHED 37. Promoting pro-environmental behaviors in students and their families by connecting the chemistry classroom to blended learning experiences. P.L. Daubenmire

4:55 CHED 38. Online videos as teaching and learning platforms for general chemistry courses. J. Ranga

5:15 CHED 39. Visualization design — how do we do this? R.M. Kelly

5:35 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 253B

Toxicology and Environmental Impact in the Chemistry Curriculum: Science and Strategies for Educators - State of the Art Symposium

Cosponsored by CEI

I. J. Levy, J. C. Warner, *Organizers*

A. S. Cannon, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 CHED 40. How Training Chemist in 21st Century Toxicology Contributes to the Design of Lower Toxicity Products. P. Spencer

2:40 CHED 41. Evolution of structure-activity relationship (SAR) methodology in 21st century toxicity prediction. R. Naven

3:40 Intermission.

4:00 CHED 42. Harnessing toxicity testing in the 21st century to help train chemists. J.R. Fowle

5:00 Panel Discussion.

5:20 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 207

Undergraduate Research Papers

Cosponsored by SOCED

J. R. Miecznikowski, J. V. Ruppel, N. Snyder, *Organizers*

C. V. Gauthier, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 43. Novel design of water soluble porphyrin containing supramolecular complex nanoparticles for enhanced photodynamic therapy. S.V. Shutthanandan, M. Zhu, J. Jayawickramarajah

1:45 CHED 44. Synthesis and characterization of water soluble zinc(II) model complexes for liver alcohol dehydrogenase. N.A. Bernier, J.R. Miecznikowski

1:55 CHED 45. Synthesis and characterization of asymmetric water soluble zinc(II) model complexes for liver alcohol dehydrogenase. C.A. Van Akin, N.A. Bernier, J.R. Miecznikowski

2:05 CHED 46. Light-activated inorganic-peptide hybrids. M. Rotondaro, E.C. Glazer

2:15 CHED 47. Reactions of 1,2-bis[(2,6-diisopropylphenyl)imino]acenaphthene (dpp-BIAN) with vanadium chloride compounds. G. Risica, N. Onishi, N. Tsamchoe, J.D. Gordon, C.D. Abernethy

2:25 Intermission.

2:35 CHED 48. Selective synthesis and characterization of a bimetallic calix[5]arene complex. M. Prieto-Cortez, B.A. Martinez-Ortega

2:45 CHED 49. Using Cheminformatics to better design of chelates to lanthanide and actinide complexes. K. Moyle, S. Vyas, P.C. Sanschagrin, S. Wiggan, J. Brennan

2:55 CHED 50. Synthesis and characterization of diazonium tetrachloroaurate(III) precursors for surface grafting. Y. Pajouhafsar, O. Tytler, J. Park, K. Kim, W. Adams, A. Mohamed, H. Abdou

3:05 CHED 51. Determining the factors that dictate carbene retention vs. displacement in ligand addition to Cp*Co(NHC). J. Andjaba, C.A. Bradley

3:15 CHED 52. Voltage tuned acidity of catalytic surfaces for non-faradaic isomerization reactions. A. Vong, I.M. Kendrick, J.H. Doan, E.S. Smotkin

3:25 Concluding Remarks.

Section D

Boston Convention & Exhibition Center
Room 208

General Papers

S. A. Fleming, *Organizer*

S. C. Timmons, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 53. Integration of undergraduate research into the chemistry curriculum using thematically linked laboratory courses in biochemistry, chemical biology, and neurobiology. R. Johnson, G.C. Hoops, J. Kowalski

1:55 CHED 54. Drug discovery research with undergraduate students: An excellent facilitator of STEM education. R.J. Doll

2:15 CHED 55. From molecule to market: Implementation and assessment of a novel experiment promoting critical thinking and entrepreneurship in the organic chemistry laboratory. J.R. Knoff, S.C. Timmons

2:35 Intermission.

2:45 CHED 56. Integrating technology in classroom by developing and implementing interactive simulations in chemistry. T. Gupta, A. Mehta, G.T. Albing

3:05 CHED 57. Nanoparticle-based paper sensors for educational use: An exploration of portable devices for colorimetric antioxidant analysis in the classroom. E.M. Sharpe, E.S. Andreescu

3:25 CHED 58. Composition and mosquitoicidal activity of the essential oil of *Monarda fistulosa* (Beebalm). C. Ardizzone, A. Rogers, Y. Shaikh, K. Jeffers, J. Hightower, M. Cochran, W. Dees, O.E. Christian

3:45 Intermission.

3:45 CHED 59. Computer-assisted student admissions based on predicted academic performance. E. Muratov, M. Lewis, D. Fouches, A. Tropsha, W. Cox

4:05 CHED 60. Using text mining to discover frequency and patterns of student study habits. L. Ye, S.E. Lewis

4:25 CHED 61. Using software to model a bifactor structure in order to capture an item-writing pattern. J.E. Lewis, X. Xu

4:45 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF and SOCED

Wikipedia and Chemistry: Collaborations in Science and Education

Sponsored by CINF, Cosponsored by CHED

SUNDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

General Posters

I. J. Levy, *Organizer*

7:00 - 9:00

CHED 62. The 2016 Biennial Conference on Chemical Education. R.W. Schwenz, J.M. Smist, M.L. Miller

CHED 63. From lecture hall to benchtop: Applying pedagogical skills to successful undergraduate research. N. Zargari

CHED 64. Design and implementation of research methods course for freshman undergraduate students. S. Sambasivan, T. Callender, C.J. Foley, N. Leonhardt

CHED 65. Withdrawn.

CHED 66. Revised baccalaureate biological chemistry program to include informatics. M.J. D'Souza, R.J. Kashmar

CHED 67. Delivering a postbaccalaureate medical sciences certificate program to working adults. J. Tierney, E. Dudkin, T. Nilier, M. Bodek, K. Geveke, D.W. Finneran

CHED 68. Building interface chemistry curriculum content system to meet the needs of different professionals. Z. Jiang, Z. Yao, L. Zhao, H. Yue, M. An, X. Han, Y. Huang

CHED 69. Student instructional enhancement strategies: Implementation of economically self-sustained peer-leading (ESSP), POGIL, service learning, and live speakers in the classroom. A. Shukla, S. Shukla

CHED 70. Implementation of an undergraduate certificate in chemistry education: A peer-instruction program. E. Buginsky, D.M. York

CHED 71. Teacher quality in the chemistry program at the University of Maryland, Baltimore County. S. Mang, H.M. Perks, W.R. Lacourse

CHED 72. Shades of green chemistry. M. Yatin, D.L. Warner

CHED 73. Increasing student exposure to chemical structures in Biochemistry and Medicinal Chemistry courses through test-enhanced learning. J. Ross, M. Hernick

CHED 74. Improving student understanding of lipids concepts in a biochemistry course using test-enhanced learning. S. Horn, M. Hernick

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:

www.acs.org/boston2015

- CHED 75.** BioSeq: Delivering genuine research experiences involving bioinformatics and next-generation sequencing to high school classrooms. C. Etson, **M.R. Hartman**, P. Braunstein, K. Harrington, T. Amondi, H. DeBaets, A. Garrity, N. Lingafelter, B. Yang, M. Fierman, K. O'Hagan, D. Slonim, D.R. Walt
- CHED 76.** Integrating content between biochemistry lecture and laboratory. T. Neumann
- CHED 77.** 3D printing in an undergraduate biochemistry lab. S.C. Meyer
- CHED 78.** Current status of IUPUI's educational Distributed Drug Discovery (D3) program. **W.L. Scott**, R.E. Denton, G. Anderson, K. Marrs, J.G. Samaritoni, J.D. Durrant, S. Colglazier, M. Abraham, J. Dilley, M. Phillips, J. Lacombe, M.J. Odonnell
- CHED 79.** Adopting the Just in Time Teaching method in an introductory organic chemistry class: Instructor and student perspectives. M. Wright, **A.E. Keirstead**
- CHED 80.** Synthesis of bicyclic *N*-heterocycles: Introducing an advanced scaffold in the undergraduate organic chemistry laboratory. **J.K. Murray**, M.J. Price
- CHED 81.** Anilinderivatives: Synthesis of Schiff base compounds with interesting fluorescent properties. M.J. Price
- CHED 82.** Synthesis of 1,1-diphenylethylene (DPE): The marriage of a Grignard reaction and a column chromatography experiment. **L.T. Alty**, M.B. France, I. Alty, C.A. Saber, D.M. Smith
- CHED 83.** Sweet side of organic chemistry: Identification of sweetness through chemical methods. **J.M. Baxter-Vu**, **G. De La Garza**, N. Patel, D.R. Oliver, J. Prince, D. Ward, S. Serfoss
- CHED 84.** Triumphs and pitfalls of having a flipped classroom in organic chemistry. **D.J. Swartling**
- CHED 85.** Hydroboration-oxidation reactions in the undergraduate teaching laboratory: Reagent and reaction condition choices for optimizing student success. **D.E. Marty**
- CHED 86.** Building a classroom teaching - experiment training - project research triune teaching mode for talent cultivation. **Z. Yao**, J. Wang, C. Li, Z. Wang, P. Yang, D. Wang, X. Han
- CHED 87.** Do verification labs affect student exam performance? **J. Xian**, D.B. King
- CHED 88.** Blending it up: Active learning in a STEM classroom through the use of on-line materials. **M.E. Keithly**, C.J. Brame, M.A. Woelfle, K.L. Friedman
- CHED 89.** On the development of academic social networks: A new model in STEM eLearning. **E. Buginsky**, K.J. Chun, D.M. York
- CHED 90.** Correlation of quiz environments with test scores in General Chemistry. **C. Rezsnyak**
- CHED 91.** Improving the office hour experience for general chemistry students. **T.S. Carpenter**
- CHED 92.** Nuclear chemistry under western New York: A lesson for general chemistry. **D. Ventura**, A. Poblacki
- CHED 93.** Assessment to improve learning in general chemistry. **P.K. Yuen**, C. Lau
- CHED 94.** Mathematics as an effective learning tool in general chemistry. **P.K. Yuen**, C. Lau
- CHED 95.** Catalyzing group work in introductory chemistry: Examining student attitudes and evidence of learning for multiple strategies. **A.C. Lamanna**, M. Thompson
- CHED 96.** Developing and implementing engaging introductory chemistry laboratories through collaborative teaching innovation. **L. Wang**, F. Schunk, P. Lynch
- CHED 97.** Standardizing representations of electrons and electron movement. **J. Mullins**
- CHED 98.** Determining total acid content in sour candies. **T.L. Marx**, A.H. Sowell, **C.H. Jaworek-Lopes**, S. Iacobucci
- CHED 99.** Reaction of orthoesters with amine hydrochlorides: An introductory organic lab experiment combining synthesis, spectral analysis, and mechanistic discovery. **S. Saba**, J.A. Ciaccio
- CHED 100.** Linking learning to real life research goals: Biofuel production and analysis in the classroom and the laboratory. **J. de la Parra**, V. Likourinou, A. Rovira, H. Harakawa, A. Stoebenau, S. Breselge, C.W. Lee-Parsons
- CHED 101.** Guided inquiry based laboratory instruction in upper undergraduate Inorganic laboratory course. **Z. Assefa**
- CHED 102.** Metal or carbonate identification via pressure measurements. **D.C. Haagenson**
- CHED 103.** User-friendly tool for the modeling and design of plasmonic nanostructures. **S.L. White**, J.G. Smith, A.N. Sobh, N.A. Sobh, P.K. Jain
- CHED 104.** New aspects of slime chemistry. **M.B. Jacobs**, D.M. Schubert, M. McCray
- CHED 105.** Use of tea bags containing orange peel for removal of toxic metals from drinking water. **A. Shukla**, S. Shukla
- CHED 106.** Determining relative quality of commercial motor oil by liquid-liquid extraction and back titration: A guided inquiry experiment. **J. Logan**, N. Abrams
- CHED 107.** Contextualized Raman spectroscopy laboratories for physical chemistry. **M.A. Crawford**, E.M. Marzluff
- CHED 108.** Examining the intermolecular interactions of ionic liquids and phenol derivatives using far-infrared spectroscopy and computational chemistry. **A.M. Fedor**, M.J. Toda
- CHED 109.** Quinine fluorescence quenching by multiple halides salts: An extension of a common physical chemistry laboratory experiment. **J. Halstead**, H. DeGraaf
- CHED 110.** One discovery leads to another: An interactive chemical sensing workshop. **A.E. Norton**, J.M. Ringo, J.M. McElveen, W.B. Connick

MONDAY MORNING

Section A

Boston Convention & Exhibition Center Room 253C

Citizens First: Using Real-World Contexts for Engaging Students in Learning Chemistry

Cosponsored by CEI

P. L. Daubenmire, C. H. Middlecamp, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 111. Science The World: Developing structured, research and real-world inspired STEM experiments for K-12 curricula. **L.J. Landherr**, C. Puzzo, C. Chamberlain, J. Podyma, G. Rapsilber

8:55 CHED 112. The *Working with Chemistry* program: A template for project-based inquiry in general chemistry. **D.J. Wink**, S. Gislason, J. Ellefson-Kuehn

9:15 CHED 113. Chemistry and energy: A life-inspired approach to enhance the transfer of the scientific energy concept into real world issues. **T. Wagner**

9:35 Intermission.

9:45 CHED 114. Citizens first: Seeing beyond plastic recycling codes. **C.H. Middlecamp**

10:05 CHED 115. Understanding organic chemistry in the context of the production of hydrocarbon fuels in Brooklyn. **P. Spellane**

10:25 CHED 116. General Chemistry assignment analyzing environmental contamination for the DePue, IL, National Superfund site. **F. Geiger**

10:45 Intermission.

10:55 CHED 117. Drug detectives: Battling counterfeit drugs with wet chemistry and analytical techniques. **M.A. Pillers**, M. Lieberman

11:15 CHED 118. Paper analytical devices for pharmaceutical testing in the analytical chemistry laboratory curriculum. **D. O'Donnell**, A.A. Weaver, T.L. Barstis, M. Lieberman

11:35 CHED 119. Got fakes? A distributed pharmaceutical analysis laboratory. **M. Lieberman**

11:55 Concluding Remarks.

Section B

Boston Convention & Exhibition Center Room 253B

Toxicology and Environmental Impact in the Chemistry Curriculum: Science and Strategies for Educators – State of the Art Symposium

Cosponsored by CEI

I. J. Levy, J. C. Warner, *Organizers*

A. S. Cannon, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CHED 120. Infusing toxicology throughout the chemistry curriculum at South Dakota State University. **D.E. Rainie**, D.P. Cartrette

9:00 CHED 121. Teaching toxicology and environmental impact: A toxicology course for chemistry majors at Simmons College. **A.S. Cannon**, J.C. Warner

9:20 CHED 122. Teaching toxicology through a laboratory safety program. **D.C. Finster**

9:40 Intermission.

10:00 CHED 123. Integrating toxicology and green chemistry into a single course? Yes, it can be done. **A. Weissfloch**

10:20 CHED 124. Incorporating principles of toxicology and environmental health into the chemistry curriculum at UC Berkeley. **M.J. Mulvihill**

10:40 CHED 125. Introducing chemical toxicology in the organic chemistry curriculum. **A. Voutchkova**

11:00 Panel Discussion.

11:20 Concluding Remarks.

Section C

Boston Convention & Exhibition Center Room 207

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits

Cosponsored by BMGT, CEI, ENVR, I&EC, MEDI, PROF, SCHB and YCC

Financially supported by Green Chemistry Institute (GCI) Network of Early-Career Sustainable Scientists & Engineers (NESSE)

A. Ivanova, M. Kipreos, *Organizers*

R. E. Borg, W. A. Lawal, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 126. Greener solutions program: A private/public partnership teaching students in advancing the design of safer chemistry. **M.J. Mulvihill**, M. Schwarzman

9:05 CHED 127. Tools for green chemistry. **D.J. Constable**

9:35 CHED 128. Challenges and opportunities in green chemistry research academic institutions. **S.O. Obare**

10:05 CHED 129. Green chemistry and entrepreneurship. **J.C. Warner**, J. Pont

10:35 Intermission.

10:45 CHED 130. Opportunities in government for students of green chemistry. **N.D. Anastas**

11:15 CHED 131. Implementing green chemistry in the pharmaceutical industry: Challenges and opportunities. **E.A. Peterson**

11:45 CHED 132. Green chemistry in action. **S. Sullivan**

12:15 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CINP, COLL, ENFL, PROF and SOCED

Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reals

Sponsored by YCC, Cosponsored by CHED, IAC, PRES and PROF

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center Room 253C

Citizens First: Using Real-World Contexts for Engaging Students in Learning Chemistry

Cosponsored by CEI

P. L. Daubenmire, C. H. Middlecamp, *Organizers, Presiding*

1:30 Introductory Remarks.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

1:35 CHED 133. Ethics and spirituality: What are they doing in my science textbook? P. Nahlik, P.L. Daubenmire

1:55 CHED 134. Making water personal. K. Anderson

2:15 CHED 135. Using the climate debate to teach general chemistry. C.H. Lisse, K.N. Cossey, C. Mills

2:35 Intermission.

2:45 CHED 136. Experiential learning through course development and implementation of green general chemistry labs. V. Lykourinou, J. de la Parra, T.R. Gilbert, C.W. Lee-Parsons, A. Rovira, S. Dufort, S. Song, H. Harakawa, A. Stoebenau

3:05 CHED 137. Application based service learning in the first year chemistry sequence. J. Deiner, N. Trun, G. Galford

3:25 CHED 138. Community-based learning in environmental chemistry: Arsenic testing in rural Maine. E. Leshner

3:45 Intermission.

3:55 CHED 139. Development of laboratory experiences that build a foundation in chemistry for pre-health students: Using context, pedagogy, and chemical principles. L. Schroeder, D.J. Wink, G. Clark

4:15 CHED 140. Fighting with food: Battling chemical toxicity with good nutrition. S.A. Hershberger

4:35 CHED 141. Spreading the industrial safety culture into classrooms: The role of corporate volunteer programs. J.L. Curtis-Fisk, T. Wilson, J. Morris

4:55 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 253B

Incorporating Green Chemistry Innovations and Applications into the Classroom and Outreach

Cosponsored by CEI, I&EC and SOCED

E. J. Brush, J. E. Wissinger, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 142. Microwave-assisted aspirin synthesis from over-the-counter pain creams using naturally acidic catalysts: A green undergraduate organic chemistry laboratory experiment. J.T. Fahey, A.E. Dineen, J. Henain

1:55 CHED 143. Teaching green chemistry with epoxidized soybean oil. H.S. Barcena, A. Tuachi, Y. Zhang

2:15 CHED 144. Modernizing the organic chemistry teaching laboratory with experiments based on new green reactions and sustainable polymer technologies. J.E. Wissinger, G. Fahnhorst

2:35 CHED 145. Green chemistry resources for the organic laboratory course: A partnership with Sigma-Aldrich. A.S. Cannon

2:55 Intermission.

3:05 CHED 146. Paper or plastic? An online approach to teaching green chemistry and sustainability to non-science majors. M. Kerr

3:25 CHED 147. Infusion of sustainable chemistry concepts in the undergraduate curricula through multiple interventions. C. Lai, D.R. Radu

3:45 CHED 148. Establishing regional student-faculty collaborations in green chemistry teaching, research, and outreach education: Project GreenLab. E.J. Brush

4:05 CHED 149. Student involvement in the development of green chemistry activities and demonstrations for grade school through undergraduate audiences: Recyclable catalysis with magnetic nanoparticles, bioplastics with lobster shells, and metrics with Legos. R. Hudson, A. Bishop, S. Glaisher, K.N. Esdale, D. Leaman, K. Kawamura, J.L. Katz

4:25 CHED 150. Chemistry Connections: Inspiring students with innovation. K. Anderson

4:45 Discussion.

5:05 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 207

Active Learning in the Chemistry Classroom

D. A. Katz, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 151. Choices for active learning. D. Rush Walker

1:55 CHED 152. Active chemistry: Classroom activities, small scale investigations, and active assessment. D.A. Katz

2:15 CHED 153. Argument based inquiry. L. Hogue

2:35 CHED 154. Active learning in General Chemistry II and Survey of Chemistry. E.L. Lebeau

2:55 Intermission.

3:05 CHED 155. Coupling the flipped classroom with automated response. J.F. Kirby

3:25 CHED 156. Active learning in chemistry: Steps toward universal implementation of strategies across curriculum. L. Benedict

3:45 CHED 157. Using learning assistants to effectively implement course transformations in general chemistry. B. Abrams, N. Bassina, D. Dill, A. Golger

4:05 Intermission.

4:15 CHED 158. Flipping the general chemistry classroom: Does it make a difference? J.A. Smieja, L. Brunell

4:35 CHED 159. Changing the culture in the general chemistry classroom in a large urban university. M. Delgado

4:55 CHED 160. Problem-based learning as a research experience. J. Poe

5:15 Concluding Remarks.

Section D

Boston Convention & Exhibition Center
Room 208

Promoting Engaged Student Learning through the ACS Guidelines

C. K. Larive, T. J. Wenzel, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 161. Pedagogies to promote skill development in the undergraduate chemistry curriculum. T.J. Wenzel

1:55 CHED 162. ACS Guidelines and student skills development at the University of Wisconsin-Madison. J.S. Hamers, C.R. Landis

2:15 CHED 163. Research-based laboratories across the foundational and in-depth courses. K. Frederick, K. Sheppard, R. Howard, K. Cetto Bales, S.T. Frey, J.G. Navea

2:35 Intermission.

2:45 CHED 164. Integrating inquiry-based learning throughout the chemistry curriculum. E.D. Niemeier

3:05 CHED 165. Curricular changes that affect content and pedagogy. M. Oliver-Hoyo

3:25 CHED 166. Chemistry major program growth and retention gains through engaged student learning at Salem State University. R.S. Mactaylor

3:45 Panel Discussion.

4:15 Concluding Remarks.

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters Agricultural and Food Chemistry

Cosponsored by AGFD and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

CHED 167. Use of the QuEChERS approach in the extraction of pesticides from imported fresh fruits and vegetables.

B. Um, K. Williams, M. Iorsh, P.D. Svoronos

CHED 168. Determination of pesticides in fruits, vegetables, and grains via the Luke method. I. Sun, K. Williams, M. Iorsh, P.D. Svoronos

CHED 169. Determining antioxidant quantities present in commercially available beverages via the Folin Ciocalteu microspectrophotometric analysis. J. Leong, D. Proano, S. Svoronos, T. Xu, P.D. Svoronos

CHED 170. Determination of the amount of gallic acid present in commercial beverages via high performance liquid chromatography (HPLC). D. Proano, S. Svoronos, B. Montalbano, P.D. Svoronos

CHED 171. Citrus-derived oil and its compounds eliminate the biofilm of *Staphylococcus aureus* and *Listeria monocytogenes* on milking equipment. C. Ma, C. Federman, D. Biswas

CHED 172. Composition and biofilm inhibitory activity of the essential oil of *Carissa grandiflora*. J. Vajko, G.E. Ritter, D. Gary, T. Lu, M. Gallier, R. Johnson, D. Lauderdale, A. Mendez, K. Landry, M. Clarke, C.G. Struchtemeyer, O.E. Christian

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Analytical Chemistry

Cosponsored by ANYL and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

CHED 173. Extraction and analysis of pigmented ommochromes in cephalopod chromatophores. C.W. DiBona, S.F. Jones Labadie, M.A. Griswold, L.F. Deravi

CHED 174. Withdrawn.

CHED 175. Solid phase extraction of illicit drugs (amphetamine and methamphetamine). N. Evans, R.L. Marvin, E.E. Mojica

CHED 176. Spectroscopic characterization of an ionic liquid (1-butyl-3-methylimidazolium thiocyanate). N. Abbas, E.E. Mojica

CHED 177. Pigment analysis of a 14th century illuminated book of hours by Raman microscopy. C.R. Sullivan, A.M. Fleshman, B.C. Tilghman

CHED 178. Determination of the refractive index of adipic acid measured by extension method. B. Um, H. Shin, J.H. Shin

CHED 179. Refractive index of adipic acid measured by zoom-in method. H. Shin, B. Um, J.H. Shin

CHED 180. Examination of endophytic fungi from Sumac wood and flowers. E.S. Lewis, C. Ibarra, C. MacTaylor

CHED 181. Zinc and copper analysis of ribbed mussel (*Geukensia demissa*) pallial cavity fluid. E.R. Pacer, A.S. Harper-Leatherman, P.C. Braun, D.J. Brousseau

CHED 182. Surface-enhanced Raman scattering based optical probes for real-time pH determination. D. Botamanenko, N. Schorr, S.R. Emory

CHED 183. Investigation of the direct electron transfer of ferritin on modified gold electrodes. B. Sturm, S. Olubajo, D. Zapfen

CHED 184. Determination of the presence of alterants in commercially available herbs and spices. C.A. Mendel, M. Yatin

CHED 185. Comparative analysis of *Phragmites australis* endophytes. C.A. Mendel, D. Antonuccio, E. Shanoski, J. Roth, A. Pepecicelli, C. MacTaylor

CHED 186. Analysis of archeological soils. J.A. Kelley, A. Scaffidi, N. Eyet

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters Biochemistry

Cosponsored by BIOL and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

CHED 187. Subcellular localization of glucose-6-phosphatase toward understanding spatiotemporal regulation of glucose metabolism. S. Bracey, C. Kohnhorst, D. Schmitt, S. An

CHED 188. Kinetics and substrate specificity of the LipN hydrolase from *Mycobacterium ulcerans*. S.N. Raynor, R. Johnson, G.C. Hoops

CHED 189. Identification of histidine 303 as the catalytic base of lysyl oxidase via site-directed mutagenesis. R.N. Oldfield, K.M. Lopez

CHED 190. Design and synthesis of capture-tag-release (CTR) probes for protein labeling. L. Etamad, M. Vessicchio, G. Naclerio, V. Jedson, A.R. Van Dyke

CHED 191. Visualizing live cell membrane binding for FTT258. W. Hart, R. Johnson

CHED 192. Determination of the biological function of OVCA2, a potential ovarian cancer related enzyme. J. Bun, R. Johnson

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- CHED 193.** In gel enzymatic activity of serine hydrolases from *M. smegmatis*. H.L. Hansen, R. Johnson
- CHED 194.** Quantitative analysis of purine nucleotide pools involved an AMPK regulatory loop. G. Balaa, D. Schmitt, S. An
- CHED 195.** Formation of symmetric and asymmetric droplet interface bilayers: Water permeability studies. S. Lee, P. Milianta, M. Muzzio, J. Denver
- CHED 196.** Effects of solvent and method of preparation on artificial biological membrane. J. Denver, P. Milianta, S. Lee
- CHED 197.** Tuning of membrane permeability via various ion interactions. M.E. Morales, S. Evangelista, S. Lee
- CHED 198.** Withdrawn.
- CHED 199.** Potential for DNA quadruplex formation in a prokaryotic genome. S. Shephardson, M. Nunez
- CHED 200.** Characterization of the HIV-1 monomeric conformation of the 5'-leader. N. Bolden, V. Van, S. Monti, M.F. Summers
- CHED 201.** Effects of ethylene glycol versus glycerol on lipid production in *Chlorella vulgaris*. P.E. Adkins, D. Kolling, A.T. Holland, M. Stickler, K. Stickler, A. Stevenson
- CHED 202.** Mechanism of HIV-1 capsid-nucleocapsid polyprotein in genome recognition. S.E. McCowin, S. Keane, M.F. Summers
- CHED 203.** Electrophilic sesquiterpene lactones modulate the heat shock response system. G. Crossland, A. Newton, R.E. Connor
- CHED 204.** Spectroscopic and thermodynamic characterization of fluorinated unnatural amino acid containing superfolder green fluorescent protein variants. C. Van Hook, L. Zack, B. Dudeck, C. Henkels
- CHED 205.** Influence of tail-group lipid chain structure on water permeability in artificial biological membrane. M. Lopez, J. Villanova, A. Armetta, S. Lee
- CHED 206.** Probing the prostate cancer secretome: Biomarker identification via bioorthogonal chemistry and MS proteomics. S. Purcell, D. Spiciariach, S.L. Maund, D.M. Peehl, C.R. Bertozzi
- CHED 207.** Antibacterial and biofilm inhibitory evaluation of Jamaican collection of *Mammea americana*. T.A. Estrada, S. Doucet, G.E. Ritter, A. Scanlan, S. Nunez, M. Turwar, C.G. Struchtemeyer, O.E. Christian

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Biotechnology

Cosponsored by BIOT and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 208.** Evolution of DNA templates for hydroxyapatite mineralization in the presence of physiological NaCl. K.R. Baillargeon, A.E. Gordon
- CHED 209.** Investigating the effects of sonication in the fluorescence properties and protein aggregation of green fluorescence protein and liquid silk fibroin protein in an undergraduate research course for non-sciences majors. C. Bennett, S. Alibeik, P. Valverde
- CHED 210.** DNA fingerprinting and genetic analysis of ALU allele distribution. T. Pierre-Louis, N. Gadura

- CHED 211.** Uncovering the genes involved in copper induced cell death pathway by screening *Saccharomyces cerevisiae* genomic library. B. Kumari, N. Gadura
- CHED 212.** Finding evolutionary relationships between New York City roaches through DNA barcoding. O. Zagalo, T. Pierre-Louis, N. Gadura
- CHED 213.** Drug delivery: Encapsulated zeolite H-Y under simulated body conditions. N. Guthrie, S. Titinchi, K. Bailey, O. Okani, A. Mack

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Chemical Education

Cosponsored by SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 214.** Soaps made by the organic research chemists are tested by biology research in their investigation of biofilm formation in a joint undergraduate research collaboration. L. Cambalaza, D. Evans, J. Callahan, M. Castaldi
- CHED 215.** Development and implementation of a novel organic chemistry lab curriculum: Evaluation of the reformed teaching method. W. Marmor, C. Ayotte, D. Saviola, T.G. Collison
- CHED 216.** Fischer esterification by microwave irradiation using various alcohols (or chemistry doesn't have to stink). J. Cheng, S.C. Pilcher
- CHED 217.** Chemistry at the farmer's market. R.L. Nispel, R. Morgan Theall, J. Pratt, E.J. Yezierski
- CHED 218.** Bridging the gap between K-12 teachers and chemistry professionals in western North Carolina: A service learning project. L.R. Sigmon, E. Miller, G. Heard
- CHED 219.** Synthesizing and evaluating cockroach pheromones as a means of interdisciplinary teaching. J.G. D'Angelo, H. Zimmler-DeLorenzo, K. Gaier, E. Robinson, B. Proctor
- CHED 220.** Mad Scientist Day Junior: Inspiring future scientists. C.M. McCulley, M.K. Triplett, J.A. Nikles
- CHED 221.** Reactivity of Cp*Co(II) equivalents towards E-E (E = N, O, and S) bonds. K. Dalphon, C.A. Bradley
- CHED 222.** Synthesis and characterization of new XL N-heterocyclic carbenes (NHCs) and their reactivity with base metals. C. Bradley, Z.D. Call
- CHED 223.** Design of a greener kinetics reaction experiment for general chemistry students utilizing an effervescent acid. F. Nampanya, H. Sevan, M. Weinrich, S. Cullipher, C. Ngai
- CHED 224.** Determining the genetic pathways involved in cell death of copper treated *Saccharomyces cerevisiae*. H. Shah, N. Gadura
- CHED 225.** Screening a *Saccharomyces cerevisiae* genomic library to determine copper induced cell death pathways. R. Shao, N. Gadura
- CHED 226.** Determination of the ionization constant of carboxylic acids at 0 °C using microscale freezing point depression measurements. U. Dewanamuni, P. Irigoyen, P.D. Svoronos
- CHED 227.** P-platinated nucleosides. R. Ciccarelli, E. Holahan, S. Casino, T. Bogaczyk, T. Lord, R.A. Stockland
- CHED 228.** Gold catalyzed addition of diphenylphosphinic acids to alkynes. K. Garcia, D. Fraccica, K. Vostal, R.A. Stockland
- CHED 229.** Base-free cross-coupling of arylphosphonates. R. Ciccarelli, K. Garcia, M.E. Richard, E. Miller, R. Bergin, R.A. Stockland
- CHED 230.** Nucleophilic aromatic substitution reactions of 2-chloropyridines: Development of an organic chemistry laboratory project. C. Gallagher, M.W. Thomsen
- CHED 231.** Generation of metallo-polymers using transesterification. K. Garcia, K. Vostal, R.A. Stockland
- CHED 232.** Application of microfluidics in teaching core organic chemistry in both classical and interactive classroom settings. H.J. Rodriguez Chavez, S.N. Ike, J. Moats, B. McCord, J.M. Quirke
- CHED 233.** Application of divided U-tubes in teaching core organic chemistry in both classical and interactive classroom settings. J.M. Quirke, J.A. Hernandez, J. Moats
- CHED 234.** Integration of paper-based analytical devices (µPADS) and classical glassware photography in teaching core organic chemistry. S.N. Ike, H.J. Rodriguez Chavez, J. Moats, B. McCord, J.M. Quirke
- CHED 235.** Synthesis of glucosamine-NSAID conjugates. C.S. Sebastiano, R.A. Jones, C.D. Hall, Y. Thillier
- CHED 236.** Development of experiments utilizing a portable Raman spectrometer for nonscience, general chemistry, and upper level laboratories. A. Kayser, C.A. Bradley
- CHED 237.** Exploring a critical thinking schema for general chemistry students. C. Gabel, J. Daniel, M. Flores
- CHED 238.** Development of a chemistry laboratory manual for blind and low-vision students. E. Miller, C.A. Supalo, A.A. Hill
- CHED 239.** Pupil diameter as an indicator of cognitive load in chemistry tasks. J. Garcia, S. Cullipher, M. Weinrich, H. Sevan
- CHED 240.** Spectrometry, colors, and equilibrium constants. J. Reinoso, C. Ngai, M. Weinrich, H. Sevan
- CHED 241.** Students' ideas of what it means to problem solve in an undergraduate chemistry class. E. Auch, M.T. Dianovsky
- CHED 242.** Visualizaton of organic molecules: An analysis of a student's visual-spatial ability. A. Garcia, L. Perez, G. Vasquez, P.A. Janowicz
- CHED 243.** Thin film production and characterization. O. Santillan, E. Valenzuela, A. Williams, R.K. Moreno, B. Veldman
- CHED 244.** Oxidation of red cabbage anthocyanin. Y.A. Leguizamon, H.S. Barcena

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Computational Chemistry

Cosponsored by COMP and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 245.** Using structural bioinformatics to design glycopeptides with enhanced secondary structure. J. Rogers, S. McHugh, Y. Lin
- CHED 246.** Molecular dynamics simulations of detergent micelles. A. Philpott, A. Hoffmaster, D. Grodi, E.L. Harvey, B. Mertz

- CHED 247.** Determination of the potential energy surface for the dissociation of hydrogen on metal decorated graphene. J.G. Quattrucci, B. Walker
- CHED 248.** Studying the structure of the mitotic checkpoint complex using computational analysis and temperature-sensitive yeast mutants. T. Van Eeuwen, J. Luginland, P. Melloy, G. Anderle
- CHED 249.** Triclosan: Substituent effects and thermochemical properties. A. Jimenez, M. Rosan, K.R. Jorgensen
- CHED 250.** Computational study on quinones, extended quinones, and their sulfur counterparts. J. Covey, M. Paone, A. Ud-Doula, P.T. Pham
- CHED 251.** Thermochemical study of halocarbons: Brominated methane, ethane, ethylene, and acetylene derivatives. M. Cadena, K.R. Jorgensen
- CHED 252.** Electronic structure studies of copper dioxygen complexes. K. Parikh, A. Dinescu
- CHED 253.** Determining the product of the reaction between chromotropic acid and formaldehyde. K.A. Leets, G.D. Gibbs, L. Tribe

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Environmental Chemistry

Cosponsored by ENVR and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 254.** Investigating the chemical composition of sealcoat emulsion collected from three sites in south-central Pennsylvania, USA. Z. Greenberg, O. Wilkins, A.E. Witter
- CHED 255.** Towards greener remediation: Removal of Cr(VI) using cellulose films. M. Dilip, K. Paradis
- CHED 256.** Phytoremediation potential of native wetland species in acid mine drainage (AMD) conditions. R.A. Wilkes, J.L. Bayline, J. Kilgore, P. Skylstad
- CHED 257.** Free cyanide: Understanding sampling, preservation, and analysis by gas diffusion separation by the NYC-DEP. S. Salamone, C. Ooi, P.D. Svoronos, P. Meleties, F. Jacques, J. Vilacis
- CHED 258.** New York City's waste water and sewage treatment by the Environmental Protection Agency. H. Shin, M. Stephen, E. Shin, P.D. Svoronos, P. Meleties, F. Jacques, J. Vilacis
- CHED 259.** Controlling the industrial heavy metal pollutants' discharge into New York City's wastewater through the Industrial Pretreatment Program (IPP) of the NYC Department of Environmental Protection (NYC-DEP). D. Proano, J. Vilacis, F. Jacques, P.D. Svoronos, P. Meleties
- CHED 260.** ArcGis: Understanding citywide infrastructural landscape through the Environmental Protection Agency. B. Um, T. Islam, J. Vilacis, F. Jacques, P. Meleties, P.D. Svoronos
- CHED 261.** Promoting health in southwest Morocco through water quality project field study. A.E. Madi, J.A. Elliot, M.A. Mesnaoui, N. Nid, M. Yatin
- CHED 262.** Estrogen in our surface water and sediment. K. Murphy, F. Fonseca
- CHED 263.** Green polymers as potential agents for removal of suspended solids from domestic wastewater. R. Srinivasan, T.B. Roberson

- CHED 264.** Effects of fruit nutrition and biochemistry on the physiological condition of wild birds. C. Carrington, S. Smith
- CHED 265.** Rice husk as a metal adsorbent: Investigation of competitive adsorption properties of Cd, Cu, Pb and Zn. D. Alexander, D.D. Amarasiriwardena
- CHED 266.** Chemistry of wastewater treatment: Monitoring a rural facultative lagoon system in a research-based environmental analysis course. T.D. Strickland, E.M. White
- CHED 267.** Effect of different power and tile conditions on the rates of growth for algal turf scrubbers. T.R. Schinasi, K. Aubrecht

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Green Chemistry & Sustainability

Cosponsored by I&EC and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 268.** Microwave-assisted synthesis of silver nanoparticles by using fresh citrus juices and antimicrobial activity: A comparative study. M. Yatin, H. Vinnikava, D. Antonuccio
- CHED 269.** "Kitchen green chemistry" approach to the kinetic study of iodine clock. M. Yatin, J. Elizabeth Hamilton
- CHED 270.** Spectroscopic characterization of malonic acid induced protein crosslinks as a greener alternative to cell fixation. D. Szlosek, P.M. Doherty, D. Finocchietti, C. Lessard
- CHED 271.** Evaluation of acid-catalyzed transesterification reactions of vegetable oil to prepare biodiesel. R.N. Goodrich, P.T. Bell
- CHED 272.** Extraction and examination of endophytes obtained from beach rose (*Rosa rugosa*). A. Vinn, C. MacTaylor

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Inorganic Chemistry

Cosponsored by INOR and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 273.** Synthesis and characterization of novel cerium(IV) aryloxide complexes as selective one-electron oxidants for organic substrates. M. Bull, C. Tyrol, M. Martin, R. Schnabel
- CHED 274.** Nickel mediated carbon dioxide and ethylene coupling for catalytic acrylate production. A. Spentzos, W. Bernskoetter
- CHED 275.** Incorporating 4-aminopyridyl groups in coordination polymers. J. Koka, D.R. Manke
- CHED 276.** Synthesis of an iron(III) containing phenyl POSS polymer. M.T. Hay, A. Adams, T. Carlin, T. Logue
- CHED 277.** Effect of excited state torsion strain yielding greater photosubstitution within a series of ruthenium(II) N,O-chelates. F. Delano, B. Sears
- CHED 278.** Investigation of 8-hydroxyquinolate photosubstitution in a series of ruthenium(II) complexes targeting dsDNA for light activated therapy. A. Cardillo, B. Sears

- CHED 279.** Investigation of the effect of N,O-chelating ligands on the absorbance and photochemistry in a series of tris-chelated ruthenium(II) complexes. E.T. Fisher, B. Sears

- CHED 280.** Photophysical and photodynamic reactivity of a series of ruthenium(II) heteroleptic 8-hydroxyquinoline and phenathroline chelates. A. Koerner, B. Sears
- CHED 281.** Reactivity of ruthenium-salicylaldehyde complexes with benzylamine. N. Spitha, D.N. Blauch
- CHED 282.** Exploiting redox switchable polymerization reactions to study electron transfer self-exchange reactions. J. Curley, A. Biernesser, K.R. Delle Chiaie, J.A. Byers

- CHED 283.** Synthesis, characterizations, and properties of organoruthenium complexes of flufenamic acid. S. Parnell, S. Pramanik, S.K. Mandal

- CHED 284.** Synthesis of metal-POCOP and metal-PNCNP pincer catalysts for transfer hydrogenation of biomass-derived substrates. M. Abele, A. Onyett, T. Thananathanachon

- CHED 285.** Synthesis of bis(amidinato)-M-heterocyclic carbene iron complexes with increased solubility and their application as catalysts for the hydrogenation of alkenes. C. Wolstenholme, H.Z. Kaplan, J.A. Byers

- CHED 286.** Synthesis and characterization of intermediates of the palladium(II) catalyzed alkyne hydroarylation. A. Azua, A. Lopez, R. Damera, C. Hahn

- CHED 287.** Electrochemistry of an electron-rich subporphyrazine. T.J. Herman, W.S. Durfee, J.R. Stork

- CHED 288.** Stabilizing transition-metal-alkylthiolate bonds via secondary sphere hydrogen bonding. R. Hall, S. Pazić

- CHED 289.** Examination of $PNC^{HC}P$ pincer catalysts in cross-coupling reactions. J.R. Hall, B. Anderson

- CHED 290.** Synthesis and characterization of heterobimetallic calix[5]arene complexes. M.A. Tiemann, B.A. Martinez-Ortega

- CHED 291.** Withdrawn.

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Medicinal Chemistry

Cosponsored by MEDI and SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 292.** Intermolecular synthesis and medicinal chemistry of cinnamate and cinnamide derived cyclobutanes. T. Lynch-Colameta, R. Telmesani, A.B. Beeler
- CHED 293.** Withdrawn.
- CHED 294.** Assessment of NEU-1090, an analog of NVP-BEZ235, as a new lead and tool compound for human African trypanosomiasis. T.J. DeLano, J.D. Seixas, S.A. Luengo-Arrata, R. Diaz, M. Navarro, M.P. Pollastr
- CHED 295.** Computational design of positive allosteric modulators of the AMPA receptor. M. Sacco, L.A. Bonner
- CHED 296.** Progress toward the synthesis of STAT3 inhibitor, CPD-188. J. Hoppe, B. Green, D.D. Grove
- CHED 297.** Synthesis of potential dopamine transporter inhibitors. T.C. Harned, L.A. Bonner

- CHED 298.** Design, synthesis, and application of fluorine-labeled biotin-linker-taxoid conjugates as ^{19}F NMR probes for the metabolic stability assessment of tumor-targeted drug delivery systems. J. Khan, B. Lichtenthal, L. Wei, J.G. Vineberg, I. Ojima

- CHED 299.** Novel dihydrofolate reductase inhibitor obtained through field-based computational modeling and SAR. K. Pearce, A.S. Piasecki, O. Hajder, D.A. Barr

- CHED 300.** Design and synthesis of novel NS3 protease inhibitors of the dengue virus. T.J. Carroll, T.C. Minors, S. Mayfield, A. Ramesh, E. Lin, P. Doyle, W. Chen, G. Bellegard-Bastos, Z. Zinsli, A. Scharf, R. Spoering, R.R. Ranatunge

- CHED 301.** Dissolution testing of chewable tablets of aspirin, ibuprofen, and acetaminophen. M. Sowers, A.F. Charlebois, S. Ibrahim

- CHED 302.** Identification of novel inhibitors for the treatment of histoplasmosis. A.J. Maurais, J. Franco, C. Berkes

- CHED 303.** Novel synthesis of (+)-catechin metabolites. K.W. Petersen, A. Lemus, J.W. Leahy

- CHED 304.** Copper mediated synthesis of 2,4-diaminopyrimidines: A potential new class of DHFR inhibitors. S. Anderson, D. Nitschmann, P.M. Pelphey

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Nanochemistry

Cosponsored by SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 305.** Colloidal dispersions of C_{60} fullerene in mixed solvent solutions. L.D. Bienski, R.N. Callahan, A.J. Kinnison
- CHED 306.** Synthesis, characterization, and catalytic application of palladium nanoparticles on carbon microsphere composites. C. Livingston, K.M. Metz
- CHED 307.** Forensic nanotechnology: Gold-carbon nanoparticles in fingerprint development. J. Park, O. Tytler, K. Kim, W. Adams, Y. Pajouhafsar, A. Altunaji, S. Altunaji, A. Mohamed, H. Abdou
- CHED 308.** Forensic nanotechnology: Gold-aniline nanocomposites in fingerprint development. K. Kim, O. Tytler, J. Park, W. Adams, Y. Pajouhafsar, S. Altunaji, A. Altunaji, A. Mohamed, H. Abdou
- CHED 309.** Collaboration between engineering students in introductory biology and chemistry courses: Synthesis, characterization, and toxicity measurements of iron oxide nanoparticles. L.E. Grove, S. Alibeik, K. Griffin, J. Nguyen, J. Penn, A. Sirois, K. Vilardi
- CHED 310.** Carbon nanotubes as molecular conduits. L.M. Nebel, L. Bricker, S. Menges, M.D. Ellison, M. Strano
- CHED 311.** Exceptional conductivity behavior of a clathrate-forming surfactant. J. Monde, C.E. Larrabee
- CHED 312.** Microwave synthesis of single-walled carbon nanotube-ruthenium nanoparticles composites for dye degradation. N. Tobar, T. Hemraj-Benny
- CHED 313.** Partial sulfonation of polyaniline nanofibers. S. Salamone, D.M. Sarno
- CHED 314.** Solvent effects on the photodegradation of the nanoparticle precursor tetrachloroaurate. C.E. Baker, J.C. Marcum

- CHED 315.** Chemical manipulation of MoS_2 and its applications in 2D heterostructures. H. Bergman, H. Tran, L.M. Campos

Section E

Boston Convention & Exhibition Center
Hall C

Undergraduate Research Posters

Organic Chemistry

Cosponsored by SOCED

N. Di Fabio, J. Roberts, *Organizers*

2:00 - 4:00

- CHED 316.** Synthesis of small molecule inhibitors against hepatitis C virus. M. Young, M. Busch, K. Strom, J.K. Snyder
- CHED 317.** Studies toward the total synthesis of trocheliophorolide A: A hydroboration approach. H. Simpson, A. Carestia, W. Spencer, J. Swartzenberg, T.G. Collison
- CHED 318.** Studies toward the total synthesis of aplydactone: A model study. A. Streit, A. Kelly, K.A. Valentine, T.G. Collison
- CHED 319.** Microwave-assisted synthesis of oligomers of α -aminoisobutyric acid. M. Rotondaro, A. Varuolo, T. Jacisin, M.A. Kubasik
- CHED 320.** Enzymatic resolution of the enantiomers of 2-ethyl-1-hexanol. L. Harris, D. Oldham
- CHED 321.** Synthesis of DEHP and its metabolites. K. McDaniel, D. Oldham
- CHED 322.** Role of directing groups in copper(I)-catalyzed oxidative decarboxylative coupling reactions. R. Goydel, K. Humphreys, C. Scaggs, J. Simmons, A. Baur, J.M. Hoover
- CHED 323.** Facile synthesis and computational studies of novel pyrazolone based monomers and dendrimers for potential use as encapsulating agents. J. Caruso III, A.M. Baijia
- CHED 324.** Synthesis of 2,6-dimethyl-4-o-methylphenyl-3-cyclohexenecarboxylic acid. W. Liang, S. Xie
- CHED 325.** Synthesis of pyrazolone derivatives from a nitrile or carboxylic acid. K.P. Tang, S. Xie
- CHED 326.** Hydrogen-bonding control of solvatochromism and non-radiative decay in the fluorescence of 3-amino-fluorenone derivatives. I. Alty, C.J. Abelt
- CHED 327.** Implementation of computational aids for Diels-Alder reaction in undergraduate organic chemistry laboratory. G. Slick, J. Jung
- CHED 328.** Photo-Fries reaction as a photochemical probe to quantify the cage effects of ionic liquids. A. Diorio, T.J. Rioux, L. Walsh, A.E. Keirstead

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- CHED 329.** Site selective Pd catalyzed intramolecular cyclization of oxygen nucleophiles. **D. Thach, G. Dong**
- CHED 330.** Solvents effects on electrophilic aromatic bromination of anilides. **J. Liegeot, M.W. Thomsen**
- CHED 331.** Functionalization of carbon fibers for use in composites. **D.E. Martyn, P.D. Bui**
- CHED 332.** Developing new experiments for the undergraduate organic chemistry laboratory: Electrophilic aromatic substitution. **M. Bader, L. Al Fhaid, T. Alrawaf, A. Alghunaim, A. Alabdullah, Y. Aloraji, Y. Alhabib, A. Rababah, Y. AlDosari**
- CHED 333.** Stereoselective synthesis of the bicyclo[2.2.2]diazoctane family. **J. Robins, K. Kim, J.R. Scheerer**
- CHED 334.** Survey of commercially available dried mushrooms for the presence of lovastatin and citrinin. **I.R. Eason, N.J. Wilson, M.C. Frazier, E. Jeong, B.A. Clement**
- CHED 335.** Fluorescence properties of 2-mercapto-6,7-diphenyl-5,6-dihydropteridin-4-ol. **E. Timothy, G.E. Greco, S. Sibley**
- CHED 336.** Synthesis of a stercoibilin isopomer: A potential biomarker of autism. **T. Puleo, K. Lewis, G.F. Pirrone, A.F. Charlebois**
- CHED 337.** Synthesis and optical properties of conjugated C-13 podocarpic acid derivatives. **N.T. Toomey, D.H. Miles**
- CHED 338.** Old reaction, new insights: The structures of all regioisomers of oxo- and dioxochlorins. **E. Kaesmann, R. Li, A. Nimthong-Roldán, M. Zeller, C. Bruckner**
- CHED 339.** Buchner ring expansion with diazoalkanes in flow. **R. Rosen, A.L. Courtney, A.B. Beeler**
- CHED 340.** Statistical analysis of tobacco for country of origin via ¹H-NMR and multivariate component analysis. **D.L. Paredes, C. McCleave, J.A. Bjorklund, N.L. Petersen**
- CHED 341.** Towards helical molecular structures. **H.S. Barcena, K. Maziarz, A. Gorbenco**
- CHED 342.** Development of alkylcobalamin derivatives for visible and near infrared light-mediated DNA cleavage. **W.M. Moreau, A.C. McCue, J.R. Shell, T.A. Shell**
- CHED 343.** Synthesis of alkyne from aldehydes and ketones via a-substituted N-tosyl hydrazones. **C. Arcand, C. Dooley, C.K. Weinreb**
- CHED 344.** Improved synthesis of 1,3,5,7-tetraethynyladamantane. **J. Pisano, C.K. Weinreb**

- CHED 345.** Surface enhanced Raman spectroscopy to study photocatalytic degradation of organic pollutants. **F.K. Wallace, M.J. Nee**
- CHED 346.** TiO₂ photocatalysis for water purification. **J. Metz, R. Liang, M.J. Shultz**
- CHED 347.** Thermal decomposition of 4-nitrosooxy-2-butanone. **E.R. Sias, J. Ellison, E.M. Wright, B. Warner, L.R. McCunn**
- CHED 348.** Determining the quantitative properties of photocatalytic plasmonic materials. **H. Somayaji, S. Lerch, B.M. Reinhard**
- CHED 349.** Eutectic behavior of binary polycyclic aromatic hydrocarbons (PAH) mixtures. **L. Zhong, E. Gunn, J.L. Goldfarb**
- CHED 350.** Porosity development and activation energies of the pyrolytic decomposition of coal-biomass blends. **A. Vyas, J.L. Goldfarb**
- CHED 351.** Infrared study of sporopollenin effect on pollen spectra. **J. Cassidy, G.A. Parodi**

- Section E**
Boston Convention & Exhibition Center Hall C
- Undergraduate Research Posters**
Polymer Chemistry
Cosponsored by PMSE, POLY and SOCED
- N. Di Fabio, J. Roberts, Organizers**
- 2:00 - 4:00**
- CHED 352.** Syntheses and antioxidant properties of lignin precursors. **A. Matsunaga, G. Bradley, P.V. Maciejczyk**
- CHED 353.** Triazine polyamide derivatives application as drug delivery systems. **M. El-Sayed, S. E. Abdel Naeem, A. O. Elzoghby, A.A. Bekhit, A.A. El Bardan, A. El-Faham, S.N. Khattab**
- CHED 354.** Investigating properties of VBT-VBA copolymer as a chemical rubber antiozonant: Development of the controlled rubber ozonization method. **R.W. Gurney, N.E. Lee, M. Voronina, A. McKeon, J. Genevich**
- CHED 355.** Hydrogel microfluidics for engineering tissue-like tubules. **Z. Nie, Q. Zhang, S. Wain**
- CHED 356.** Ring opening polymerization of six membered cyclic carbonates using bimetallic catalysts. **W.F. Schwandt, S. Poland**
- CHED 357.** Utilization of a catalyst-free, strain-promoted reaction between azides and norbornenes in dendrimer synthesis. **C. Tovar, A. Lopez, C.E. Hobbs**
- CHED 358.** Functionalization of polymer using thio-bromo click reactions. **C. De Los Santos, C.E. Hobbs**
- CHED 359.** Phosphonium polyelectrolytes: Film formation, supramolecular assembly, and antibacterial properties. **R. Smith, C.A. Conrad, E.H. Freeman, E.F. Colter**

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- Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais**
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- Section E**
Boston Convention & Exhibition Center Hall C
- Undergraduate Research Posters**
Physical Chemistry
Cosponsored by SOCED
- N. Di Fabio, J. Roberts, Organizers**
- 2:00 - 4:00**
- CHED 360.** Statistical analysis of tobacco for country of origin via ¹H-NMR and multivariate component analysis. **D.L. Paredes, C. McCleave, J.A. Bjorklund, N.L. Petersen**
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- CHED 371.** Infrared study of sporopollenin effect on pollen spectra. **J. Cassidy, G.A. Parodi**

Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais

Sponsored by YCC, Cosponsored by CHED, IAC, PRES and PROF

Technical program information known at press time. The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

†Cooperative Cosponsorship

MONDAY EVENING

Section A

Boston Convention & Exhibition Center Room 213

From Raw to Varoom: The Science Behind Getting a Car on the Road

Cosponsored by PMSE, POLY, RUBB and SCC†

Financially supported by IPEC board
S. C. Rukes, Organizer, Presiding

4:00 Introductory Remarks.

4:05 CHED 360. Raw materials for making a car: Where do they come from? **S.C. Rukes, A. Nydam, D. Goodwin, E.J. Escudero**

4:40 CHED 361. Making of the car: The building of the chassis and other parts. **S.C. Rukes, A. Nydam**

5:15 CHED 362. Under the hood: What makes the engine work? **S.C. Rukes, A. Nydam**

5:40 CHED 363. Getting rid of the excess heat: The cooling system. **S.C. Rukes, D. Goodwin**

6:05 Intermission.

6:15 CHED 364. Let the car roll: The making of tires. **S.C. Rukes, E.J. Escudero**

6:50 CHED 365. Roads, roads, we drive on. **S.C. Rukes, D. Goodwin, E.J. Escudero**

7:30 CHED 366. Extra features: Options to protect and beautify the car. **S.C. Rukes**

7:55 CHED 367. What does the future hold for automobiles? **S.C. Rukes, A. Nydam**

8:15 Concluding Remarks.

Section A

Boston Convention & Exhibition Center Hall C

Sci-Mix

I. Black, I. J. Levy, B. E. Rios McKee, Organizers

8:00 - 10:00

38, 62-63, 66, 69, 71-72, 75, 77, 89, 92, 95, 98, 100, 104-106, 110, 146. See previous listings.

468, 482. See subsequent listings.

Section A

Boston Convention & Exhibition Center Hall C

Successful Student Chapters

Cosponsored by SOCED

N. Di Fabio, Organizer

8:00 - 10:00

CHED 368. ACS Alexandria University: Activities, events, and community outreach. **S.N. Khattab, M. El-Sayed, B.A. Ali, H. Yosry, M.N. Hassanien, D. Reda, A.M. Hafez, A. Elmaamoun, M. Fathi, Y.G. Ahmed, M.M. Abd Elbadia, A. Saad, M. Gaaffer**

CHED 369. University of Maryland, Baltimore County's chemistry community. **N. Steenrod, M. Shin, G. Balaa**

CHED 370. Contribution of ACS USM Student Chapter towards chemical education in Malaysia. **D. Nithiaselvan, J. Quah, N. Zaulkiflee, H. Lee, J. Lim, S. Low**

CHED 371. Chemistry on the coast: Student activities at the University of New England. **B.E. Boe, R. Juneau, M. Perry, A.E. Keirstead**

CHED 372. Creating links and polymers: The ACS Student Affiliate Chapter at the University of Richmond. **B. Zhang, D. Stevens, K. Josloff, S. Houck, T. Bui, W. Case**

CHED 373. Accomplishments of the UMD American Chemical Society student affiliates chapter. **C. Ma, C. Tsui**

CHED 374. Greening a student chapter. **A. Goranov, S.L. Carberry**

CHED 375. University of Utah American Chemical Society Student Chapter. **A. Anamisis, C.J. White, C. Jennings, M.R. Kiley, N. Pratt, R. Parkin, R. Carlisle, A. Burton, H.L. Sebahar, J.D. Rainier, T.G. Richmond**

CHED 376. Wilkes University's ACS Student Chapter: Educating the community about green chemistry principles. **B.S. Clem, K.M. Rehrg, A. Dinescu, C. Henkels**

CHED 377. Northeastern University Student Affiliates of the American Chemical Society: Enriching the chemistry community in the greater Boston area. **J. Conway, W. Timson**

CHED 378. Saint Anselm College Chemistry Club: We work periodically. **C.I. Muldoon, J. Cassidy, A. Scaffidi, C. Dooley, W.M. Moreau, N. Eyet**

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center Room 253C

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Cosponsored by ANYL†, BIOL†, BIOT†, BMGT†, CORP†, DAC†, ENFL†, PHYS† and POLY†

Financially supported by UMN College of Science and Engineering, UMN Office of the Vice President of Research, ACS Minnesota Local Section, UMN College of Biological Sciences, UMN Department of Chemical Engineering and Materials Science, Valspar, BASF, STREM Chemicals, UMN Department of Chemistry
L. M. Johnson, Organizer, Presiding

9:00 Introductory Remarks.

9:05 CHED 379. Opening presentation: Building successful collaborations. **C. Arnold**

9:15 CHED 380. Fundamental research to commercial products. **R.H. Grubbs**

9:50 CHED 381. Toward the practical application and commercial translation of layer-by-layer assembly. **P.T. Hammond**

10:25 Intermission.

10:40 CHED 382. From bench to market in the capital intensive energy market. **D.G. Nocera**

11:15 CHED 383. Understanding and Using Nature's Design to Develop New Commercial Technologies. **A.M. Belcher**

11:50 Concluding Remarks.

Section B

Boston Convention & Exhibition Center Room 253B

Chemistry Education Research

Teaching and Learning in Introductory Chemistry

T. Greenbowe, Organizer

G. Bhattacharyya, Organizer, Presiding

8:30 Introductory Remarks.

8:35 CHED 384. Pilot of a blended general chemistry laboratory course to increase course capacity and improve learner success in a large enrollment course. **S. Burchett, K.H. Woelk, J.L. Hayes**

8:55 CHED 385. Team based learning reduces attrition in a first semester general chemistry course. **L.L. Comeford**

- 9:15 CHED 386.** Improving student engagement in general chemistry laboratory through group discussions. M. Mahalingam, J. Väilisaari
- 9:35** Intermission.
- 9:45 CHED 387.** Relationship between student study time, satisfaction, and exam grade in an introductory chemistry course. J.R. Pribyl, B.J. Brown, E.A. Doss
- 10:05 CHED 388.** Studio chemistry at CalPoly: An examination of student outcomes. A. Kiste, G.E. Scott
- 10:25 CHED 389.** Free and interactive chemistry lab manuals through collaborations: Project at a community college. V. Kumar
- 10:45** Intermission.
- 10:55 CHED 390.** Integrating scale across the general chemistry curriculum. J.M. Trate, A. Blecking, P. Geissinger, K.L. Murphy
- 11:15 CHED 391.** Reading to promote conceptual change for redox and bonding concepts: Investigating the interaction between reading skill and text type. R. Buell, S. Paziemi
- 11:35 CHED 392.** Investigation of general chemistry textbook usage: Development of a survey to probe how and why students use textbooks. R.W. Buell, S. Paziemi
- 11:55** Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 207

Active Learning in the Chemistry Classroom

D. A. Katz, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 CHED 393.** Accessible picture of what light is and how it interacts with matter. B. Abrams, N. Bassina, D. Dill, A. Golger
- 8:55 CHED 394.** Teaching using a hybrid course model: Crafting and using effective out-of-class activities that engage and prepare students. B. Abrams, E. Allen, N. Bassina, D. Dill, P. Garik, A. Golger
- 9:15 CHED 395.** Modeling instruction: A research-based guided-inquiry approach to high school chemistry curriculum. D. Sun, L.E. Slocum, L. Dukerich
- 9:35** Intermission.
- 9:45 CHED 396.** Coordinated response to student deficiencies and their performance in "General Chemistry". K.A. Asala, R.L. Jew, S.K. Michael, J.C. Poler, M.M. Rabinovich, C.D. Striplin
- 10:05 CHED 397.** Student-driven interactive chemistry lab assessment tool to evaluate lab instructors and learners. S. Burchett, J.L. Hayes
- 10:25 CHED 398.** Withdrawn.
- 10:45** Intermission.
- 10:55 CHED 399.** Engaging students in learning analytical chemistry: Active learning through integrated labs, learning groups, and case studies. R.E. Goacher
- 11:15 CHED 400.** Partnering with a local middle school to enhance science curriculum: A service learning opportunity. F. Yopez Castillo
- 11:35 CHED 401.** Engaging organic chemistry students with group activities. C. Gabel, S. Gordon, S. Norris, N. Kuehl
- 11:55 CHED 402.** Creating an active learning environment and providing formative assessment in Organic Chemistry large enrollment lecture course using iPads with airserver. M. Chatterjee
- 12:15** Concluding Remarks.

Section D

Boston Convention & Exhibition Center
Room 208

From Discovery to Application: Implementing the Last 50 Years of Innovation into the Undergraduate Chemistry Classroom

A. C. Banerjee, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 CHED 403.** From discovery to application: Innovations in heterogeneous catalysis and implementation in undergraduate research and teaching. A.C. Banerjee
- 8:55 CHED 404.** Computational chemistry in the undergraduate curriculum. M.A. Boucher, D.A. Barr
- 9:15 CHED 405.** Simplified molecular dynamics simulations for teaching viscosity and self-diffusion. M.J. Neel
- 9:35 CHED 406.** From discovery to application: Incorporating 50 years of the glass transition into a polymer chemistry course. D.W. Holley
- 9:55** Intermission.
- 10:05 CHED 407.** Modern biochemical techniques in foundation chemistry labs. E.J. McIntee, H.V. Jakubowski, C.P. Schaller, K.J. Graham, R.A. Hutcheson
- 10:25 CHED 408.** Chemical education via biodiesel production. M.B. Jacobs, T.C. Vogt, E.S. Ball, S. Ahsan, J. Zimmerman, S. McManus, C. Farman, J.J. Holloway
- 10:45 CHED 409.** Inorganic molecular design: A two-credit advanced course designed to provide an introduction to modern inorganic chemistry. B.J. Johnson
- 11:05** Concluding Remarks.

Current Topics in Chemical Safety Information

Use Cases for Chemical Safety Information

Sponsored by CHAS, Cosponsored by AGFD, CCS, CHED and CINF†

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253C

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Cosponsored by ANYL†, BIOT†, BMGT†, CHED†, CORP†, DAC†, ENFL†, PHYS† and POLY†

Financially supported by UMN College of Science and Engineering, UMN Office of the Vice President of Research, ACS Minnesota Local Section, Valspar, BASF, STREM Chemicals, UMN Department of Chemistry, UMN College of Biological Sciences, UMN Department of Chemical Engineering and Materials Science

L. M. Johnson, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35 CHED 410.** Holistic approach to biomaterials, healing, and commercialization. B.D. Ratner
- 2:10 CHED 411.** Bioorthogonal chemistry: An enabling tool. C.R. Bertozzi
- 2:45** Intermission.
- 3:00 CHED 412.** Step and flash imprint lithography: From the lab to the fab. C.G. Willson
- 3:35 CHED 413.** Miniaturizing a measurement: Nanoliter volume nuclear magnetic resonance and single cell mass spectrometry. J.V. Sweedler

- 4:10 CHED 414.** Breakthroughs in imprint lithography and 3D additive fabrication. J.M. Desimone
- 4:45** Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 253B

Chemistry Education Research Organic Chemistry in the Classroom and Lab

G. Bhattacharyya, T. Greenbowe, *Organizers*
T. Gupta, *Presiding*

- 1:30** Introductory Remarks.
- 1:35 CHED 415.** Mixed methods study of green chemistry understanding from the organic laboratory. T.L. Kishbaugh, R. King
- 1:55 CHED 416.** Transforming the organic chemistry experience: Development, implementation, and evaluation of organic lab modules. T.G. Collison, J.A. Cody, T.D. Kim, B.L. Edelbach, J.P. Anderson, C. Ayotte, D. Saviola, W. Marmor
- 2:15 CHED 417.** Measurement of graduate student instructors' pedagogical content knowledge related to solution-state concepts. J.C. Lutter, G.V. Szymczak
- 2:35 CHED 418.** Graduate student instruction in organic chemistry laboratory: How is pedagogical content knowledge of thin layer chromatography developed? L. Hale, G.V. Szymczak
- 2:55** Intermission.
- 3:05 CHED 419.** Representation mapping to understand students' abstraction capacity. M. Weinrich, H. Sevia
- 3:25 CHED 420.** Visualization of organic molecules: An analysis of a student's visual-spatial ability. A. Garcia, L. Perez, P.A. Janowicz, G. Vasquez
- 3:45 CHED 421.** Construction of student-friendly and scientifically-valid descriptions of electron-pushing diagrams. G. Bhattacharyya
- 4:05** Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 207

Active Learning in the Chemistry Classroom

D. A. Katz, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:35 CHED 422.** Well, how did I get here? The evolution of an organic chemistry experience. N.E. Carpenter
- 1:55 CHED 423.** Active learning in a large organic chemistry class. D.A. Canelas
- 2:15 CHED 424.** Flipped classroom in undergraduate and post-baccalaureate premedical organic chemistry classes at Goucher College. G.E. Greco
- 2:35** Intermission.
- 2:45 CHED 425.** Using 'clickers' to encode and decode conceptual knowledge in organic chemistry. S.M. Graham
- 3:05 CHED 426.** Multiple choice testing in college organic chemistry courses: Using immediate feedback – assessment technique (IF-AT) forms to assess learning from mistakes. P.M. Schwartz, J.D. Merrel, P.F. Cirillo, J.A. Webb
- 3:25 CHED 427.** International organic chemistry competition: A thrilling, unique experience. L.I. Khallil, K.M. Chahine, B.R. Kaafarani
- 3:45** Intermission.

- 3:55 CHED 428.** Teaching flavor chemistry through the design and synthesis of artificial scents. J.L. Epstein
- 4:15 CHED 429.** Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: An active-learning approach. S. Riegel
- 4:35 CHED 430.** MitoNEET folding and iron sulfur cluster stability investigations in the undergraduate lab course as a unique experiential learning environment. T. Leeper, W.J. Goldenhuys, D. Morris
- 4:55** Concluding Remarks.

Current Topics in Chemical Safety Information

Sponsored by CHAS, Cosponsored by CCS, CHED and CINF†

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 253C

Process-Oriented Guided Inquiry Learning (POGIL)

R. S. Moog, *Organizer*

A. L. Smith, *Presiding*

- 8:30** Introductory Remarks.
- 8:35 CHED 431.** Guided inquiry vs. traditional approaches for learning introductory nutrition. A.L. Smith, R.J. Purcell, J.M. Vaughan
- 8:55 CHED 432.** Enhancing success in general chemistry by implementing POGIL activities in workshops. S. Russo-Rodriguez
- 9:15 CHED 433.** iPOGIL: Developing interactive process-oriented guided inquiry learning activities. D.W. Kuykendall
- 9:35** Intermission.
- 9:45 CHED 434.** Development of POGIL activities for teaching new content in analytical chemistry courses. I. Kimaru, M.C. Koether, K. Chichester, K.M. Lantzky Eaton
- 10:05 CHED 435.** Guided inquiry experiment to determine the configuration of a polymer in aqueous solution. A.L. Marsh
- 10:25** Panel Discussion.

Section B

Boston Convention & Exhibition Center
Room 253B

Chemistry Education Research

Cognitive and Affective Factors in CER

T. Greenbowe, *Organizer*

G. Bhattacharyya, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 CHED 436.** Persistence in STEM: Using a subset instrument to measure subtle changes in self-efficacy and outcome expectations. S. Srinivasan, K.L. Murphy
- 8:55 CHED 437.** Study of the effectiveness of single shot, case study-based responsible conduct of research workshops in research experiences for undergraduates programs. P.A. Mabrouk
- 9:15 CHED 438.** Withdrawn.
- 9:35** Intermission.
- 9:45 CHED 439.** Being an expert in chemistry: Students' views of the novice-expert spectrum. M.T. Dianovsky

10:05 CHED 440. Nationwide survey of the undergraduate physical chemistry course. L. Fox, G. Roehrig

10:25 CHED 441. Analysis of scientific argumentation in two POGIL physical chemistry classrooms. A.C. Moon, C.L. Stanford, R.S. Cole, M.H. Towns

10:45 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 207

General Papers

Totals

S. A. Fleming, *Organizer*

A. Gupta, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 442. Real research/real genres: Integrating research-based writing into an introductory quantitative chemistry lab sequence for majors. B. Abrams

8:55 CHED 443. Peer-assessment based learning in chemical education. A. Gupta

9:15 CHED 444. Student-generated content: PeerWise use in undergraduate chemistry classrooms. A. Kay, J. Hardy

9:35 Intermission.

9:45 CHED 445. Transforming learning pathways in the undergraduate chemistry laboratories. K. Hess

10:05 CHED 446. Entirely student-created wiki textbook to accompany a sophomore-level course in bio-organic chemistry. B.C. Goess

10:25 CHED 447. Withdrawn.

10:45 CHED 448. Improving student outcomes: Implementing study strategies. I. Sawchyn

11:05 CHED 449. Developing critical thinking skills using student group presentations in biochemistry. S.M. Tremain

11:25 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253C

Polymer Concepts in Inorganic Chemistry Courses

Cosponsored by INOR, PMSE and POLY

W. T. Ford, C. Tessier, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CHED 450. Tutorial on inorganic and organometallic backbone polymers. F. Jaekle

1:35 CHED 451. Introduction to silicone chemistry. M.S. Ferritto

2:05 CHED 452. Teaching organometallic chemistry to polymer students. L. Jia

2:35 Intermission.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:

www.acs.org/boston2015

2:45 CHED 453. Mixing it up: Integrating inorganic and polymer concepts in undergraduate courses. D.P. Gates

3:05 CHED 454. Polymer concepts in an inorganic chemistry laboratory and lecture course sequence. C. Tessier, W.J. Youngs

3:25 CHED 455. Withdrawn.

3:45 CHED 456. Teaching polymer chemistry in green chemistry: An inorganic approach. D.J. Darensbourg

4:05 CHED 457. Using independent literature and laboratory research projects to introduce polymer concepts in advanced inorganic chemistry. C. Goh

4:25 CHED 458. Incorporation of polymer chemistry topics in inorganic and materials chemistry courses at Florida Atlantic University. D.T. de Lill, C.E. Carraher

4:45 CHED 459. Polymers in inorganic chemistry: A first-hand account. G. Arbuckle-Keil

5:05 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 253B

Teaching Organic Chemistry for Biology Majors

R. Swisher, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 CHED 460. Offering an elective medicinal chemistry course and a targeted chemistry minor in an attempt to engage more science majors to take additional chemistry courses at a small liberal arts university. M.J. Castaldi, J.L. Epstein

2:00 CHED 461. Approaches to improve the teaching effectiveness of organic chemistry for biology majors. Z. Wang

2:20 CHED 462. Reactivity 2: A new integrated foundation course. E.J. McIntee, C.P. Schaller, K.J. Graham, B.J. Johnson, T.N. Jones

2:40 CHED 463. One course to bring them all, and in the science prime them: New approaches for teaching students in a world of convergent science. J. Kritzer

3:00 Intermission.

3:10 CHED 464. Teaching organic chemistry for biology and environmental science majors. R. Swisher

3:30 CHED 465. Examining the nicotine-triggered dopamine response in *pho-chromocytoma* rat cells (PC-12) in the organic chemistry laboratory: Engaging life science students in their home turf. J. Osko, F. Yopez Castillo, J. Ulrich

3:50 CHED 466. Organic chemistry for Life Science students: The Purdue NEXUS program. J.A. Chmielewski

4:10 Discussion.

Section C

Boston Convention & Exhibition Center
Room 207

General Papers

Diversity/Retention Issues

S. A. Fleming, *Organizer*

F. Damkaci, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 467. Attaining chemistry faculty diversity: A case study at a public, four-year liberal arts college. D.P. Pursell, P. Bell

1:55 CHED 468. Lighting the pathway to academic careers for Native Americans in STEM: Preliminary report. K.M. Hughes, S. EchoHawk, M.J. Ondrechen

2:15 CHED 469. Comprehensive study of talking lab equipment in chemistry and other science laboratory classes to integrate students who are blind. C.A. Supalo

2:35 Intermission.

2:45 CHED 470. Chemistry camp for middle school girls. M. Levine, N. Serio, B. Radaram, S. Chaudhuri, W. Talbert

3:05 CHED 471. STEM educational enhancement in Oklahoma: Teaching chemistry to 4th-6th grade by high school students. A. Rahman

3:25 CHED 472. Peer mentorship program using general chemistry labs: Impact on retention. F. Damkaci

3:45 CHED 473. Development of technical chemistry language skills for non-native speakers. D. Ramella

4:05 Concluding Remarks.

THURSDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 253C

General Papers

Undergrad Lab

S. A. Fleming, *Organizer*

C. S. Hamann, *Presiding*

8:00 Introductory Remarks.

8:05 CHED 474. Implementing an embedded chemistry research experience in an undergraduate Instrumental Analysis course. K.S. Wendling

8:25 CHED 475. Feasible screening method for antimicrobial activity of natural products for the interdisciplinary research project at a small liberal-arts college. H. Shin

8:45 CHED 476. 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

9:05 Intermission.

9:15 CHED 477. Synthesis, characterization, and toxicity measurements of iron oxide nanoparticles: An interdisciplinary collaboration between introductory chemistry and biology labs for engineering students. L.E. Grove, S. Alibeik

9:35 CHED 478. Incorporating faculty research into upper-level chemistry courses when schedule and budget make it seem otherwise impossible. C.E. Mactaylor, D. Hamill, J. Cotter

9:55 CHED 479. First physical chemistry lab: Monte Carlo calculations of π . D. Riccardi, L. Pegrar

10:15 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 253B

General Papers

Courses

S. A. Fleming, *Organizer*

A. Fazal, *Presiding*

8:00 Introductory Remarks.

8:05 CHED 480. Research-based course for introducing nanoscience to 1st year students from a chemist's perspective. T.J. Sorensen

8:25 CHED 481. Case study review of a problem based learning approach used to educate and train young forensic scientists through the use of six sigma investigative tools. D. Wallace Duckworth

8:45 CHED 482. Introduction of quantum mechanics principles at mesoscopic and macroscopic levels to first-year undergraduates through hands-on chemistry laboratory activities. F. Schunk, A. Mendoza-Garcia, I. Pirozzi, L. Wang

9:05 Intermission.

9:15 CHED 483. General chemistry for Life Science students: The Purdue NEXUS program. C. Hrycyna

9:35 CHED 484. Inorganic and bioinorganic chemistry: A foundational course in inorganic chemistry. K.E. Kristian

9:55 CHED 485. Practical course in physical organic chemistry suitable for the primarily undergraduate institution. D. Jacobs

10:15 CHED 486. Chemical measurement laboratory: A foundation level laboratory course for the new chemistry curriculum. A. Fazal, R.M. White, M.R. Ross

10:35 Concluding Remarks.

CHAS

Division of Chemical Health and Safety

D. Decker, J. Pickel and F. Wood-Black,
Program Chairs

SUNDAY MORNING

Combining Scientific Evidence for Health Policy and Regulation

Sponsored by AGRO, Cosponsored by CHAS and TOXI

SUNDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Waterfront 1A/1B

Lab Safety 25 Years After Promulgation of the OSHA Laboratory Standard

Cosponsored by CCS

P. A. Reinhardt, *Organizer*

L. DeBerardinis, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHAS 9. University laboratory safety in 2015: Was it the lab standard or what? G. Hall

1:55 CHAS 10. Enhancing safety culture through collaborative development of laboratory specific chemical hygiene plan (LSCHP) and Standard Operating Procedures (SOPs). T. Chandra

2:15 CHAS 11. What constitutes a laboratory? Princeton laboratory safety programs today and beyond. B.S. Chance

2:35 CHAS 12. From accident analysis to accident prevention at UCLA. C.A. Merlic, I. Schroeder

2:55 Intermission.

3:10 CHAS 13. Impact of the OSHA Laboratory Standard on basic laboratory safety education for undergraduates. R.H. Hill

3:30 CHAS 14. Where are we with lab safety education: Who, what, when, where, and how? K.P. Fivizzani

3:50 CHAS 15. Should science departments have their own safety departments? An assessment of a centralized approach. K.S. Hylton

4:10 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF, SOCED and WCC

MONDAY MORNING

Section A

Seaport Hotel and World Trade Center
Waterfront 1A/1B

Lab Safety 25 Years After Promulgation of the OSHA Laboratory Standard

Cosponsored by CCS

L. DeBerardinis, *Organizer*

P. A. Reinhardt, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHAS 1. Reflections of an OSHA regulator on the Laboratory Standard. F. Malaby

8:55 CHAS 2. Meandering towards OSHA's lab standard compliance. M.D. Finucane

9:15 CHAS 3. "Compliance" does not mean "safe". M.E. Mulcahy

9:35 CHAS 4. Developing a model for chemical safety literacy in the lab. R. Stuart

9:55 Intermission.

10:10 CHAS 5. Chemical hygiene plans: The vision and the reality. M. Weil, C. Pires, N. Kielbania

10:30 CHAS 6. DOE Energy Innovation Hub's effort to influence laboratory safety among its funded researchers. S. Rupkey, D. Hodge

10:50 CHAS 7. Withdrawn.

11:10 CHAS 8. Laboratory safety: Engaging 600+ research groups. S. Tumidajski

11:30 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF, SOCED and WCC

MONDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Waterfront 1A/1B

Chemical Health & Safety Awards

Cosponsored by CCS

D. B. Walters, *Organizer, Presiding*

D. M. Decker, *Presiding*

1:30 Introductory Remarks.

1:35 CHAS 16. Musings of a founder of the Chemical Health and Safety Division. E.M. Pearce

1:55 CHAS 17. Laboratory safety in the 21st century. R. Stuart

2:25 CHAS 18. 12,000 thoughts on laboratory safety in 20 minutes or less. R. Toreki

2:55 Intermission.

3:10 CHAS 19. SafetyStratus Collegiate Safety Award. M.D. Finucane

3:40 CHAS 20. From the safety beat: The UCLA fatality and beyond. J. Kemsley

4:10 CHAS 21. Science, safety, and human suffering. N. Sangji

4:20 Concluding Remarks.

TUESDAY MORNING

Section A

Seaport Hotel and World Trade Center
Waterfront 1A/1B

Current Topics in Chemical Safety Information

Use Cases for Chemical Safety Information

Cosponsored by AGFD, CCS, CHED and CINF†

L. McEwen, R. Stuart, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 CHAS 22. Organizing chemical information to support lab safety. R. Stuart, L. McEwen

9:25 CHAS 23. Keeping your kids away from poisonous chemicals: Chemical safety in the household. N. Qin

9:45 CHAS 24. Updating NFPA 45: Fire protection for laboratories using chemicals. L. Montville

10:05 CHAS 25. Blueprint for successful chemical management at Yale's West Campus. C.D. Incarvito, K.M. Heard

10:25 Intermission.

10:40 CHAS 26. Chemistry lab safety information resources for academic user. G. Baysinger

11:00 CHAS 27. Teaching future chemists how to create meaningful risk assessment tools. S.B. Sigmann

11:20 Panel Discussion.

Transforming University-Industry Partnerships for an Innovative Future

Envisioning, Enabling and Executing

Sponsored by PRES, Cosponsored by AGRO, BMGT, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

TUESDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Waterfront 1A/1B

Current Topics in Chemical Safety Information

Cosponsored by CCS, CHED and CINF†

L. McEwen, R. Stuart, *Organizers, Presiding*

1:30 CHAS 28. Designing a hazard and risk assessment protocol for undergraduate instruction and use. D.C. Finster

1:50 CHAS 29. Experience with data handling in large chemical databases. N.R. Langerman

2:10 CHAS 30. Ensuring that lessons learned are not forgotten: Leveraging ELN to transform the safety paradigm. M. Manfredi, R. Durvasula, W. Bullock, B. Cavallaro, C. McNab, M. Nolte, D. Vanderwall

2:30 CHAS 31. Encoding reactive chemical hazards and incompatibilities in an alerting system. J.W. May, R.A. Sayle

2:50 Panel Discussion.

3:05 Intermission.

3:20 CHAS 32. Biological and ecological toxicity of engineered nanomaterials. I.L. Gunsolus, T. Qiu, V. Feng, C.L. Haynes

3:40 CHAS 33. eNanoMapper: A database and ontology framework for nanomaterials design and safety assessment. B. Hardy, E.L. Willighagen, J. Hastings, M. Hegl, N. Jellazkova, H. Sarimveis

4:00 CHAS 34. Data, data everywhere, nor any bit processable: Opportunities for amalgamating and opening up chemical data and information relevant to hazard recognition and safety planning. J. Zhang, P. Thiessen, G. Fu, E. Bolton, L. McEwen

4:20 CHAS 35. It's all in how you do it: Annotating process conditions in laboratory chemical hazard recognition and risk management. L. McEwen, Y. Li

4:40 Panel Discussion.

Transforming University-Industry Partnerships for an Innovative Future

Energizing and Education

Sponsored by PRES, Cosponsored by AGRO, BMGT, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

CINF

Division of Chemical Information

E. Davis, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Integrated Approaches in Structure-Based Drug Design (see *COMP, Sunday*)

Designing Chemical Libraries for Screening: Past, Present & Future (see *COMP, Sunday*)

Education for Sustainable Development and Innovative Technologies Across Culture (see *CHED, Sunday*)

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits (see *CHED, Sunday*)

Informatics 2.0 for the Analytical Sciences: Big Data, the Semantic Web, and Metadata (see *ANYL, Sunday*)

Advances in Predictive Toxicology: In Silico & In Vitro Approaches (see *MEDI, Monday*)

SOCIAL EVENTS:

Careers in Chemical Information and Cheminformatics Panel Discussion & Brunch, 9:00 AM: Sunday

Reception, 6:30 PM: Sunday

Luncheon, 12:00 PM: Tuesday

Skolnik Award Symposium
Reception, 6:30 PM: Tuesday

Wikipedia Edit-a-thon, 1:30 PM: Wednesday

BUSINESS MEETINGS:

Business Meeting, 1:00 PM: Saturday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 104A

Substance Identifiers, Addressing the Challenges Presented by Chemically Modified Biologics: The Role of InChI & Related Technologies

S. R. Heller, K. Taylor, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 1. Generating canonical identifiers for glycoproteins and other chemically modified biopolymers. R.A. Sayle, J.W. May, N. O'Boyle

9:05 CINF 2. Toward addressing informatics challenges presented by antibody drug conjugates. S.K. Sukuru, T. Zhang, L.N. Tumey, E. Muszynska, M. Tran, F. Loganzo

9:35 CINF 3. Representation of chemically modified proteins in the Substance Index SPL Files. Y. Borodina, G. Schadow

10:05 Concluding Remarks.

Section A

Boston Convention & Exhibition Center
Room 104A

Applications of Cheminformatics to the Diverse World of Natural Products

R. Schenck, A. J. Williams, *Organizers, Presiding*

10:30 Introductory Remarks.

10:35 CINF 4. Naming algorithms for derivatives of peptide-like natural products. R.A. Sayle, N. O'Boyle, C. Southan

11:00 CINF 5. Applications of cheminformatics to the diverse world of natural products. A.J. Williams, S. Dabb

11:25 CINF 6. Reliable structure characterization and elucidation: Finding and confirming the truth. P.D. Wheeler, A. Williams

11:50 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 104B

The Growing Impact of Big Data in the World of Chemical Information

S. Ekins, R. Potenzzone, A. J. Williams, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 7. Challenges in big data chemistry using publicly available chemical information. S. Kim, G. Fu, V.D. Hähneke, L. Han, B. Yu, L. Geer, B. Shoemaker, A. Gindulyte, S. He, P. Thiessen, E. Bolton, S.H. Bryant

9:00 CINF 8. Multiplexing analysis of 1000 approved drugs across 70 million PubChem entries: Will the correct structures please stand up? C. Southan

9:25 CINF 9. How the availability of online data and datasets can underpin a platform of connected data. A.J. Williams

9:50 Intermission.

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10:05 CINF 10. Applying cheminformatics and bioinformatics approaches to neglected tropical disease big data. **S. Ekins**, J. Lage De Siqueira, L. McCall, M. Sarker, M. Yadav, E. Ponder, A. Kallel, B. Bunin, J. McKerrow, C. Talcott

10:30 CINF 11. Chemocentric informatics novel analysis of “omics” data identifies novel associations between histone deacetylase inhibitors and neurodegeneration. **M.P. Bradley**

10:55 CINF 12. Chemical biology informatic approaches to identify and validate new therapeutic targets. **P. Kutchukian**

11:20 CINF 13. Analyzing ToxCast data using nebula (neighbor-edges based and unbiased leverage algorithm). **H. Hong**

11:45 Closing Remarks.

Integrated Approaches in Structure-Based Drug Design

Sponsored by COMP, Cosponsored by CINF and MEDI

Best in Class Computational Software by Integration

Sponsored by COMP, Cosponsored by CINF

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 104A

Wikipedia and Chemistry: Collaborations in Science and Education

Cosponsored by CHED

Y. Li, M. A. Walker, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CINF 14. Chemistry and Wikipedia: Coverage, evolution, and citations. **E. Alvaro**, A. Yanguas-Gil

1:25 CINF 15. Chemistry collaborations on Wikipedia. **M.A. Walker**

1:45 CINF 16. Improving the knowledge about chemistry: The two leading encyclopedias, Wikipedia and RÖMPP, cooperate in Germany. **G.F. Herrmann**

2:05 CINF 17. PubChem Wikipedia integration and potential for future collaboration. **J. Zhang**, P. Thiessen, A. Gindulyte, E. Bolton

2:25 CINF 18. Wikipedia and Wiktionary as resources for chemical text mining. **R.A. Sayle**, D.M. Lowe

2:45 Intermission.

3:00 CINF 19. Tools and strategies: Incorporating Wikipedia-based assignments into a course. **E. Salvaggio**, J. Mathewson

3:20 CINF 20. Wikipedia editing in chemistry classrooms: Resonance and gaps between educational needs and Wikipedia community practices. **Y. Li**

3:40 CINF 21. Improving Wikipedia topics, a chemistry outreach activity. **K. Lindblom**

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

4:00 CINF 22. Value of the Mediawiki platform for providing content to the chemistry community. **A.J. Williams**

4:20 CINF 23. Chemical collaborations in the wiki realm. **A. Mabbett**

4:40 CINF 24. Panel Discussion: Wikipedia and MediaWiki: Collaborations and Education in Chemistry. **Y. Li**, M.A. Walker

5:00 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 104B

Visualizing Chemistry Data to Guide Optimization

Guiding Compound Optimization

E. Davis, M. D. Segall, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CINF 25. Integrating data visualization into the drug discovery workflow. **P. Walters**, G. Bemis, J. Feng, B. Goldman, G. McGaughey, J. Orr, E. Perola, S. Roberts, J. Yuen, J. Weiss

1:30 CINF 26. Data visualization: New directions or just familiar routes? **E. Champness**, P. Hunt, M.D. Segall

1:55 CINF 27. Reaction discovery and optimization tools for visualizing chemistry data. **J. Bishop**, P. McHale, P. Skinner, M. Schoenberg

2:20 CINF 28. Visualization of structure-activity relationship patterns and compound design using the SAR Matrix method. **D. Dimova**, J. Bajorath

2:45 Intermission.

3:00 CINF 29. Visualization and manipulation of Matched Molecular Series for decision support. **N. O'Boyle**, R.A. Sayle

3:25 CINF 30. Design and characterization of chemical space networks. **M. Vogt**, G.M. Maggiora, J. Bajorath

3:50 CINF 31. Interactive web-based tools for navigating the biologically relevant chemical space. **O. Rabal**, J. Oyarzabal

4:15 CINF 32. Compact models for compact devices: Visualisation of SAR data using mobile apps. **A. Clark**

4:40 CINF 33. Fast, visual, and compelling analysis of datasets from similarity to SAR. **M. Hartshorn**, D. Ormsby, C. Mueller, R. Brown, J. Gordon, T. Mansley, C. Tudge

5:05 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF and SOCED

Integrated Approaches in Structure-Based Drug Design

Sponsored by COMP, Cosponsored by CINF and MEDI

SUNDAY EVENING

Section C

Seaport Hotel and World Trade Center
Lighthouse 1

CINF Scholarships for Scientific Excellence: Student Poster Competition

Financially supported by Royal Society of Chemistry
G. Grethe, *Organizer*

6:30 - 8:30

CINF 34. P-OSRA: Polymer Optical Structure Recognition Application. **B. Reinstadler**, H. Horn

CINF 35. Modeling electronic properties of molecular systems using machine learning and informatics. **M. Haghighatlar**, G. Kumar, J. Hachmann

CINF 36. Knowledge-based approach to the parameterization of small molecule force fields based on crystal structures. **F. Roessler**, O. Korb, R.C. Glen, P. Bond

CINF 37. Pilot study of clustering based safety assessment for fragrance ingredients. **J. Shen**, L. Kromidas

CINF 38. Investigation of the endocrine disruption potential of bisphenol A replacement compounds. **H. Ng**, R. Perkins, W. Tong, H. Hong

CINF 39. Chemical alerts and QSAR models based on dynamically-generated annotated linear structural fragments. **D. Mehta**, J.F. Rathman, C. Yang

CINF 40. Developing group contributions for predicting transition state structures. **P. Bhoorasingh**, R.H. West

CINF 41. Changes in scholarly publishing practices in the chemical sciences: A focus on early career chemists. **M. Noel**

CINF 42. Predicting Tox21 assay outcome by quantitative structure-activity relationship and machine learning methods. **M. Lee**, D. Nguyen, R. Huang

CINF 43. Chess-like algorithms behind Chematica's retrosynthetic planning. **S.A. Szymkuc**, E.P. Gajewska, T. Klucznik, P. Dittwald, M. Startek, K. Molga, M. Bajczyk, B. Grzybowski

CINF 44. Retrosynthesis of complex molecules using Chematica. **E.P. Gajewska**, S.A. Szymkuc, T. Klucznik, P. Dittwald, M. Startek, K. Molga, M. Bajczyk, B. Grzybowski

CINF 45. Mining chemical databases to obtain knowledge based information of non-covalent interactions. **M. Koebel**, S. Sirimulla

CINF 46. In silico assessment of toxicity endpoints: Case-studies using CORINA Symphony and ChemTunes Studio. **C.H. Schwab**, J. Maruszczyk, A. Tarkhov, T. Kleinoeder, D. Hristozov, B. Bienfait, O. Sacher, J.F. Rathman, C. Yang

CINF 47. Chemogenomics-assisted anti-obesity drug discovery. **R. Hajjo**, A. Tropsha

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 104A

Retrosynthesis, Synthesis Planning, Reaction Prediction: When Will Computers Meet the Needs of the Synthetic Chemist?

D. Evans, W. A. Warr, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 48. What are the next steps in your synthesis? The Reaxys experience. **J. Swienty Busch**

9:05 CINF 49. Green chemistry in synthesis planning systems: A role for biocatalysis data and sustainability metrics? **P. Johnson**, V. Valko, A.P. Cook

9:35 CINF 50. Synthetically accessible virtual inventory (SAVI). **Y. Pevzner**, W. Ihlenfeldt, M.C. Nicklaus

10:05 CINF 51. Analyzing success rates of supposedly “easy” reactions. **R.A. Sayle**

10:35 CINF 52. Computer-inspired organic synthesis: Building on success. **J.M. Goodman**

11:05 CINF 53. Using reaction driven de novo design as a “retrosynthetic” analysis tool. **B.B. Masek**, S. Nagy, D. Baker, R. Dorfman, F. Soltanshahi, K. Dubrucq

Section B

Boston Convention & Exhibition Center
Room 104B

Enabling Machines to “Read” the Chemical Literature: Techniques, Case Studies & Opportunities

Extracting Chemical Information from Patents

D. M. Lowe, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 CINF 54. CHEMDNER-Patents: Automatic recognition of chemical and biological entities in patents. **M. Krallinger**, F. Leitner, **O. Rabal**, M. Vazquez, J. Oyarzabal, A. Valencia

10:00 CINF 55. SureChEMBL: An open patent chemistry resource. **G. Papadatos**, M. Davies, N. Dedman, A. Hersey, J.P. Overington

10:25 CINF 56. Deuterogate: Causes and consequences of automated extraction of patent-specified virtual deuterated drugs feeding into PubChem. **C. Southan**

10:50 Intermission.

11:05 CINF 57. Evaluating US patent full text documents with chemical ontologies. **L. Weber**

11:30 CINF 58. Text-mining to produce large chemistry datasets for community access. **A.J. Williams**, D.M. Lowe, I.V. Tetko, C. Coba, V. Tkachenko, A. Pshenichnov, K. Karapetyan

Section C

Boston Convention & Exhibition Center
Room 103

Workflow Tools & Data Pipelining in Drug Discovery

E. Davis, T. Dudgeon, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CINF 59. When command line tools meet KNIME: Using the best of the two worlds to support drug discovery teams. **M. Lee**

8:30 CINF 60. Pipelining in mind: Compound library preprocessing in an interactive workflow. **M. Hilbig**, **M. Rarey**

8:55 CINF 61. New web based collaborative environment for cheminformatics workflows. **T. Dudgeon**

9:20 Intermission.

9:30 CINF 62. Workflows supporting drug discovery against malaria. **B. Hardy**

9:55 CINF 63. Accessing knowledge and design insights from a fully-annotated kinase-focused compound collection. **N. Brooijmans**

Section C

Boston Convention & Exhibition Center
Room 103

CINFlash: Workflow Tools Lightning Round

E. Davis, *Organizer, Presiding*

10:30 Introductory Remarks.

10:35 CINF 64. CINFlash: Workflow tools lightning round. **E. Davis**

21st Century Chemistry Education: Formal and Informal

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MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 104A

Retrosynthesis, Synthesis Planning, Reaction Prediction: When Will Computers Meet the Needs of the Synthetic Chemist?

D. Evans, W. A. Warr, *Organizers, Presiding*

1:00 CINF 65. SynTree, chemical synthesis on a PC. J. Figueras

1:30 CINF 66. Empowering chemists in synthesis planning — lessons from the evolution of ARChem. O. Ravitz, A.P. Cook, Z. Zsoldos, P. Johnson

2:00 CINF 67. Computer-aided synthesis design (CASD) and forward reaction prediction tools for both idea generation in new synthesis route planning and for de novo molecule design. V. Eigner Pitto, F. Huerta, M. Hutchings, H. Saller, P. Loew

2:30 CINF 68. Chematica — the Deep Blue of chemistry. B. Grzybowski

3:00 CINF 69. Reaction mining with condensed graphs of reactions: Problems and perspectives. A. Varnek

3:30 CINF 70. Assessment of optimal conditions for selective deprotection reactions resulted from analysis of large reaction database. T.I. Madzhidov, A. Lin, I. Antipin, O. Klimchuk, A. Varnek

4:00 CINF 71. Energy refinement of reactive molecular dynamics pathways. L. Wang, R.T. McGibbon, V.S. Pande, T.J. Martinez

Section B

Boston Convention & Exhibition Center
Room 104B

Enabling Machines to “Read” the Chemical Literature: Techniques, Case Studies & Opportunities

Turning Chemical Text & Structures into Chemical Knowledge

D. M. Lowe, *Organizer, Presiding*

1:30 CINF 72. Identifying chemical species in combustion models. R.H. West

1:55 CINF 73. Text mining the chemical literature to find chemicals in context. T. Wu, A.C. Hinton, D.R. Milward

2:20 CINF 74. Unlocking chemical information from tables and legacy articles. D.M. Lowe, R.A. Sayle, A.J. Williams

2:45 Intermission.

3:00 CINF 75. Chemical structure identification and retrieval with OSRA. I. Filippov, I. Weidlich

3:25 CINF 76. P-OSRA: Translating polymer images to text using extensions of open source software. B. Reinstadler, H. Horn

3:50 CINF 77. Practical case studies of the application of CLIDE for the efficient extraction of chemical structures from documents. A.T. Valko, P. Johnson

Section C

Boston Convention & Exhibition Center
Room 103

The Growing Impact of Openness in Chemistry: A Symposium in Honor of JC Bradley

A. Lang, A. J. Williams, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CINF 78. Contributions of Jean-Claude Bradley to the vision and execution of Open Notebook Science. A.J. Williams, A. Lang

1:25 CINF 79. Making it open: Putting cheminformatics to use against the Ebola virus. S. Ekins

1:45 CINF 80. Opening up and connecting up antimalarial data: Progress but with caveats. C. Southan

2:05 CINF 81. Context of crowdsourcing: A driver of organizational openness? D.C. Thompson, J. Bentzien

2:25 Intermission.

2:35 CINF 82. Promoting, supporting, and incentivizing openness in scientific research. S. Bowman

2:55 CINF 83. OpenTox — an open community and framework supporting predictive toxicology and safety assessment. B. Hardy

3:15 CINF 84. Topliss batchwise scheme reviewed in the era of Open Data. L. Richter, G.F. Ecker

3:35 CINF 85. Anatomy of a chemical reaction: Dissection by machine learning algorithms. A. Clark

3:55 CINF 86. Cheminformatics OLCC. R.E. Belford, D.J. Wild, L. McEwen, A.J. Williams, S.J. Chalk, J.L. Muzyka, J.H. Penn, J.L. Holmes

4:15 Intermission.

4:25 CINF 87. PubChem project and annotations. J. Zhang, P. Thiessen, S. Kim, A. Gindulyte, R. Geer, E. Bolton

4:45 CINF 88. Open Spectral Database: Open data, open code, open concept. S.J. Chalk

5:05 CINF 89. DeepLit WikiHyperGlossary. M.A. Bauer, A.P. Cornell, D. Berleant, R.E. Belford

5:25 CINF 90. Changing landscape of scientific publishing: Open access, open data, and more. C. Hollingworth

5:45 Concluding Remarks.

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

E. Davis, *Organizer*

8:00 - 10:00

13, 19, 31, 34-35, 43, 45-46, 54, 69, 80. See previous listings.

CINF 91. Chemistry enabling Chinese, Japanese, and Korean patents. D.M. Lowe, R.A. Sayle

94, 109, 118, 138, 149, 160, 166, 168. See subsequent listings.

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 104A

Herman Skolnik Award Symposium

Cosponsored by COMP and MEDI

Financially supported by Pfizer

J. Bajorath, *Organizer*

V. Shanmugasundaram, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CINF 92. Force fields for biomolecular simulations. A. Hagler

8:45 CINF 93. Paradigm which permits the parsing of information content arising from receptor-independent ligand activity models and receptor-dependent activity models. A.J. Hopfinger

9:25 CINF 94. Non-specificity of drug-target interactions: Consequences for drug discovery. G.M. Maggiora, V. Gokhale

10:05 CINF 95. Molecular similarity approaches in chemoinformatics: Early history and bibliometric analysis. P. Willett

10:45 Intermission.

11:00 CINF 96. Generative topographic mapping: Universal tool for chemical space analysis. A. Varnek

11:30 CINF 97. Development of a knowledge-generating platform driven by big data in drug discovery through production processes. K. Funatsu

Section B

Boston Convention & Exhibition Center
Room 104B

Scientific Integrity: Can We Rely on the Published Scientific Literature?

Integrity and Peer Review

Cosponsored by COMSCI

J. N. Currano, *Organizer*

W. G. Town, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 CINF 98. Integrity, ethics, and trust in scientific research literature. C. Leonard

9:35 CINF 99. Policy making at the American Chemical Society: Developing a statement on scientific integrity. S. Cooney, C.J. Proctor

10:05 CINF 100. Publishability. M.G. Hicks

10:35 Intermission.

10:50 CINF 101. What is the role of peer review in protecting the integrity of scientific research? N. Qin

11:20 CINF 102. Open, network-based answer to the reproducibility crisis: The ScienceOpen peer review concept. S.R. Dawson

11:50 CINF 103. Managing new threats to the integrity of the scientific literature. J.N. Currano, K.R. Foster

12:20 Concluding Remarks.

Current Topics in Chemical Safety Information

Use Cases for Chemical Safety Information

Sponsored by CHAS, Cosponsored by AGFD, CCS, CHED and CINF‡

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 104A

Herman Skolnik Award Symposium

Cosponsored by COMP and MEDI‡

Financially supported by Pfizer

J. Bajorath, *Organizer*

V. Shanmugasundaram, *Organizer, Presiding*

1:00 CINF 104. Enabling drug discovery by computational molecular design. G. Schneider, P. Schneider

1:30 CINF 105. Integrating public data sources into the drug discovery workflow. P. Walters, A. Aronov, B. Goldman, J. Feng, B. McClain, L. Meireles, H. Shih, J. Weiss

2:00 CINF 106. Going beyond R-group tables: Close-in analog prioritization using neighborhood information derived from SAR matrices. L. Zhang, K. Johnson, J. Starr, C. Poss, J.B. Milbank, M. Kuhn, V. Shanmugasundaram

2:30 Intermission.

2:45 CINF 107. AnalogExplorer: A new method for graphical analysis of analog series and associated structure-activity relationship information. Y. Hu

3:15 CINF 108. How many fingers does a compound have? The various ways to define molecular similarity. E. Loukine

3:45 CINF 109. Dark chemical matter: Could “inactive” compounds be good starting points for drug discovery? A.M. Wassermann

4:15 CINF 110. Complexity and heterogeneity of data for chemical information science. J. Bajorath

4:45 Awards Presentation.

Section B

Boston Convention & Exhibition Center
Room 104B

Scientific Integrity: Can We Rely on the Published Scientific Literature?

Publisher Safeguards to Scientific Integrity

Cosponsored by COMSCI

W. G. Town, *Organizer*

J. N. Currano, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 111. Toward a more reproducible corpus of scientific literature. C. Berrios

2:05 CINF 112. Extraordinary public access to scientific evidence in the FDA modified risk tobacco product process. J.M. Solyst

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- 2:35 CINF 113. Validation and fraud in small-molecule crystallography. S. Conway
- 3:05 CINF 114. Scientific integrity: A crystallographic perspective. I. Bruno
- 3:35 Intermission.
- 3:50 CINF 115. Ways publishers help, maintain, and support responsible research. R.J. Boucher
- 4:20 CINF 116. Integrity, trust, and reproducibility: How scientific publishers can contribute. G.F. Herrmann
- 4:50 CINF 117. The write stuff — scientific integrity and publishing. J. Humphrey, R. Kidd
- 5:20 Concluding Remarks.

Current Topics in Chemical Safety Information

Sponsored by CHAS, Cosponsored by CCS, CHED and CINF†

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 104A

Chemical Information Skills: The Essential Toolkit for Chemical Research

G. Baysinger, J. M. Goodman, *Organizers, Presiding*

9:00 Introductory Remarks.

- 9:05 CINF 118. Chemical Information Sources Wikibook — the open source created by chemical information professionals for chemical information professionals. C.F. Huber
- 9:30 CINF 119. Soft skills of chemical research: Academic integrity and research ethics. D. Wrublewski, M. Leonard, A. Buhler, N. Bharti
- 9:55 CINF 120. Integrating bibliographic management tools in chemical information literacy instruction. S.P. Baykoucheva, J. Houck
- 10:20 CINF 121. Replacing the traditional graduate chemistry literature seminar with a chemical information literacy course. V.F. Scalfani, S.A. Woski, P.A. Frantom
- 10:45 Intermission.
- 11:00 CINF 122. Chemical information skills: A searcher's perspective. E.N. Cheeseman
- 11:25 CINF 123. Withdrawn.
- 11:50 CINF 124. Patents — the essential multifunctional tool for science, business, and intellectual property information. E.S. Simmons
- 12:15 CINF 125. Career information resources for graduate students and postdocs. G. Baysinger

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

Section B

Boston Convention & Exhibition Center
Room 104B

Find the Needle in a Haystack: Mining Data from Large Chemical Spaces

D. Deng, *Organizer, Presiding*

- 8:30 Introductory Remarks.
- 8:35 CINF 126. Frequency of activity cliffs and distribution over different potency ranges. D. Stumpfe, D. Dimova, J. Bajorath
- 9:05 CINF 127. Random indexing for comparing path-based chemical fingerprints. P. Devaney, D. Lancia, J. Milbank, M.P. Bradley
- 9:35 CINF 128. Withdrawn.
- 10:05 Intermission.
- 10:20 CINF 129. Resolving cryptic needles to molecular structures: The GtoPdb experience. C. Southan, A.J. Pawson, J.L. Sharman, H.E. Benson, E. Faccenda
- 10:50 CINF 130. Current and future developments of Markush technology in drug discovery. D. Deng, Á. Figyelmesi
- 11:20 CINF 131. GPU-accelerated virtual screening: Rationale, challenges, and case studies. O. Isayev, D. Fourches
- 11:45 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 103

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Cosponsored by AGRO, COMP, ENVR and MEDI

M. AbdulHameed, *Organizer, Presiding*

- 8:15 Introductory Remarks.
- 8:20 CINF 132. Using mode-of-action (MOA) data to guide the development of local quantitative structure-activity relationship (QSAR) models for molecular and early cellular events in an adverse outcome pathway (AOP). J.L. Tunkel, J. Melia, K. Salinas, L. Morlacci, J. Rhoades, M. Kawa, C.A. Rudisill, H. Carlson-Lynch
- 8:40 CINF 133. QSAR models could replace LLNA test for predicting human skin sensitization potential of chemicals. V.M. Alves, R. Braga, E. Muratov, D. Fourches, N. Kleinstreuer, J. Strickland, C.H. Andrade, A. Tropsha
- 9:00 CINF 134. Assessing skin sensitization potential by combining AOP-informed chemotype alerts, QSAR models, and in vitro biological assay data. J.F. Rathman, C. Yang, A. Mostrag-Szlichtyng, B. Bienfait, J. Maruszczyk, C.H. Schwab
- 9:20 CINF 135. Using OpenTox to map toxicity data to adverse outcome pathways. B. Hardy
- 9:40 CINF 136. Cheminformatic tools in support of pharmacokinetics and ADME profiling. M.R. Goldsmith, D.T. Chang
- 10:00 Intermission.
- 10:15 CINF 137. Predicting off target profiles using local 3D QSAR models generated "on the fly". B.B. Masek, A. Steudle, L. Wang, B. Wendt
- 10:35 CINF 138. Linking transporter interaction profiles to in vivo side effects. E. Kotsampasakou, S. Escher, A. Jurik, H. Sitte, L. Pezawas, G.F. Ecker
- 10:55 CINF 139. Enhancing structural alerts for toxicity with mechanism-based metabolism and reactivity models. S. Swamidass, T. Hughes, G.P. Miller

- 11:15 CINF 140. Toxicity biomarker identification and drug repurposing using gene co-expression modules. G.J. Tawa, M. AbdulHameed, D. Ippolito, K. Kumar, J. Lewis, J.D. Stallings, A. Wallqvist

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 104A

Chemical Information Skills: The Essential Toolkit for Chemical Research

G. Baysinger, J. M. Goodman, *Organizers, Presiding*

- 1:30 Introductory Remarks.
- 1:35 CINF 141. So I have an SD File... what do I do next? R. Guha, N. O'Boyle
- 2:00 CINF 142. Chemical literacy for the ages: Essential skills in 2D chemical representation. L. McEwen, E. Hepler-Smith
- 2:25 CINF 143. From lab to the libraries: A new journey. N. Bharti
- 2:50 CINF 144. Experiments with chemists and information. J.M. Goodman
- 3:15 Intermission.
- 3:30 CINF 145. ChemData: A web application for learning chemical informatics. S.J. Chalk
- 3:55 CINF 146. Improving geographically distributed research with real time collaboration. A. Stracz, A.D. Costache
- 4:20 CINF 147. Chemical research toolkit: An end-to-end solution. J. Bishop, P. McHale, P. Morieux
- 4:45 CINF 148. ELN, RegMol and inventory: From synthesis to registration to inventory. R. Hotchandani
- 5:10 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 104B

Find the Needle in a Haystack: Mining Data from Large Chemical Spaces

D. Deng, *Organizer, Presiding*

- 1:00 Introductory Remarks.
- 1:05 CINF 149. Data driven multi-object optimization (MOO) in drug design. S. Keinan, E. Hobbs, E. Hatcher-Flush
- 1:30 CINF 150. Multiobjective transformation based de novo design: A case study of surfactants. C. Kannas, W. Read, N. Ruddock, M. Fletcher, T. Jackson, R. Stevens, J. Winter, P. Willett, V.J. Gillet
- 1:55 CINF 151. Mapping chemical data with Diversity Genie. I. Filippov, I. Weidlich
- 2:20 Intermission.
- 2:30 CINF 152. Extraction of structure-activity relationship information from activity cliff clusters. D. Dimova, D. Stumpfe, J. Bajorath
- 2:55 CINF 153. Withdrawn.
- 3:25 Intermission.
- 3:35 CINF 154. Drug discovery tool pipeline — the best of all worlds. C. Detering
- 4:00 CINF 155. 3D characteristics of efficient protein-protein interactions inhibitors: A big data analysis. M. Kuenemann, L. Bourbon, C. Labbé, B. Villoutreix, O. Sperandio
- 4:25 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 103

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Cosponsored by AGRO, COMP, ENVR and MEDI

M. AbdulHameed, *Organizer, Presiding*

- 1:30 Introductory Remarks.
- 1:35 CINF 156. Differential network analysis of chemical-mediated cancer induction. F. Mulas, D. Gusenleitner, S. Monti
- 1:55 CINF 157. Massively orthogonal search engine for mechanism of action and toxicity studies. D.W. Seinger, V. Shivashankar, M. Larbaoui, I. Mendelev, M. Steeves, S. Litster, P. Marc
- 2:15 CINF 158. Combining predicted biological descriptors with chemical descriptors affords reliable hybrid QSAR models of rodent carcinogenicity. R. Politi, S. Capuzzi, S. Farag, A. Tropsha
- 2:35 CINF 159. Mining big datasets to create and validate machine learning models. A. Clark, S. Ekins
- 2:55 CINF 160. From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. M.T. Kim, H. Zhu
- 3:15 Intermission.
- 3:30 CINF 161. ChEMBL database and its application in toxicity assessment. P. Bento
- 3:50 CINF 162. Modeling ABC transporters as potential DILI targets. M.D. Segall, P. Hunt, J. Tyzack
- 4:10 CINF 163. Addressing a key hurdle in translational research: Predicting mouse liver microsomal stability using machine learning. A.L. Perryman, S. Ekins, J. Freundlich
- 4:30 CINF 164. Using supervised Latent Dirichlet Allocation for structure-activity relation modeling in Tox21 2014 data challenge. I. Weidlich, I. Filippov
- 4:50 CINF 165. Cheminformatics-based signal boosting for predicting drug adverse events. A.D. Fant, N.L. Kruhlak, K.K. Burkhart

THURSDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 104A

General Papers

E. Davis, *Organizer, Presiding*

- 9:00 CINF 166. CIIPro: An online cheminformatics portal for large scale chemical data analysis. D.P. Russo, W. Wang, M.T. Kim, D. Pinolini, H. Zhu
- 9:30 CINF 167. Improving virtual screening performance through identification of molecular descriptor features sensitive to specific biological activities. M. Vogt, J. Bajorath
- 10:00 CINF 168. "Graphical abstracts only": The changing use of periodicals among early career chemists. M. Noel
- 10:30 CINF 169. QSPR/QSAR studies of antifouling/fouling-release surface coatings containing quaternary ammonium salts. F. Jabeen, B. Rasulev, M. Ossowski, B.J. Chisholm, S. Stafslien, P. Boudjouk

THURSDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 104A

General Papers

E. Davis, *Organizer, Presiding*

1:00 CINF 170. Experimental chemoinformatics study of tautomerism of commercial screening samples. L. Guasch, M.C. Nicklaus

1:30 CINF 171. Which kinase to hit in NCI-60? From a selectivity problem to a multitarget solution. O. Méndez Lucio, A. Chavan Ravindranath, Q. Ain, K. Birchall, C. Mpamhanga, S. Knapp, A. Bender

2:00 CINF 172. HackaMol: An object-oriented Modern Perl library for molecular hacking on multiple scales. D. Riccardi

2:30 CINF 173. Programmatic access to chemical information in PubChem. S. Kim, P. Thiessen, E. Bolton, S.H. Bryant

SUNDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Blrm II

Founders Award Lecture & Symposium

A. P. Grollman, *Organizer, Presiding*

1:00 TOXI 6. Aflatoxins — another “A” in the library of naturally-occurring human carcinogens. T.W. Kensler, J.D. Groopman

1:40 TOXI 7. Proteogenomic analysis of human colon and rectal cancer. D.C. Liebler

2:20 Intermission.

2:45 TOXI 8. Somatic mutations in tumor DNA present in biological fluids as markers for the early detection of cancer. N. Papadopoulos

3:25 TOXI 9. Chemical toxicology of a novel human carcinogen, aristolochic acid. A.P. Grollman

MONDAY MORNING

Section A

Westin Boston Waterfront
Harbor Blrm II

You ng Investigator Symposium

P. J. Beuning, *Organizer, Presiding*

8:00 TOXI 10. Replication bypass and mutagenesis of the C1'- α -anomeric lesions of 2'-deoxyribonucleosides in *Escherichia coli* cells. N.J. Amato, Q. Zhai, Y. Wang

8:15 TOXI 11. In vitro replication studies of O²- and O⁴-alkylthymidine lesions with human DNA polymerase η . N. Williams, P. Wang, J. Wu, Y. Wang

8:30 TOXI 12. N'-nitrososornicotine 5'-hydroxylation causes DNA damage in rats. A.T. Zarth, P. Upadhyaya, J. Yang, S.S. Hecht

8:45 TOXI 13. Human DNA polymerase η is impeded by nucleotides with altered hydrogen bonding capacities. A. Nilforoushan, A. Furrer, L.A. Wyss, B. Van Loon, S.J. Sturla

9:00 TOXI 14. Quantitation of pyridyloxobutyl-DNA adducts in tissues of F-344 rats treated with (R)-, (S)-, or racemic N'-nitrososornicotine. J. Yang, P.W. Villalta, P. Upadhyaya, S.S. Hecht

9:15 TOXI 15. Urinary biomarkers of exposure to N'-nitrososornicotine in African-American and Caucasian smokers. H.R. Baniasadi, G. Yakovlev, S.E. Murphy, Y. Patel, J. Jensen, D. Hatsukami, I. Stepanov

9:30 TOXI 16. Replicative bypass and mutagenic properties of O²-alkylthymidine lesions in *E. coli*. P. Wang, Q. Zhai, Y. Wang

9:45 Intermission.

10:05 TOXI 17. Biomonitoring the cooked meat carcinogen 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) in dyed hair by ultra performance liquid chromatography-orbitrap high resolution multistage mass spectrometry. J. Guo, K. Yonemori, K.K. White, L.R. Wilkens, L. Le Marchand, R.J. Turesky

10:20 TOXI 18. Rapid throughput DNA isolation from formalin-fixed paraffin embedded tissues for biomonitoring DNA adduct. B. Yun, L. Yao, T.A. Rosenquist, K.G. Dickmann, A.P. Grollman, R.J. Turesky

10:35 TOXI 19. Metabolic activation of 3-nitrobenzanthrone by aldo-keto reductases (AKR1C1—AKR1C4): evidence for 6 electron reduction. J.R. Murray, M. Huang, T. Zang, I.A. Blair, C. Mesaros, V. Arlt, H. Schmeiser, T.M. Penning

10:50 TOXI 20. Rat liver nuclear extracts oxidize M₁dG in duplex DNA to 6-oxo-M₁dG. M. Mitchener, J. Galligan, L.J. Marnett

11:05 TOXI 21. Platelet biomarkers of metabolic disturbances in Friedreich's ataxia. A. Worth, N. Snyder, I.A. Blair

11:20 TOXI 22. Uncovering the broader roles of redox partner proteins for cytochrome P450 enzymes. W. Zhang, D.H. Sherman, S. Li

11:35 TOXI 23. Synthesis and analysis of DNA lesions generated from oxidative damage at the C-3' position of deoxyribonucleotides. F.M. Bedi, P. Bhatkhande, W. Li, S. Ayoub, A.C. Bryant-Friedrich

Innovation in Health and Medicine

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Global Research Needs: Identifying and Prioritizing Efforts to Sustain Environmental Quality

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MONDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Blrm II

New Approaches to the Study of Chemical Toxicology in Human Health: Accelerator Mass Spectrometry

P. T. Henderson, *Organizer, Presiding*

1:00 TOXI 24. Biomedical applications of accelerator mass spectroscopy: Past, present, and future. K. Turteltaub, G. Bench, T. Ognibene, M. Malfatti, G. Loots, B.A. Buchholz, H. Enright

1:40 TOXI 25. Application of accelerator mass spectrometry in drug development — vismodegib as a case study. C. Hop, R. Graham, H. Wong, M. Dresser, C. Khojasteh, Y. Shin

2:20 TOXI 26. Accelerator mass spectrometry (AMS) to study ADME of carcinogenic polycyclic aromatic hydrocarbons following microdosing in humans. D.E. Williams, E. Madeen, R. Corley, K. Turteltaub, T. Ognibene, M. Malfatti, T. McQuistan

3:00 Intermission.

3:25 TOXI 27. Perinatal exposure to trilocarban results in altered lipid metabolism. H. Enright, M. Falso, V. Lao, M. Malfatti, E. Kuhn, N. Hum, Y. Shi, K. Haack, K. Kulp, B.A. Buchholz, G. Loots, G. Bench, K. Turteltaub

4:05 TOXI 28. Use of radiocarbon-labeled cytotoxic drugs for pre-clinical medicine applications in cancer therapy. P. Henderson

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

A. C. Bryant-Friedrich, *Organizer*

8:00 - 10:00

21. See previous listings.

54, 56-58, 60-61, 63, 66, 76, 80-82, 89-90, 93, 98, 101, 104, 106. See subsequent listings.

TUESDAY MORNING

Section A

Westin Boston Waterfront
Harbor Blrm II

The Exposome

S. Balbo, *Organizer, Presiding*

8:00 TOXI 29. Exposome: A tool for untargeted discovery in the environmental health sciences. D. Balshaw

8:40 TOXI 30. Breath biomarkers to investigate the human exposome. J. Pleil

9:20 Intermission.

9:45 TOXI 31. Protein adductomics — a strategy to detect internal exposure to electrophiles. M. Törnqvist

10:25 TOXI 32. High resolution mass spectrometry-based DNA adductomics approach for the investigation of the exposome. S. Balbo

TUESDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Blrm II

The Role of Gut Microbiota in Carcinogenesis

S. J. Sturla, *Organizer, Presiding*

1:00 TOXI 33. Chemical discovery in the human microbiota. E.P. Balskus

1:40 TOXI 34. Biological chemistry of phosphorothioate DNA modifications in gut microbiota. P.C. Dedon

2:20 Intermission.

2:45 TOXI 35. Biotransformation of carcinogens by gut microbes. S.J. Sturla

3:25 TOXI 36. Role of gut microbiome in chemical toxicity and individual susceptibility. K. Lu

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TOXI

Division of Chemical Toxicology

A. Bryant-Friedrich, *Program Chair*

SUNDAY MORNING

Section A

Westin Boston Waterfront
Harbor Blrm II

Chemical Research in Toxicology Young Investigator Award Symposium

P. J. Beuning, *Organizer, Presiding*

8:00 Award Presentation.

8:15 TOXI 1. Multiple conformations of a chimeric Y-family polymerase define a pathway for docking primer-template DNA into the active site. R. Nelson, R. Wilson, N. Banavali, J.D. Pata

8:55 TOXI 2. Supraholoenzyme DNA polymerase complex for coupled replication and lesion bypass. M. Cranford, A. Chu, R.J. Bauer, M.A. Trakselis

9:35 TOXI 3. Crosstalk between DNA polymerase beta, nucleotide excision repair, and mismatch repair modulates the cellular response to cisplatin. A. Nemeč, L. Abriola, J.B. Sweasy

10:15 Intermission.

10:40 TOXI 4. Watching base excision repair glycosylases search for and find oxidized DNA bases. S. Wallace

11:20 TOXI 5. Recognition of DNA damage by specialized DNA polymerases. P.J. Beuning

Combining Scientific Evidence for Health Policy and Regulation

Sponsored by AGRO, Cosponsored by CHAS and TOXI

TUESDAY EVENING

Section A

Westin Boston Waterfront
Harbor Blrm II

Division of Chemical Toxicology
Keynote Address

P. F. Hollenberg, *Organizer, Presiding*

5:00 Introductory Remarks.

5:10 TOXI 37. B lymphocyte as a sensitive cellular target for impairment by dioxin and dioxin-like compound. **N. Kaminski**

Section B

Westin Boston Waterfront
Grand Blrm A/B

General Poster Session

A. C. Bryant-Friedrich, *Organizer*

6:30 - 8:00

TOXI 38. Replication dependent DNA repair of DNA interstrand cross-links by human translesion DNA polymerases. **W. Xu, S. Ghosh, A. Ouellette, M.M. Greenberg, L. Zhao**

TOXI 39. Moving toward full quantum chemical methods for physicochemical property estimates in toxicity, fate, and transport models of emerging environmental contaminants: Lessons learned from the 2014 Elk River chemical spill in West Virginia. **W.A. Alexander, N.J. Deyonker**

TOXI 40. Withdrawn.

TOXI 41. Synthesis and properties of backbone extended nucleosides. **R.S. Das, E. Hardter, L. McLaughlin**

TOXI 42. Change on antibacterial activity of enrofloxacin due to permanganate oxidation. **Y. Xu, S. Liu, F. Cui, W. Shi**

TOXI 43. Adaptation and application of computational and cheminformatics methods in nanomaterials toxicity prediction: An overview. **B. Rasulev**

TOXI 44. Biomarkers of asbestos exposure: From discovery to the identification of their structures. **C. Mesaros, N. Snyder, A. Worth, I.A. Blair**

TOXI 45. X-ray absorption spectroscopy study of evolution of Ag nanomaterials in the rat lung. **T. Guo, A. Davidson, D. Anderson, L. Van Winkle, K. Pinkerton**

TOXI 46. Rapid and precise localization of cell cultures on semipermeable membranes for cytotoxic and cell-to-cell responses in microfluidic systems. **B.J. Nablo, D. Reyes-Hernandez**

TOXI 47. Simultaneous determination of 8-oxo-2'-deoxyguanosine and 8-oxo-2'-deoxyadenosine in human retinal pigment epithelium DNA by liquid chromatography nano-electrospray-tandem mass spectrometry. **B. Ma, M. Jing, P.W. Villalta, R.J. Kapphahn, D.A. Ferrington, I. Stepanov**

TOXI 48. Mobile apps for transporter drug-drug interaction prediction: A tool of the future, now. **S. Ekins, A. Clark, J.E. Polli, S. Wright**

TOXI 49. Probing Mn(II) over-exposure induced neuronal deficits in a zebrafish model system. **S. Bakthavatsalam, S. Das Sharma, M. Sonawane, V. Thirumalai, A. Datta**

TOXI 50. Screening of DNA adducts induced by the experimental anticancer prodrug PR104A as biomarkers for drug susceptibility. **A. Stornetta, S. Balbo, S.S. Hecht, P.W. Villalta, S.J. Sturla**

TOXI 51. Withdrawn.

TOXI 52. Mass spectrometric characterization of human serum albumin adducts formed with *N*-oxidized metabolites of 2-amino-1-methyl-phenylimidazo[4,5-*b*]pyridine in human plasma and hepatocytes. **Y. Wang, L. Peng, M. Bellamri, S. Langouët, R.J. Turesky**

TOXI 53. Toward an MIE atlas — tools for toxicity prediction. **T.E. Allen, S. Liggi, J.M. Goodman, S. Gutsell, P.J. Russell**

TOXI 54. Impact of minor groove alkylation on transcription by RNA polymerase II. **S. Malvezzi, T. Angelov, L. Farnung, F. Eichenseher, P. Cramer, S.J. Sturla**

TOXI 55. DNA polymerase switching during translesion synthesis across (5'S)-8,5'-cyclo-purine DNA lesions. **W. Xu, C. Yang, A. Ouellette, L. Zhao**

TOXI 56. Quantification of thiazolidine-4-carboxylic acid in toxicant-exposed cells by liquid chromatography-mass spectrometry reveals an intrinsic antagonistic response to oxidative stress-induced toxicity. **J. Liu, W. Chan**

TOXI 57. Lesion recognition by the nucleotide excision repair protein XPC: Binding pathways and free energy profiles. **H. Mu, N.E. Geacintov, Y. Zhang, S. Brodye**

TOXI 58. Oncometabolites inhibit AlkB family DNA repair enzymes. **Q. Tang, K. Bian, F. Chen, D. Li**

TOXI 59. Characterization and evaluation of mutagenic nucleoside compounds that can cause virus population collapse. **N.A. Sayeh, D. Li**

TOXI 60. Effect of glyphosate, its metabolites and impurities on lymphocyte viability and apoptosis. **M. Kwiatkowska, P. Jarosiewicz, B. Huras, J. Michalowicz, B. Bukowska**

TOXI 61. Noninvasive measurement of Aristolochic Acid-DNA adducts in urine samples from Aristolochic Acid-treated rats by liquid chromatography coupled electrospray ionization tandem mass spectrometry. **M. Leung, W. Chan**

TOXI 62. Biological evaluation of the AlkB protein on DNA repair in cell. **F. Chen, K. Bian, Q. Tang, D. Li**

TOXI 63. Toxic metals inhibit AlkB family DNA repair enzymes. **K. Bian, Q. Tang, F. Chen, D. Li**

TOXI 64. Quantitative analysis of 5'-hydroxycytosine in smokers' urine by liquid chromatography-electrospray ionization-tandem mass spectrometry. **P. Upadhyaya, S.S. Hecht**

TOXI 65. pH-Dependent equilibrium between 5-guanidinothymine and iminoallantoin in nucleoside and oligodeoxynucleotide context. **J. Zhu, A.M. Fleming, C.J. Burrows**

TOXI 66. Toxicogenomic analyses of liver fibrosis. **M. AbdulHameed, D.L. Ippolito, G.J. Tawa, K. Kumar, J. Lewis, J.D. Stallings, A. Walkvist**

TOXI 67. Safety of nanosized iron intended for food fortification: Effect of primary particle size, agglomerate size, and effective density. **I.A. Trantakis, L. von Moos, M. Schneider, F. Hilty, S. Pratsinis, M. Zimmermann, S.J. Sturla**

TOXI 68. Moving beyond risk quotients: Comparing dose-response effects to reproductive natural variability. **A.B. Francisco, M. Buonanduci, J. Gravenmier, J. Iannuzzi, S. Selden, T. Negley**

TOXI 69. Identification of a DNA adduct of *N*'-nitrosocotinine, a potential metabolite of *N*'-nitrosornicotine. **P. Upadhyaya, A.T. Zarth, E. Carlson, S.S. Hecht**

TOXI 70. Regio and stereospecific structural perturbations resulting from 3,4-epoxybutene derived hydroxyalkyl deoxyinosine adducts in the human *N*-ras codon 61 sequence. **D.W. Kuo, M.P. Stone**

TOXI 71. Design and development of new tools for mapping 3-nitrotyrosine containing proteins. **C. Turrado, D. Rivera-Burgos, G. Gong, J.S. Wishnok, S.R. Tannenbaum**

TOXI 72. Sequence effects on translesion synthesis of an aminobiphenyl-DNA adduct: Conformational, thermodynamic, and binding studies. **A. Cai, R. Wiesner, B. Cho**

TOXI 73. Metabolism of an oxygenated polycyclic aromatic hydrocarbon (PAH) acenaphthenequinone in human HepG2 and Caco-2 cells. **M. Huang, C. Mesaros, I.A. Blair, T.M. Penning**

TOXI 74. Urinary biomarkers of 4-(methyl-nitrosamino)-1-(3-pyridyl)-1-butanone metabolic activation in African-American and European-American smokers. **A. Jain, G. Yakovlev, P. Upadhyaya, Y. Patel, J. Jensen, D. Hatsukami, I. Stepanov**

TOXI 75. LC-MS evaluation of corticosteroid metabolism in an in vitro microphysiological model of the human airway. **D. Rivera-Burgos, U. Sarkar, R. Prantli-Baun, A.R. Lever, J.R. Coppeta, J.S. Wishnok, J.T. Borenstein, S.R. Tannenbaum**

TOXI 76. DNA-protein cross-links: DNA-peptide cross-link preparation and DNA polymerase miscoding. **K.M. Johnson, F. Guengerich**

TOXI 77. Hydroxyphenyllysine residues in histones following intracellular exposure to 3,5-dimethylaminophenol: A model for induction of oxidative stress by aromatic amines. **R. Channaveerappa Kodihalli, P.L. Skipper, L.J. Trudel, J.S. Wishnok, G.N. Wogan, S.R. Tannenbaum**

TOXI 78. Assessment of potential ecological and health impact of coal ash spill in Dan River North Carolina. **M. Hu, L. Fernandez, P. Laresse-Casanova, A. Wang, M. Schreiber, B. Williams, A. Gu**

TOXI 79. On the use of EPR for rapid phototoxicity determination. **L. Whitehead, J. Kublbeck, J. White**

TOXI 80. Tributyltin exposures alter interleukin 6 secretion and production from lymphocytes. **S. Brown, W. Wilburn, M. Whalen**

TOXI 81. Putative human tRNA methyltransferase is a tumor growth suppressor that promotes senescence and death of cancer cells by management of reactive oxygen species. **C. Gu, L. Endres, U. Begley, T.J. Begley, P.C. Dedon**

TOXI 82. Specificity and activity of Y-family DNA polymerases. **N.M. Antczak, J. Walsh, P. Ippolito, P.J. Beuning**

TOXI 83. Meta-analysis of ionic liquid literature and toxicology. **M.E. Heckenbach, R.U. Halden**

TOXI 84. Gene expression microarray analysis of fish exposed to organohalide pollutants in a feeding study. **V.D. Dang, K.J. Kroll, S. Supowit, R.U. Halden, N.D. Denslow**

TOXI 85. Occurrence of carcinogenic *N*-nitrosamines in freshwater sediments collected near wastewater treatment plants. **A. Gushgari, R.U. Halden, A. Venkatesan**

TOXI 86. Gender-specific effect of diazinon exposure on gut microbiome structures and its function. **B. Gao, X. Bian, T. Glenn, K. Lu**

TOXI 87. Nuclear metabolism of an inflammation-linked DNA adduct in the genome. **O.R. Wauchope, J. Galligan, W.N. Beavers, P.J. Kingsley, L.J. Marnett**

TOXI 88. Metabolomic response of staged human neural stem cells to neurotoxic compounds. **X. Bian, S. Wallace, A. Majumde, M. Amosu, M. Smith, S. Stice, K. Lu**

TOXI 89. Thermodynamic studies of DNA duplexes containing the spiroiminodihydroant lesion. **B. Gruessner, M. Dwarakanath, M. Martel, E.R. Jamieson**

TOXI 90. Strategy for identifying unknown adducts based on adductome LC-MS data and incubation experiments with corresponding electrophiles. **H. Carlsson, U. Nilsson, M. Törnqvist**

TOXI 91. Nucleosome packaging of a hantavirus lesion on DNA. **M. Klureza, L. Goehring, E. Norabuena, S. Barnes, E.R. Jamieson, M. Nunez**

TOXI 92. DNA polymerase η is the most active human Y-family polymerase for the bypass of O²-(4-(3-pyridyl)-4-oxobutyl) thymidine, a DNA adduct derived from tobacco smoke. **A. Gowda, T. Spratt**

TOXI 93. Generation of a C5'-uridyl radical. **M. Ellis, R. Shaik, A.C. Bryant-Friedrich**

TOXI 94. Small molecule biomarker of oxidative damage from low energy electrons. **P. Bhattachande, A.C. Bryant-Friedrich**

TOXI 95. Quantification of gemcitabine incorporation into DNA to determine drug sensitivity and mechanisms of resistance in bladder cancer cells. **T. Scharadin, H. Zhang, M. Zimmermann, S. Wang, M. Malfatti, G. Cimino, C. Pan, P.T. Henderson**

TOXI 96. Stepped MRM LC-MS/MS for discovery of novel DNA modifications. **S. Mohapatra, S. Senyo, D. Bryant, C.K. Malik, R.B. Indrakanti, C.J. Rizzo, R.T. Lee, P.C. Dedon**

TOXI 97. Absolute quantification of apolipoprotein A1 in human serum by LC-MRM/MS using fully SILAC labeled protein standard. **Q. Wang, S. Zhang, L. Guo, C.M. Busch, W. Jian, N. Weng, N. Snyder, C.A. Mesaros, I.A. Blair**

TOXI 98. Impact of core composition and surface chemistry of semiconductor quantum dots on their stability in biological solutions and toxicity in zebrafish. **M. Muth, R.P. Brown, Z. Rosenzweig**

TOXI 99. Analysis of polar metabolites in biological samples by ion-pairing liquid chromatography-mass spectrometry. **L. Guo, A. Worth, C. Mesaros, I.A. Blair**

TOXI 100. Drug and toxicant exposures cause reprogramming of tRNA modifications in rat tissues in a mechanism of translational control of cellular response. **S. Kellner, S. Auerbach, T. Begley, P.C. Dedon**

TOXI 101. Probing conformational equilibria in site-specific 2'-deoxyribose DNA adducts by high field NMR spectroscopy. **A.H. Kellum, R. Bowen, V. Jasti, A.K. Basu, M.P. Stone**

TOXI 102. Method development for the spectrophotometric analysis of arsenic in aqueous media. **N.P. Jenkins, M.T. Buthelezi**

TOXI 103. Co-exposure studies: Infectious agents and arsenic exposure. **C.G. Knutson, G. Gong, L. Cheaney, C. Kaufman, S. Muthupalani, S.R. Tannenbaum, J.G. Fox**

TOXI 104. Epigenetic regulation of cytosine methylation, hydroxymethylation, formylation, and carboxylation by TET methylcytosine dioxygenase. **C. Seiler, J. Song, M. Andersen, J. Fernandez, F. Kassie, N.Y. Tretyakova**

TOXI 105. Spectrophotometric analysis of copper and lead in human nails and hair. **M.T. Buthelezi, E. Labovitis**

TOXI 106. Identification and structural characterization of 3,4-epoxybutene-induced formamidopyrimidine DNA adducts. **A. Groehler**, N.Y. Tretyakova

TOXI 107. Characterization of metipranolol metabolism in rat, rabbit, and human ocular and liver S9 fraction. **J.L. Bushee**, C. Dunne, U.A. Argikar

TOXI 108. Characterization of carteolol metabolism in rat, rabbit, and human ocular and liver S9 fractions. **U.A. Argikar**, J.L. Bushee, C. Dunne

WEDNESDAY MORNING

Section A

Westin Boston Waterfront
Harbor Blrm II

General Papers

A. C. Bryant-Friedrich, *Organizer, Presiding*

8:00 TOXI 109. Noninvasive measurement of carcinogen exposure by quantifying urinary DNA/RNA adducts using liquid chromatography coupled tandem mass spectrometry. **W. Chan**

8:20 TOXI 110. Meconium for targeted and untargeted quantitation of prenatal exposure and metabolism. **N. Snyder**

8:40 TOXI 111. Base-displaced intercalated solution structure of the DNA adduct N-(2'-deoxyguanosin-8-yl)-3-aminobenzanthrone. **D.A. Politica**, M.P. Stone, C. Malik, A.K. Basu

9:00 TOXI 112. Bioaccessibility of fipronil sorbed to paired soil and house dust samples. **J. Starr**, W. Li, D.M. Stout, K. Bradham, B. Schumacher

9:20 TOXI 113. Integrated assessment of drug metabolism, pharmacokinetics, toxicity, and biomarker discovery in a liver and a gut microphysiological system. **U. Sarkar**, S.R. Tannenbaum, R.L. Carrier, K. Chen, M. Cirit, L. Griffith, D.J. Hughes, R. Channaveerappa Kodihalli, E. Large, J.S. Wishnok, J. Wu

9:40 TOXI 114. Gold nanoprobe for in-gene colorimetric detection of DNA adducts. **I.A. Trantakis**, S.J. Sturla

10:00 Intermission.

10:10 TOXI 115. Analysis of phosphate adducts in hepatic and pulmonary DNA of rats treated with 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone. **B. Ma**, P.W. Villalta, A.T. Zarth, D. Kotandeniya, P. Upadhyaya, I. Stepanov, S.S. Hecht

10:30 TOXI 116. Decoding the S-nitroso proteome in a mouse model of Alzheimer's by SNOTRAP and mass spectrometry — clues for altered signaling pathways. **U.I. Seneviratne**, R. Channaveerappa Kodihalli, A. Nott, V. Bhat, J.S. Wishnok, L. Tsai, S.R. Tannenbaum

10:50 TOXI 117. Unusually strong XPC-HR23B/DNA complexes could lead to an "unproductive" form of human nucleotide excision repair. **B. Cho**, B. Hilton, S. Gopal, L. Xu, S. Mazumder, P. Musich, Y. Zou

11:10 TOXI 118. Processing of oxidatively generated guanine lesions in DNA by competitive base and nucleotide excision repair pathways. **V. Shafirovich**, K. Kropachev, T. Anderson, Z. Liu, M. Kolbanovskiy, N.E. Geacintov

11:30 TOXI 119. Individual differences in sensitivity to cytotoxic and genotoxic effects of a tobacco carcinogen. **L.A. Peterson**, I. Ignatovich, A.E. Grill, Y. Ho

11:50 TOXI 120. Human DNA polymerase γ catalyzes correct and incorrect DNA synthesis with high catalytic efficiency. **T. Spratt**, A. Gowda, G. Moldovan

WEDNESDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Blrm II

DNA Polymerases: From Mutagenesis to Biotechnology

Y. Wang, *Organizer, Presiding*

1:00 TOXI 121. Novel DNA polymerases — creating the engines for nucleic acid based diagnostics and the life sciences. **T.W. Myers**

1:40 TOXI 122. Improved Illumina sequencing by polymerase engineering. **M. He**

2:20 TOXI 123. Structural and functional studies of human translesion synthesis DNA polymerases η , ι , and κ and their interactions with damaged DNA. **F.P. Guengerich**, Q. Zhang, Y. Su, J. Choi, A. Patra, M. Egli

3:00 Intermission.

3:25 TOXI 124. Tautomerization as a principle to force evolution and extinction. **J.M. Essigmann**

4:05 TOXI 125. Novel shuttle vector-based methods for assessing the impact of DNA lesions on transcriptional and replicative bypass of DNA lesions in cells. **C. You**, B. Yuan, P. Wang, **Y. Wang**

CHAL

Division of Chemistry and the Law

K. Bianco, J. Hasford and J. Kennedy,
Program Chairs

SOCIAL EVENTS:

Reception, 5:00 PM: Monday
Luncheon, 12:00 PM: Monday

BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Sunday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 152

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

X. Pillai, *Organizer, Presiding*

9:30 CHAL 1. Top 10 reasons to file a patent application. **R.G. Bone**

10:00 CHAL 2. Top 10 problems with the patent system. **R.G. Bone**

10:30 CHAL 3. 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

Boston Convention & Exhibition Center
Room 152

Beyond the Bench: Careers in Intellectual Property

K. E. Bianco, *Organizer, Presiding*

1:30 CHAL 4. Top 10 reasons to become a patent attorney. **R.G. Bone**

2:00 CHAL 5. Navigating the path from graduate school to a career in patent law. **C. Rodrigo**

2:30 CHAL 6. Exploring a career as a patent examiner at the U.S. PTO. **S. Hasford**

3:00 CHAL 7. Careers in patent law: A litigator's perspective. **K.E. Bianco**

3:30 CHAL 8. Careers in university technology transfer. **J. Cho**

4:00 Panel Discussion.

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 152

Best Practices in Identifying, Protecting and Managing your Intellectual Portfolio

K. E. Bianco, J. J. Hasford,
Organizers, Presiding

9:00 CHAL 9. Identifying inventions — your own and others. **J. Jacobstein**

9:30 CHAL 10. Practical considerations for patent portfolio management. **M. McGurk**

10:00 CHAL 11. Enforcing your patent portfolio: A primer on U.S. patent infringement litigation. **J.J. Hasford**

10:30 CHAL 12. Know thy enemy: The different ways to attack a U.S. patent and tips to avoid becoming a victim. **K.E. Bianco**

11:00 Panel Discussion.

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 152

The Importance of Scientific Information in Patent-related Endeavors

E. N. Cheeseman, *Organizer, Presiding*

1:30 CHAL 13. Approaches to the searching for chemical information. **E.N. Cheeseman**

2:00 CHAL 14. Scientific information at the nexus of pharmaceutical research and patents. **C. Goddard**

2:30 CHAL 15. Finding a needle in a patent haystack. **R. Schenck**

3:00 CHAL 16. Resources for searching biological sequence patent information. **K. Hoppe**

3:30 CHAL 17. Importance of scientific information in patent exclusivity and drug development. **D. Farmer**

4:00 CHAL 18. Importance of being earnest — in your searching: Or, what you don't know can hurt you. **B.A. Stembridge**

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

K. E. Bianco, *Organizer*

8:00 - 10:00

CHAL 19. Chocolate — a religious experience. **H.M. Peters**, S.B. Peters

CHAL 20. 2015 National Inventors Hall of Fame inductees. **H.M. Peters**, S.B. Peters

CHAL 21. New changes in the America Invents Act for inventors: New section 102. **A. Berks**

CHAL 22. Provisional patent applications for fun and profit. **A. Berks**

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 152

Developments in Pharmaceutical Patent Law

B. Trinque, *Organizer, Presiding*

9:00 CHAL 23. Pharmaceutical patent prosecution primer. **B. Trinque**

9:30 CHAL 24. Markush claims: Efficient chemical claiming. **S.A. Sullivan**

10:00 CHAL 25. Small molecule Federal Circuit case law. **D. Cauble**

10:30 CHAL 26. Harmonizing the doctrines of enablement and obviousness with working examples: An in-house counsel's perspective. **A. Zink**

11:00 CHAL 27. Prosecution of chemical and pharmaceutical patent applications in Europe. **J. Harris**

GMOs and the Entanglement of Intellectual Property Rights

Sponsored by AGRO, Cosponsored by CHAL, ENVR and SCHB

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 152

Developments in Pharmaceutical Patent Law

B. Trinque, *Organizer, Presiding*

1:30 CHAL 28. Obtaining biomarker and diagnostic claims. **S. Coughlin**

2:00 CHAL 29. Combination therapies: Federal Circuit case law and application drafting strategies. **E. Karnas**

2:30 CHAL 30. Patenting of biologics in the biosimilars era. **J. Velema**

3:00 CHAL 31. What you need to know about Inter Partes Review proceedings. **J. Poplin**

3:30 CHAL 32. Patent examination in the pharmaceutical arts. **J. Lundgren**

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 152

Strategic Planning for Your IP Portfolio: Patents, Trade Secrets, and Government Funding, What Should I Do?

J. L. Kennedy, D. Lorentzen, *Organizers, Presiding*

9:00 Introductory Remarks.

9:15 CHAL 33. Patent portfolio strategies: What should my patent portfolio look like? L. DiLorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

10:00 CHAL 34. Alternative protection strategies. L. DiLorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

10:45 CHAL 35. When do I need or want a non-infringement or freedom-to-operate opinion relating to my company's technology? L. DiLorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 152

Strategic Planning for Your IP Portfolio: Patents, Trade Secrets, and Government Funding, What Should I Do?

J. L. Kennedy, D. Lorentzen, *Organizers, Presiding*

1:00 CHAL 36. How does government funding or joint development affect patent rights? L. DiLorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

1:45 CHAL 37. Foreign patent protection. L. DiLorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

2:30 CHAL 38. Enforcing IP rights. L. DiLorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

3:15 CHAL 39. Panel Discussion. L. DiLorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

THURSDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 152

The Many Faces of CHAL: Where Chemistry Meets the Law

K. E. Bianco, *Organizer, Presiding*

9:00 CHAL 40. Divided infringement: Is any one person liable for infringing your patent claims? J.L. Blackburn

9:30 CHAL 41. Best practices for patenting chemical and material compositions. J.V. Suggs, A.C. Palma

10:00 CHAL 42. Effective invention disclosures. J. Schuchardt

10:30 CHAL 43. Pharmaceutical products: At the intersection of patent and regulatory law. A.D. Sabatelli

11:00 CHAL 44. 2.6 billion dollars per drug: Can you afford not to file for patent protection for your R&D investment? C. Alpha

THURSDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 152

The Many Faces of CHAL: Where Chemistry Meets the Law

K. E. Bianco, *Organizer, Presiding*

1:00 CHAL 45. Impact of generic drug user fee amendment (GDUFA) for submission of drug master files for API mixtures and amorphous solid dispersion (ASD). R. Randad

1:30 CHAL 46. Identification of emerging drugs of abuse. E. Gardner

2:00 CHAL 47. Software for exposure calculation of chemicals migrated from food packaging to foods in Europe. K. Salmen

2:30 CHAL 48. 19th Century chemicals and petroleum production in New York City and 21st century environmental law. P. Spellane

COLL

Division of Colloid and Surface Chemistry

R. Nagarajan, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Protein-nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact (see *PHYS*, Sunday, Monday, Tuesday, Wednesday, Thursday)

Coacervation: Principles & Applications (see *AGFD*, Monday, Tuesday)

Environmental Applications and Implications of Graphene-based Nanomaterials (see *ENVR*, Tuesday, Wednesday)

In-Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles (see *CATL*, Tuesday, Wednesday, Thursday)

Adhesion Science and Adhesive Materials (see *PMSE*, Tuesday, Wednesday, Thursday)

Nanotechnology for Analytical Sensing and Spectroscopy Based Applications (see *ANYL*, Wednesday, Thursday)

SOCIAL EVENTS:

Social Hour, 6:00 PM: Sunday

Luncheon, 12:00 PM: Tuesday

BUSINESS MEETINGS:

Executive Committee Meeting, 4:00 PM: Saturday

Open Business Meeting, 5:30 PM: Sunday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 107A

Basic Research in Colloids, Surfactants & Nanomaterials

Nanomaterial Synthesis

R. Nagarajan, *Organizer*

K. Bandyopadhyay, *Presiding*

8:30 COLL 1. Colloidal synthesis and characterization of size tunable luminescent Zn₃P₂ nanocrystals. M. Ho, R.J. Esteves, I.U. Arachchige

8:50 COLL 2. One-step seeded growth of quasi-spherical silver nanoparticles through a thermal process using hydroquinone as a selective reductant. Z. Guo, P. Lu, X. Lu

9:10 COLL 3. Palladium nanoparticle seed mediated growth of palladium nanoshell on silica core. K. Bandyopadhyay, R. Teh

9:30 COLL 4. Generation of surface active species through hydrolytic conversion of organotrialkoxysilanes and their use in particle synthesis. M. Segers, D.J. Kraft, P. Buskens, M. Moller

9:50 COLL 5. Multifunctional colloidal magnetic nanoparticles by surface initiated atom transfer radical polymerization. M. Zeltner, R.N. Grass, C. Hofer, E.M. Schneider, W.J. Stark

10:10 COLL 6. Toward an improved understanding of the synthesis of alkanethiolate-protected Pd and Pt nanoparticles. J. Sidletsky, J.J. Zurmuhlen, P. Goulet

10:30 COLL 7. Morphogenesis of shapes and porosity of mesoporous silica particles. I. Sokolov, V. Kalaparthi

10:50 COLL 8. One-pot synthesis, anisotropic blue emission, and gas sensing behaviors of ZnO supercrystals with controlled structures. F. Li, F. Gong, C. Liu, H. Liu, Y. Zhang

11:10 COLL 9. Tragedy of TOPO-bound CdSe nanocrystals: Illustrative lessons in failed synthesis. N.C. Anderson

11:30 COLL 10. Single-micelle-templating synthesis of mesoporous silica and organosilica nanotubes. A.S. Manchanda, M. Mandal, L. Huang, M. Kruk

11:50 COLL 11. Pseudomorphic transformation: Simultaneous functionalization of silica microspheres and synthesis of bimodal SBA-15/MCM-41 with bottleneck pores. M.J. Reber, D. Brühwiler

Section B

Boston Convention & Exhibition Center
Room 107B

Theory & Modeling of Nanoparticles Interactions With Biomolecules & Polymers

M. Dutt, Y. G. Yingling, *Organizers, Presiding*

8:30 COLL 12. Condensation of nucleic acids by multivalent ions. A.V. Onufriev

9:00 COLL 13. Self-assembled gene carriers of DNA and graft copolymers. E. Luijten, H. Mao, Y. Ren, Z. Wei, J. Williford

9:30 COLL 14. Effect of NP shape and ligand flexibility in the design of nucleic acid wrapping NPs. J.A. Nash, A. Singh, N.K. Li, Y.G. Yingling

9:50 COLL 15. Using graphene-DNA interactions to control nanopore transport. A. Aksimentiev

10:20 Intermission.

10:30 COLL 16. Prediction of surface and pH-specific binding of peptides to metal and oxide nanoparticles. H. Heinz

11:00 COLL 17. Simulation of surface-peptide interactions in an aqueous environment. S.A. Barr, R.J. Berry, A.N. Camden, G.M. Leuty, C. Muratore, C.H. Turner, V. Varshey, C. Welch

11:30 COLL 18. Effect of surface polarity on physisorption of biomolecules: Molecular modeling. H. Kim, Y.G. Yingling

11:50 COLL 19. Designing sterically stable drug delivery vehicles via bio-inspired hybrid soft biomaterials. F. Aydin, G. Uppaladadiam, M. Dutt

Section C

Boston Convention & Exhibition Center
Room 107C

Biochemical Ligands at Interfaces: From Molecular Scale Characterization to Devices

Financially supported by JPK Instruments and NT MDT

T. Ye, *Organizer*

G. Liu, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL 20. Applications of model membrane architectures. S.G. Boxer

9:15 COLL 21. Patterned polysaccharide networks on surfaces control the phase behavior of lipid membranes. A.B. Subramanian

9:45 COLL 22. Covalent and sequence-specific DNA surface attachment chemistry for multiplexed single molecule measurements. **G.R. Abel**, X. Hao, B.H. Cao, J. Hein, T. Ye

10:10 Intermission.

10:25 COLL 23. Discovery of DNA codes for controlling the morphologies of nanomaterials and elucidation of its mechanisms for such a control. **Y. Lu**, L. Tan, A. Ali, N. Satyavolu

11:05 COLL 24. Interactions of bacterial lipopolysaccharides with gold nanorod surfaces investigated by plasmonic sensing. **N.S. Abadeer**, G. Fülöp, S. Chen, M. Kall, C.J. Murphy

Section D

Boston Convention & Exhibition Center
Room 108

Basic Research in Colloids, Surfactants & Nanomaterials

Self-Assembly

R. Nagarajan, *Organizer*

M. Tsianou, *Presiding*

8:30 COLL 25. Polysaccharide and oligosaccharide effects on surfactant micelle structure and interactions in aqueous solution. **A. Fajalila**, P. Alexandridis, **M. Tsianou**

8:50 COLL 26. Rationalizing the self-assembly of poly-(3-hexylthiophene) using solubility and solvatochromic parameters. **M.P. Gordon**, **D.S. Boucher**

9:10 COLL 27. Self-assembly of nucleic acid amphiphiles. **K. Zhang**

9:30 COLL 28. Surfactant self-assembly on singled-walled carbon nanotubes (SWCNTs): Hydrodynamic properties. **F.R. Phelan**

9:50 COLL 29. New insights to distinct increase of spontaneous lipid transfer rate in bicelles. **Y. Xia**, K. Charubin, F. Heberle, D. Marquardt, Y. Liu, J. Katsaras, B. Hammouda, M. Nieh

10:10 COLL 30. Incorporation behavior of lipophilic molecules into lipid bilayer membrane-based nanotubes. **Y. Okazaki**, R. Sakaguchi, M. Takafuji, H. Ihara

10:30 COLL 31. Sphorolipids: Tailoring biological and physical properties by modification chemistry. **R.A. Gross**, Y. Peng, F. Totsingan, A. Koh, M.A. Meier, F. Wurm

10:50 COLL 32. Role of hydration in lecithin reverse micelle structure and gelation in cyclohexane: A molecular dynamics study. **S. Vierros**, **M. Sammakorpi**

11:10 COLL 33. Shape persistence micelles having the same aggregation numbers with the Platonic solids. **K. Sakurai**

11:30 COLL 34. Toward a better understanding of the self-assembly of poly(ethylene glycol)-functionalized hexaphenylbenzenes. **K. Wunderlich**, M. Klapper, G. Fytas, K. Muellen

11:50 COLL 35. Time and concentration dependent assembly of amyloid-like peptides into supramolecular nanostructures. **G. Cinar**, M.O. Guler

Section E

Boston Convention & Exhibition Center
Room 109A

Colloid-Polymer Architectures & Mixtures

Films and Coatings

T. Kreer, *Organizer*

S. M. Balko, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL 36. Nanostructured thin polymer films with ordered fullerene-like nanoparticles arrays: Dissipative particle dynamics simulation. **O. Guskova**, C. Seidel, J. Sommer

9:05 COLL 37. Waterborne nanoceria/polymer nanocomposites: Enhanced properties through designed nanostructure. **I. Martin-Fabiani**, A.M. Cenacchi-Pereira, F. D'Agosto, M. Lansalot, E. Bourgeat-Lami, J. Keddie

9:25 COLL 38. Investigating the efficiency of polymer dispersants on aggregation and adsorption of asphaltenes with different functional groups: A molecular dynamics simulation study. **J. Wise**, L. Goual, M. Sedghi

9:45 Intermission.

10:00 COLL 39. Polymer brushes in restricted geometries. **T. Kuhl**, W. Liao, D. Mulder, S. Balko

10:30 COLL 40. Orientational assembly of anisotropic zirconium phosphate nanoplate in polyionic salt matrix. **X. Huang**, X. Wang, J. Li, Z. Cheng

10:50 COLL 41. Surface forces associated with hierarchically structured layer-by-layer films of polymer brush grafted nanoparticles and star polymers. **J.K. Riley**, K. Matyjaszewski, R.D. Tilton

11:10 COLL 42. Particle-sorption in wobbling polymer films. **B.D. Keviet**, L. Dos Ramos, L.I. Mensink, G. Lajoinie, M. Versluis, G. Vancso, S. de Beer

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Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-resolved Spectroscopies

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Protein-nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Fundamentals and Applications

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SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 107A

Basic Research in Colloids, Surfactants & Nanomaterials

Surface Modification

R. Nagarajan, *Organizer*

I. Sokolov, *Presiding*

2:00 COLL 43. Influencing surface functionalization of aluminum fillers with acrylic-monomers through the onset of instability in Taylor Couette flow. **M. Aljishi**, Y.L. Joo

2:20 COLL 44. Current challenges in quantitative measurement of ligand binding and interactions at quantum dot surfaces. **A.B. Greytak**

2:40 COLL 45. Surface modification of inorganic oxide particles for improved dispersion in waterborne coatings. **J. Jankolovits**, A.M. Van Dyk, J. Bohling, J. Roper, C.J. Radke, A.S. Katz

3:00 COLL 46. Colloidally suspended 3-MPA capped PbS quantum dots. **C.C. Reinhart**, E. Johansson

3:20 COLL 47. Electrochemical characterization of selenium-modified gold surfaces. **E. Karnaukh**, H. Wang, **M.C. Buzzeo**

3:40 COLL 48. Smart materials based on thiol-functionalized pNIPAM and gold nanoparticles. **Y. Li**, J.W. Soares, D.M. Steeves, J.E. Whitten

4:00 COLL 49. 1-Adamantanethiol as a versatile nanografting tool. **C.I. Drexler**, C. Causey, **T.J. Mullen**

4:20 COLL 50. On-surface redox chemistry to control well-defined oxidation states of transition metal centers by ligand design. **S.L. Tait**

4:40 COLL 51. Omniphobic bio-based coatings on polyolefinic substrates. **J.H. Lavoie**, E. Shim, S. Khan, O.J. Rojas

5:00 COLL 52. Purification of carboxylated carbon nanotubes. **Z. Wu**, S. Mitra

5:20 COLL 53. Eliminating ions from polyelectrolyte multilayers: A recipe high in salt. **H. Fares**, Y. Ghoussoub, R. Surmaitis, J.B. Schlenoff

Section B

Boston Convention & Exhibition Center
Room 107B

Theory & Modeling of Nanoparticles Interactions With Biomolecules & Polymers

M. Dutt, Y. G. Yingling, *Organizers, Presiding*

2:00 COLL 54. Lessons learned from inverse design of interactions for assembly. **T. Truskett**

2:30 COLL 55. Thermal conduction by clustered colloids. **T. Matsoukas**

3:00 COLL 56. Combined experimental and molecular modeling studies of nanodiamonds. **D.W. Brenner**, F. Saberi Movahed, Z. Liu, A. Koolivand, A.I. Smirnov, J. Krim, O. Shenderova

3:30 COLL 57. Self-assembly simulations of polymer functionalized nanoparticles. **L. Chong**, S. Libring, V. Karra, M. Dutt

3:50 Intermission.

4:00 COLL 58. Ghost tweezers method for studies of nanoparticle interaction with polymer brushes and lipid membranes. **A.V. Neimark**, S. Burgess, J. Cheng, Z. Wang, A. Vishnyakov

4:30 COLL 59. Multiscale modeling of polymers. **A. Yethiraj**

5:00 COLL 60. Towards the virtual laboratory: modelling clay-polymer nanocomposites using a multiscale approach. **P.V. Coveney**, J. Suter, D. Groen

5:20 COLL 61. Controlling non-covalent dispersion of hydrophobic objects with lipids and polymers. **J. Määttä**, S. Vierros, P.R. Van Tassel, M. Sammakorpi

Section C

Boston Convention & Exhibition Center
Room 107C

Biochemical Ligands at Interfaces: From Molecular Scale Characterization to Devices

Financially supported by JPK Instruments and NT MDT

G. Liu, *Organizer*

T. Ye, *Organizer, Presiding*

2:00 COLL 62. Withdrawn.

2:30 COLL 63. Electrochemical protease profiling toward cancer analyses using peptide-functionalized carbon nanofiber nanoelectrode arrays. **L. Swisher**, D.H. Hua, T. Nguyen, **J. Li**

3:00 COLL 64. Nucleic acid biosensing at interfaces: Physicochemical perspectives and future prospects. **R. Levicky**

3:30 Intermission.

3:45 COLL 65. Aptamer-functionalized chemomechanically-modulated biomolecule catch-and-release system. **A. Shastri**, L. McGregor, H. Nan, M. Mujica, Y. Liu, O. Kuksenok, M. Aizenberg, A.C. Balazs, J. Aizenberg, **X. He**

4:15 COLL 66. Using electrochemical DNA-based (E-DNA) sensors to monitor cooperative DNA-protein interactions. **F.C. Macazo**, R.L. Karpel, R.J. White

Section D

Boston Convention & Exhibition Center
Room 108

Basic Research in Colloids, Surfactants & Nanomaterials

Emulsions and Interfaces

R. Nagarajan, *Organizer*

M. N. Kobrak, *Presiding*

2:00 COLL 67. To model chemical reactivity in heterogeneous emulsions: Think homogeneous microemulsions. **L. Romsted**

2:30 COLL 68. Understanding co-surfactant-sphorolipid combinations for improved interfacial properties. **A. Koh**, J. Han, R.A. Gross

2:50 COLL 69. Location and influence of added block copolymers on oil-in-oil emulsions. **I. Asano**, T.P. Lodge

3:10 COLL 70. Thermodynamic approach to interfacial concentration gradients. **M.N. Kobrak**

3:30 COLL 71. New generation of smart surfactants for miniemulsion. **S. Wald**, K. Landfester, F. Wurm

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3:50 COLL 72. Dynamically reconfigurable complex emulsions via tunable interfacial tensions. **L.D. Zarzar**, V. Sresht, E.M. Sletten, J.A. Kalow, D. Blankschtein, T.M. Swager

4:10 COLL 73. Understanding the interactions of epoxides and amines as reactive compartments in aqueous dispersions. **A. Bijlard**, S. Winzen, A. Kaltbeitzel, Y. Avlasevich, D. Crespy, K. Landfester, A. Taden

4:30 COLL 74. Investigating surfactant-based oil recovery process in reservoirs with heterogeneous mineralogy. **G. Javanbakht**, L. Goual

4:50 COLL 75. Framboidal triblock copolymer vesicles: A new class of efficient Pickering emulsifier. **C. Mable**, N. Warren, K.L. Thompson, O.O. Mykhaylyk, S.P. Armes

5:10 COLL 76. Characterizing the effect of modification on cellulose nanocrystal pickering emulsions. **A. Koh**, S. Spinella, A. Maiorana, R.A. Gross

5:30 COLL 77. Multibody coalescence in Pickering emulsions. **C. Na**, T. Wu

Section E

Boston Convention & Exhibition Center
Room 109A

Colloid-Polymer Architectures & Mixtures

Functional or Patterned Colloids & Surfaces

S. M. Balko, T. Kreer, *Organizers*

T. Kuhl, *Presiding*

2:00 COLL 78. Multicompartmental colloids: Synthesis, properties, and function. **J. Lahann**

2:30 COLL 79. Conformation and diffusion of DNA-coated nanoparticles. **E. Luijten**, C. Ramavarapu, H. Wu

3:00 COLL 80. Colloidal nanomaterials-encapsulated microcapsule for biomolecular sensing. **X. Xie**, W. Zhang, A. Abbaspourrad, D. Weitz, D.G. Anderson

3:20 Intermission.

3:35 COLL 81. Power-free mechanochromic sensors from force-recording, elastoplastic inverse opsals. **Y. Cho**, S. Lee, L. Ellerthorpe, G. Feng, G. Lin, J. Yin, G. Wu, S. Yang

3:55 COLL 82. How do surfaces alter the structure in multicomponent polymer systems and vice versa? A computer simulation study. **M. Mueller**, F. Leonforte, Q. Tang

4:25 COLL 83. Tortuosity and branching of worm-like micelles accessed by small-angle neutron scattering. **K. Vogt**, G. Beaucage, M.R. Weaver, H. Jiang

4:45 COLL 84. Artificial biomembrane models using giant vesicles comprised of amphiphilic random block copolymers. **E. Yoshida**

5:05 COLL 85. Sliding tethered ligands: Lock and key colloidal interactions with a topological twist. **M. Bauer**, C. Fajolles, T. Charitat, J. Iss, P. Kékicheff, J. Daillant, **C.M. Marques**

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Protein-nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact Fundamentals and Applications

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SUNDAY EVENING

Section A

Westin Boston Waterfront

Galleria

Fundamental Research in Colloids, Surfaces & Nanomaterials

R. Nagarajan, *Organizer, Presiding*

6:00 - 8:00

COLL 86. Thermal stabilization effect of multilayer graphene-coated metal nanostructures. **P. Wilson**, A. Zobel, A. Lipatov, T. Hofmann, A. Sinitzki

COLL 87. First principles simulations of pure water. **S. Gelpi**, M. Morales-Silva

COLL 88. Flame-retardant surfaces from green vinyl ester resin. **P. Shah**, A. Kokil, R.F. Kovar, Y. Lee

COLL 89. Molecular modeling and DFT analysis of theoretical covalent cross-linkages between hydroxyproline stereoisomers and galacturonic acid. **M.H. Andersen**, L. Tribe

COLL 90. Long range nanorolar for cancer cell sensing. **S.S. Sinha**, A. Pramanik, R. Kanchanapally, S.R. Chavva, B. Viraka Nellore, S.J. Jones, P.C. Ray

COLL 91. Magnetic-nanoparticle conjugated hybrid graphene oxide for prostate cancer detection and treatment. **S.R. Chavva**, A. Pramanik, B. Viraka Nellore, P.C. Ray

COLL 92. Fabrication of stable, low-density, self-assembled monolayers on gold by click thiol-yne reaction. **L. Safazadeh Haghghi**

COLL 93. Efficient removal and killing of multidrug-resistant *Staphylococcus aureus* (MRSA) using polycyclic antibacterial peptide-functionalized 3D porous graphene oxide membrane. **A. Pramanik**, R. Kanchanapally, B. Viraka Nellore, S.S. Sinha, S.R. Chavva, S.J. Jones, P.C. Ray

COLL 94. DFT study of formaldehyde coupling reaction on rutile TiO₂ (110) surface. **M. Tang**, Q. Ge, Z. Zhang

COLL 95. Alpha-ketoglutaric acid for neutralization of hydrazine and monomethylhydrazine waste streams. **C. Yestrebtsky**, C. Franco, D. Glass, R. Martinez, C. Davis

COLL 96. Surface-enhanced Raman spectroscopic (SERS) detection with submonolayer nanoparticle arrays. **R. Osgood**

COLL 97. Tunable thermochromism of anthraquinone induced by reversible microparticle/nanoparticles switching in blended block copolymers. **N. Alexandridi**, Y. Zhang, J.F. Lovell

COLL 98. Characterization of surface area burial upon formation of biomolecular interfaces. **L. Pegram**, D. Riccardi

COLL 99. Control of radiation sensitivity of inorganic resists by exchanging ligands. **D. Park**, J.M. Amador, S.R. Decker, D.A. Keszler

COLL 100. Development and characterization of surface modified metal oxide nanoparticles. **A. Torres**, O. Santillan, B. Veldman

COLL 101. Tuning surface chemistry on layer-by-layer nanoparticles to target ovarian cancer. **S. Correa**, P.T. Hammond

COLL 102. Temperature-dependent SPR measurement of the influence of probe density on the denaturation temperature of hybridized DNA on surfaces. **L. Alves de Macedo**, A. Opdahl

COLL 103. C₆₀-functionalized flavin (FC60) toward nanotube-based photovoltaics. **M. Mollahosseini**, F. Papadimitrakopoulos

COLL 104. Thermodynamics of ionic liquid polymer solutions. **Z. He**, **P. Alexandridis**

COLL 105. Withdrawn.

COLL 106. Pralidoxime functionalized polydiacetylene for colorimetric detection of organophosphates. **Y. Zhang**, L. Bromberg, T. Halton

COLL 107. Quantification of viral surface lipids using plasmon-coupling based UV-Vis spectrophotometry. **C. Wong**, A. Feizpour, H. Akiyama, S. Gummuluru, B.M. Reinhard

COLL 108. Fundamental catalytic studies of bimetallic and oxide nanomaterials for CO oxidation and the reverse water gas shift reaction. **A. Baber**, D.T. Boyle, C. Stopak

COLL 109. Protein adsorption on silica nanoparticles and oxidized silicon: Effect of surface wettability and chemistry. **B. Mondal**, Q. Xu, M. Barahman, A.M. Lyons

COLL 110. Role of tyrosines within Amot as a driver for protein-lipid association. **A.C. Kimble Hill**, N. Abufares, H.I. Petrasche, T.D. Hurley, C.D. Wells

COLL 111. Effect of aromatic and hydrophobic interactions in amphiphilic supramolecular assemblies in response to temperature changes. **O. Munkhbat**, M. Garzon, G.M. Pavan, S. Thayumanavan

COLL 112. Size- and shape-controlled synthesis of gold nanoparticles using chitosan as a stabilizer. **L. Liu**

COLL 113. Stimuli-responsive nanomaterials for detection and active decontamination of chemical and biological threats. **R.S. McDonald**, J. Owens, W.B. Salter, K. Simpson, **G. Strack**, D. Volkov

COLL 114. Spatial frequency heterodyne imaging of water filled multi-walled carbon nanotubes. **F. Schunk**, D. Rand, C.G. Rose-Petrucci

COLL 115. Withdrawn.

COLL 116. Self-assembled monolayers of amphiphilic macromolecules as bioactive cardiovascular stent coatings. **J.W. Chan**, Y. Zhang, K.E. Uhrich

COLL 117. Molecular simulations of phospholipid self-assembly: Curvature and nanoscale forces in vesicles and upon substrate adhesion. **J. Määttä**, M. Sammalkorpi

COLL 118. Fabrication of single neural cell chip to analyze cellular redox state by spectroelectrochemical technique. **K. Kim**, T. Kim, Y. Chung, W. El-Said, J. Choi

COLL 119. Bridging the pressure and materials gap between surface science and catalysis: Probing the surface of metal oxide nanoparticles. **M. Kipreos**, M.C. Foster

COLL 120. Preparation of large-area graphenes via mild oxidation followed by millstone exfoliation. **T. Yoon**

COLL 121. Design and evaluation of ligand-conjugated amphiphilic macromolecule nanoparticles for mitigation of atherosclerosis. **A.E. Moretti**, R. Chmielowski, P. Moghe, K.E. Uhrich

COLL 122. Co-engineering the supramolecular nanoparticle-protein interface. **M. Ray**, Z. Jiang, R. Landis, V.M. Rotello

COLL 123. Structured surfaces for adhesion and friction experiments. **R. Jin**, X. Xu, S. Kaur, M. Ruths

COLL 124. Robust network microcapsules with tunable permeability based on sole cellulose nanocrystals. **c. ye**, **R. Geryak**, M. Chyasnachyus, V.V. Tsukruk

COLL 125. Nonlinear optical probe of chemical reactions and photonics at the surface of silver nanoparticles. **B. Xu**, W. GAN, G. Gonella, B.G. DeLacy, H. Dai

COLL 126. Nanomechanical properties of eutectic gallium-indium particles by atomic force microscopy. **S.S. Akhter**, I. Tevis, M.M. Thuo, M.C. Foster

COLL 127. Kinetic release of micellized PEG-PLL block copolymer complexed with siRNA using FRET assay. **C.M. Bailey**, R. Nagarajan, T.A. Camesano

COLL 128. Photoreactive sulfobetaine copolymers for the modification of biomedical devices. **F. Torok**, M. Bouchard, J. Li, Z. Zhang

COLL 129. Characterization and antibacterial effect of silica-silver nanocomposite particles. **J. Kim**, S. Oh

COLL 130. Cytosolic delivery of therapeutic siRNA and miRNA using self-assembled gold nanoparticle-stabilized nanocapsules for breast cancer therapy. **J. Hardie**, Y. Jiang, R. Landis, E. Tetrault, P. Ghazi, M.E. Farkas, V.M. Rotello

COLL 131. Triethanolamine-stabilized silver nanoparticles as substrates for surface-enhanced Raman scattering. **E. Honarvarfarid**, Y. Chen, P. Goulet

COLL 132. Characterization of hybrid microspheres with silica nanoparticles-embedded surface. **N. Hano**, N. Ryu, S. Nagaoka, M. Takafuji, H. Ihara

COLL 133. Correlating excitonic and structural properties of lead sulfide (PbS) nanocrystal films. **M. Weidman**, W.A. Tisdale

COLL 134. Comparative study on the single particle optical properties of binary CdSe and ternary alloyed CdS_{1-x}Se_x semiconductor nanocrystals. **S. Dey**, S. Chen, M. Shakil, S.L. Suib, J. Zhao

COLL 135. Synthesis and stabilization of CuO nanorods in alkane based solvents. **M. Hossain**, G.C. Mills

COLL 136. Reactive fibrous adsorbents for decontamination of chemical threats. **L. Bromberg**, V. Martis, Y. Zhang, **X. Su**, T. Hatton

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

- COLL 137.** Advances in the use of gel permeation chromatography (GPC) to nanocrystals: Purification, solvent change, and surface modification. **Y. Shen,** R. Tan, M.Y. Gee, A. Roberge, A.B. Greytak
- COLL 138.** Adaptation of FTIR spectrometer to the external reaction chambers for surface analysis studies. S.V. Shilov, **T. Tague,** G. Zachmann, X. Stammer
- COLL 139.** Atomically precise gold nanoclusters for the electrocatalytic reduction of carbon dioxide. **M. Kim,** W. Choi, K. Kwak, D. Lee
- COLL 140.** Modified electrodes using Au₂₅ nanoclusters for electrochemical sensing applications. **M. Jang,** U.P. Azad, E. Ko, D. Lee
- COLL 141.** Iron chalcogenide nanoparticle precursors for solution processed photovoltaics and other applications. **B. Gebear-Eigzabher,** P. Hwang, C. Lai, D.R. Radu
- COLL 142.** Photocatalytic performance of a trifold nanocomposite material for the hydrolysis of 2-chloroethyl ethyl sulfide (CEES). **C.A. Zoto**
- COLL 143.** Silver seeds and aromatic surfactants facilitate the growth of anisotropic metal nanoparticles: Gold triangular nanoprisms and ultrathin nanowires. **Z. Qian,** S. Park
- COLL 144.** Synthesis of metal sulfide nanoparticles in toluene at room temperature. **L. Bian,** K. Ring, J. Sidletsky, P. Goulet
- COLL 145.** Quantifying the surface coverage of mercaptohexadecanoic acid on nanocrystalline SnO₂ thin films. **G.R. Soja,** M.J. Awad
- COLL 146.** Single-phase synthesis of thiolate-protected metal nanoparticles. **J. Sidletsky,** B.G. Root, P. Goulet
- COLL 147.** Nisin protection from degradation and controlled release via polyacrylate acid encapsulation. **L.W. Place,** S. Flocamo
- COLL 148.** Versatile gold nanobowl arrays for size-selective plasmonic biosensing. **E. Lehnhoff,** D. Jana, I. Bruzas, L. Sagile
- COLL 149.** Directed self-assembly of nanoparticles: Template control of nanostructure configurations. **K. Lim,** M. Asbahi, S. Mehraeen, F. Wang, J. Cao, M. Tan, J. Yang
- COLL 150.** Magneto-responsive hybrid colloidal architectures: Preparation, processing, and opal film formation. **D. Scheid,** M. Gallei
- COLL 151.** Synthesis and self-assembly of copper nanowires. **S. Darmakkolla**
- COLL 152.** Electron induced surface reactions of organometallic precursors. **J. Spencer,** R. Thorman, M. Barclay, J.A. Brannaka, Y. Wu, O. Ingolfsson, L. McElwee-White, H. Fairbrother
- COLL 153.** Modification of nitinol nanoparticles with self-assembled monolayers. **R. Quinones,** S. Garretson
- COLL 154.** Modification of zinc oxide nanoparticles with perfluoro phosphonic acids. **R. Quinones,** C. Peck
- COLL 155.** Proton coupled electron transfer through 2-2'-6'-2" terpyridine molecular wire between graphene - gold nanoparticle junction. **G.V. Jacob,** A. Patnaik
- COLL 156.** Study of thermal diffusivity in metallic and bimetallic Fe and Au nanoparticles. **K.A. Fudimura,** M. Da Cruz Santos, P.S. Haddad, A. Alves
- COLL 157.** Fabrication of liquid-like-surface and evaluation of anti-frosting property. **T. Moriya,** K. Manabe, S. Shiratori
- COLL 158.** Mechanistic study using a quartz crystal microbalance: Effect of spacer length on the antimicrobial activity of the bound peptide, Chrysothysin-1. **T. Alexander,** L.D. Lozeau, T.A. Camesano
- COLL 159.** Preparation of lipid bilayer membrane-based nanotubes-enclosed polymer composite film. **Y. Okazaki,** S. Konomi, M. Takafuji, H. Ihara
- COLL 160.** Biomemory regulator device composed of metalloprotein/DNA/nanoparticle. **J. Yoon,** S. Kim, T. Lee, J. Min, J. Choi
- COLL 161.** Molecular interactions between gold nanoparticles and model cell membranes. **P. Hu,** X. Zhang, C. Zhang, Z. Chen
- COLL 162.** Withdrawn.
- COLL 163.** Making colors from black and white. **Y. Takeoka**
- COLL 164.** Gene delivery by polyethyleneimine-functionalized graphene oxide suppresses breast cancer cell migration. **Y. Huang,** W. Wang, C. Zhong, **M. Lee**
- COLL 165.** QCM-D based mechanistic study of Alzheimer's disease: Membrane-amyloid peptide interactions. **E. Kamaloo,** T.A. Camesano
- COLL 166.** 2D nanoparticle cluster formation in supercritical fluid CO₂. **J. Wang,** G. Brown, C.M. Wai
- COLL 167.** Effect of incorporation of lysolipid on the stability of dipalmitoyl phosphatidyl choline bilayer membrane: Molecular dynamics simulation approach. **K. Lee,** Y. Kim, S.S. Jang
- COLL 168.** Magneto-fluorescent core-shell supernanoparticles. **O. Chen**
- COLL 169.** DNA-polypeptide polyplexes. **M.J. Lueckheide,** J. Viereg, L. Leon, M.V. Tirrell
- COLL 170.** Upconversion of trapped charge carriers in coupled lead sulfide quantum dot solids. **R.H. Gilmore,** W.A. Tisdale
- COLL 171.** Mechanisms of metal deposition on colloidal gold nanoparticle substrates. **P. Straney,** J. Millstone
- COLL 172.** Light scattering from concentrated eye lens beta crystallin solutions. **K.P. Van Nostrand,** L.V. Michel, G.M. Thurston
- COLL 173.** pH Sensitive delivery of Pt²⁺ based therapeutics in lipid-coated PLGA nanoparticles. **M.T. Wlodarczyk,** O. Camacho-Vanegas, P. Dottino, J.A. Martignetti, A.J. Mieszawska
- COLL 174.** Withdrawn.
- COLL 175.** Smart drug delivery system using magnetic core-shell gold nanoparticles. **H. Ilkhani,** M.R. Hepel, J. Li, Z. Skeete, J. Luo, C. Zhong
- COLL 176.** Preparation of modified poly(ethylene-co-acrylic acid) (PEAA) usary ammonium with aliphatic chains as antibacterial polymer. **H. Noh,** J. Ryu, S. Oh
- COLL 177.** Interpenetrating network polymer gel for improving oil recovery. **Y. Long,** Z. Chen, B. Bai
- COLL 178.** Tunable intermolecular interaction in N-methylfulleropyrrolidine (8-NMFP) mediated with assembly of gold nanoparticles. **S. Sutradhar,** A. Patnaik
- COLL 179.** Novel photothermal-based release mechanism for controlled release on Au nanoparticles through light. **E. Goren,** H. Cavusoglu, E. Yavuz, H. Usta, M. Yavuz
- COLL 180.** Omniphilic superparamagnetic iron oxide core-shell nanoparticles. **B. Shirmardi Shaghasemi,** E. Reimhult
- COLL 181.** Understanding the effect of TMA⁺ on the condensation behavior of [H₂Ta₂O₇]²⁻. **R. Mansergh,** L.B. Fullmer, D. Park, M.D. Nyman, D.A. Keszler
- COLL 182.** Size-dependent cellular uptake of sub-10 nm zwitterionic gold nanoparticles. **Y. Jiang,** S. Huo, S. Hou, T. Mizuhara, D. Moyano, V.M. Rotello
- COLL 183.** Assembling discrete nanoparticle clusters via weakly interacting DNA linkages. **A. Lewis,** T.L. Doane, M. Bowick, M.M. Maye
- COLL 184.** Understanding the assembly and aligning of semiconductor quantum rods on DNA origami. **Y. Chen,** T.L. Doane, M.M. Maye
- COLL 185.** Designing stable foams in the presence of alkanes and brine for oil field operations. **V. Sansen,** U. Suriyapraphadilok, A. Chareonsang, B.J. Shiau
- COLL 186.** Vitamin E- conjugated lipidic mixed micellar system as nanocarrier for the delivery of curcumin in cancer. **O. Muddineti,** P. Jha, B. Ghosh, S. Biswas
- COLL 187.** Withdrawn.
- COLL 188.** Antibacterial efficacy of carbohydrate-conjugated nanomaterials. **S.A. Wijesundera,** B. Wu, K. Jayawardana, M. Yan
- COLL 189.** Preparation of double emulsions using hybrid polymer/silica particles: New Pickering emulsifiers with adjustable surface wettability. **M. Williams,** N. Warren, L.A. Fielding, S.P. Armes, P. Verstraete, J. Smets
- COLL 190.** Blockcopolymer based cross linkable surfactant for preparation of polymeric nanoparticles by miniemulsion process. **K. Kim,** R.W. Zentel
- COLL 191.** Silica supported zirconaziridine for hydroaminoalkylation of olefin: Evidence for the mechanism. **B. Hamzaoui,** J.M. Basset, J. Pelletier
- COLL 192.** Low water activity materials for moisture harvesting. **S.A. Ferdousi,** K.L. Yeung, **Z. Liu**
- COLL 193.** Withdrawn.
- COLL 194.** Study of the relationship between cationic degree and the performance of nanoparticle dispersion. **J. Geng,** B. Bai, T.P. Schuman
- COLL 195.** Poly(ethylene glycol)-b-olaamphiphiles for highly stabilized liposomes. **Y. Zhang,** K.E. Uhrich
- COLL 196.** Withdrawn.
- COLL 197.** Controlling hydrosilylated pin-printed feature sizes on porous silicon. **D.T. McCall,** Y. Zhang, D.J. Hook, F.V. Bright
- COLL 198.** Surface properties of xerogel materials with unusual patterns and tunable topography for antifouling applications. **J.F. Destino,** Z. Jones, A. Craft, C.M. Gatlley, M.R. Detty, F.V. Bright
- COLL 199.** Aerosol-based ultrasonic synthesis of polymer-conjugated metallic nanobunches to fabricate transparent antimicrobial layers. **J. Byeon**
- COLL 200.** Carbon nanotube scaffolded self organized silica gels. **B.P. Chauhan,** **Q. Johnson,** A. Patel, S. Matam, M. Chauhan
- COLL 201.** Catalytic investigations of hybrid metallic nanoparticle nanogels: The effect of silylation on self assembly and activity. **K. Moran,** A. Patel, S. Chaudhry, **Q.R. Johnson,** S. Matam, B.P. Chauhan
- COLL 202.** SIRB, Sans Iron Oxide Rhodamine B, a novel cross linked dextran nanoparticle. **E.V. Groman,** J.S. Weinberg, A. Ramalingam
- COLL 203.** SIRB, Sans Iron Oxide Rhodamine B, a novel crosslinked dextran nanoparticle, labels human neuroprogenitor and SH-SY5Y neuroblastoma cells and serves as a USPIO cell labeling control nanoparticle. **W. Shen,** E.V. Groman, P. Fishman, P. Yarowsky
- COLL 204.** Novel plasmonic platform for label-free biosensing with membrane-associated species. **I. Bruzas,** S. Unser, L. Sagile
- COLL 205.** Eco-friendly scratch resistant wood coatings based on silica nanoparticles. **C. Alt,** C. Cordt, R. Klein
- COLL 206.** Promotion of the halide effect in the formation of metal nanocrystals via a hybrid cationic, polymeric stabilizer: Octahedra, cubes, and anisotropic growth. **M. Golden,** B.T. Sneed, C. Tsung
- COLL 207.** Chlorinated protein films for antimicrobial coatings. **L. Wang,** B. Duncan, A. Gupta, R. Ramanathan, V.M. Rotello
- COLL 208.** National synchrotron X-ray scattering facility dedicated for the studies of molecular ordering and dynamics at liquid surface/interfaces. **W. Bu,** B. Lin, M. Meron
- COLL 209.** Histamine-functionalized copolymer micelles as a drug delivery system in 2D and 3D models of breast cancer. **Y. Zhang,** P. Lundberg, **M. Diether,** C. Porsch, C. Janson, N.A. Lynd, C. Ducani, M. Malkoch, E.E. Malmstrom, C.J. Hawker, A.M. Nystrom
- COLL 210.** Metal chelating polyphenol coatings for antioxidant active packaging. **M. Roman,** E.A. Decker, J.M. Goddard
- COLL 211.** Phospholipid/aromatic thiol hybrid bilayers. **C. Li,** M. Wang, W. Zhan
- COLL 212.** All-lipid assembled photosynthetic mimics. **M. Wang,** C. Li, W. Zhan
- COLL 213.** Photoinitiated covalent surface functionalization for enhanced control over electroless deposition on silicon nitride. **Y.D. Bandara,** B.I. Karawadeniya, J. Whelan, B. Velleco, J.R. Dwyer
- COLL 214.** Electroless plating of thin gold films directly onto silicon nitride thin films and into micro- and nanopores. **J. Whelan,** N.D. Bandara, B.I. Karawadeniya, C. Masterson, B.D. Velleco, J.R. Dwyer
- COLL 215.** Molecular layers on nanoporous gold electrodes. **E.C. Landis,** D. Patel, C.L. Chevalier, R.B. Chevalier
- COLL 216.** Rapid, electroless surface modification through surface-directed azo coupling. **N. Marshall,** T. Mikhailova, B. Taylor
- COLL 217.** Electrospun polytetrafluoroethylene thin film with high heat transfer coefficient. **H. Tsuchiya,** K. Manabe, K. Kyung, T. Gaudalet, F. Gillot, S. Shiratori

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- COLL 218.** Toward the synthesis of ordered mesoporous organosilicas with closed mesopores. **A.S. Manchanda**, M. Mandal, M. Kruk
- COLL 219.** KillerRed conjugated upconversion nanoparticles for cancer imaging and photodynamic therapy. **L. Liang**, R. Zhang, V. Sreenivasan, S.M. Deyev, Y. Qian, A. Zvyagin
- COLL 220.** Dynamic coupling at the Ångström scale. **F.Y. Pong**, K.K. Dey, J. Breffke, E. Hatzakis, A. Sen
- COLL 221.** Enhanced cell performance with control of ZnO buffer layer using nanoparticles of various morphology for inverted organic photovoltaic cells (OPVs). **S. Oh**, S. Oh
- COLL 222.** Silver sulfadiazine-immobilized inorganic fillers: Preparation, characterization, and antimicrobial functions. **R. Srivastava**, Y. Sun
- COLL 223.** Removal of oxidation debris from carboxylated carbon nanotubes. **Z. Wu**, R.F. Hamilton Jr, A. Hollan, S. Mitra
- COLL 224.** Characterization of carbon nanotube composites by imaging X-ray photoelectron spectroscopy: Employing differential charging to detect carbon in carbon. **J.M. Gorham**, W.A. Osborn, J.W. Woodcock, K.C. Scott, J.M. Heddlston, A.R. Hight Walker, J.W. Gilman
- COLL 225.** Zwitterionic amphiphile based magnetofluorescent nanoparticles. **V.G. Demillo**, X. Zhu
- COLL 226.** Size-exclusive protein adsorption on plasmonic gold nanoparticles measured via optical dark-field spectroscopy. **V. Wulf**, J. Heidrich, D. Schneider, C. Soennichsen
- COLL 227.** Seed-mediated self-assembly to form core-shell and Janus nanostructure using nanoparticles-loaded thermo-cleavable polymer. **K. Sansanaphongpricha**, H. Chen, K. Sun, D. Sun
- COLL 228.** Synthesis and characterization of highly stable ligand protected quantum sized silver nanoclusters. **K. Pyo**, D. Lee
- COLL 229.** Thermal decomposition based synthesis of AgInS₂/ZnS quantum dots and their cellular imaging applications. **S. Chen**, X. Zhu
- COLL 230.** Withdrawn.
- COLL 231.** Tumor targeted poly(ethylene glycol)-poly(D,L-lactic acid)-based copolymeric micelles as a potential chemotherapeutic drug delivery system: Synthesis, physico-chemical, and in vitro characterization. **P. Kumari**, O. Muddineti, B. Ghosh, S. Biswas
- COLL 232.** Stimulus-responsive water-soluble graphene nanodevices for tunable biomarker detection. **M. Balcioglu**, B. Buyukbekar, M.S. Yavuz, M.V. Yigit
- COLL 233.** Tuning the detection capacity and specificity of polymer protected graphene nanoassemblies using endonucleases. **N.M. Robertson**, M. Hizir, M. Rana, M. Balcioglu, M.S. Yavuz, M.V. Yigit

Technical program information known at press time. The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

- COLL 234.** Two-color detection of circulating miRNAs from liquid biopsies for prostate cancer screening using graphene nanoassemblies. **M. Hizir**, N.M. Robertson, M. Rana, M. Balcioglu, M.V. Yigit
- COLL 235.** Highly sensitive enzyme-free detection of multiple miRNAs using gold nanoparticles and hybridization chain reaction. **M. Rana**, M. Balcioglu, N.M. Robertson, M. Hizir, M.V. Yigit
- COLL 236.** Withdrawn.
- COLL 237.** Withdrawn.
- COLL 238.** Withdrawn.
- COLL 239.** Synthesize and characterization of bis-cationic surfactant and self-assembly into worm-like viscoelastic fluids. **C. Yang**, Z. Hu, Q. Jiang
- COLL 240.** Stepwise functionalization method for nanostructure-based Mg_xZn_{1-x}O biosensor with increased sensitivity and selectivity. **Y. Chen**, P. Reyes, S. Misra, E. Galoppini, Y. Lu
- COLL 241.** Hydrophobicity of treated graphene oxide surfaces: Experimental and molecular dynamics simulation studies. **H. Mortazavian**, C.J. Fennell, B.R. Sedai, F.D. Blum
- COLL 242.** Porous polymeric membrane formed by charge and amphiphilicity dually driven self-assembly. **J. Xu**, Z. Zhu, H. Xue

Section C

Westin Boston Waterfront Galleria

Nanotheranostics for Cancer Applications

S. A. Morris, *Organizers, Presiding*

6:00 - 8:00

- COLL 243.** Multifunctional theranostic silica-gold core-shell nanoparticles for breast cancer applications. **D. VanDyke**, P. Rai
- COLL 244.** Mg@porous SiO₂ particles: Preparation, controlled hydrogen release, and hydroxyl radicals scavenging activities. **L. Kong**, F. Mou, C. Chen, L. Xu, J. Guan
- COLL 245.** Synthesis and optimization of colloidal gold nanoparticles for cancer therapy. **B. Yassini**, P. Rai

MONDAY MORNING

Section A

Boston Convention & Exhibition Center Room 107A

30 Years of Langmuir: Looking Back & Forward

F. M. Winnik, *Organizer*

R. M. Crooks, *Organizer, Presiding*

M. M. Santore, *Presiding*

8:30 COLL 246. Charge transport by tunneling through SAMs. **G.M. Whitesides**

9:00 COLL 247. Longing for Langmuir. **C.J. Murphy**

9:30 COLL 248. Adsorption at the bio/nano interface: DNA, liposomes, and inorganic nanoparticles. **J. Liu**

10:00 Intermission.

10:15 COLL 249. Biological and environmental media control oxide nanoparticle surface composition: The roles of biological components (proteins, peptides and amino acids), inorganic oxyanions, and humic acid. **V.H. Grassian**

- 10:45 COLL 250.** Wetting of solids by liquids. **T.J. McCarthy**
- 11:15 COLL 251.** Synthetic compounds/materials-biological interface: A doorway to new opportunities for sensing, antimicrobial activity, and therapeutics. **D.G. Whitten**, H. Pappas

Section B

Boston Convention & Exhibition Center Room 107B

Surface Modification to Control Cell/Surface Interactions

H. Moehwald, *Organizer*

A. M. Peterson, *Organizer, Presiding*

8:30 COLL 252. Maintenance and differential regulation of stem cells using functionalized nanoparticle monolayer. **R. Tang**, Z. Jiang, Y. Yeh, R. Landis, D. Moyano, V.M. Rotello

8:50 COLL 253. Retaining protein and fluorophore activity attached to graphene oxide. **C. Sun**, K.L. Walker, D. Wakefield, W. Dichtel

9:10 COLL 254. Increasing the stability of semiconductor quantum dots in biological solutions through surface chemistry. **R.P. Brown**, M. Muth, Z. Rosenzweig

9:30 COLL 255. Lasting alteration of compositional membrane asymmetry by LiCoO₂ nanoplates. **F. Geiger**

9:50 Intermission.

10:10 COLL 256. Mimicking complex virus-cell interactions with rationally engineered nanoparticle surfaces. **B.M. Reinhard**

10:30 COLL 257. pH-Responsive framboidal vesicles prepared using polymerization-induced self-assembly via RAFT aqueous dispersion polymerization as virus mimics. **C. Mable**, I. Canton, O.O. Mykhaylyk, P. Chambon, S.P. Armes

10:50 COLL 258. Surface modification to control cell/surface interactions. **S. Ashraf**, W. Parak

11:10 COLL 259. Correlating nanoparticle surface chemistry with antimicrobial activity via NMR techniques. **J. Millstone**

11:30 COLL 260. Modeling of selenium nanoparticle formation and implications on bacterial and cellular responses. **M. Stolzoff**, T. Webster

11:50 COLL 261. Heterogeneous particles to model dynamic cell/surface interactions. **M. Shave**, M.M. Santore

Section C

Boston Convention & Exhibition Center Room 107C

Biochemical Ligands at Interfaces: From Molecular Scale Characterization to Devices

Financially supported by JPK Instruments and NT MDT

G. Liu, T. Ye, *Organizers*

R. Levicky, *Presiding*

8:30 COLL 262. Single molecule resolution of interfacial biomacromolecule dynamics. **D.K. Schwartz**

9:00 COLL 263. Super-resolution imaging of fluorescently-tagged ligands on gold nanoparticle surfaces. **K.A. Willets**, K.L. Blythe

9:30 COLL 264. Nanoscale insight into the impact of heterogeneous probe spatial distribution on surface hybridization. **G.R. Abel**, X. Hao, T. Ye

10:00 Intermission.

- 10:15 COLL 265.** High-resolution, fast-scanning Atomic Force Microscopy for studying dynamic processes. **S. Kaemmer**, H. Haschke, D. Stamov
- 10:45 COLL 266.** Energetic basis for the molecular-scale organization of bone and enamel. **J. Tao**, B.J. Tarasevich, W.J. Shaw, A. Wierzbicki, J.J. De Yoro

Section D

Boston Convention & Exhibition Center Room 108

Basic Research in Colloids, Surfactants & Nanomaterials Particle Systems

R. Nagarajan, *Organizer*

M. C. Buzzeo, *Presiding*

8:30 COLL 267. Withdrawn.

8:50 COLL 268. From phenomenon to formulation: Investigating excipients that enhance the stability of colloidal drug aggregates in biological milieu. **C.K. McLaughlin**, A.N. Ganesh, B. Shoichet, M.S. Shoichet

9:10 COLL 269. Dispersant interactions at oil-water interface: Insights from molecular dynamics simulation. **D. Yu**, A. Savo, M.D. Reichert, A.K. Schultz

9:30 COLL 270. Withdrawn.

9:50 COLL 271. Star diblock copolymer concentration dictates the degree of dispersion of carbon black particles in nonpolar media: Bridging flocculation vs. steric stabilization. **S.P. Armes**, D.J. Growney, O.O. Mykhaylyk

10:10 COLL 272. Molecular Janus particles based on functionalized fullerenes: Precise synthesis and assembly in solution. **Z. Lin**, S.Z. Cheng

10:30 COLL 273. Evolution of polymeric nanoparticles formation during condensation of hydrophobic alkoxysilanes in an organic solvent free sol-gel method. **A.M. Giasuddin**

10:50 COLL 274. Anti-agglomeration Ni@yolk-ZrO₂ structure with sub-10 nm Ni core: Preparation, characterization, and catalysis in steam reforming of methane reaction. **Z. Lim**, H. Yin, K. Choy, C. Wu

11:10 COLL 275. Interface bonding effect between ternary sulfide solid solution and TiO₂NTs composite by solvothermal synthesis. **Z. Yao**, F. Jia, Z. Jiang

11:30 COLL 276. Withdrawn.

Section E

Boston Convention & Exhibition Center Room 109A

Colloid-Polymer Architectures & Mixtures

Ordered Colloidal Architectures & Structures

S. M. Balko, T. Kreer, *Organizers*

C. M. Marques, *Presiding*

8:30 COLL 277. Self organization of oligopeptides: From molecules to fibrils to spheres. **H. Braun**

9:00 COLL 278. Micelle-polyelectrolyte complexation in buffered aqueous solution. **J. Laaser**, Y. Jiang, D. Sprouse, T.M. Reineke, T.P. Lodge

9:20 COLL 279. Polymer brush colloidal particles as building blocks for functional materials. **I. Zharov**

9:40 Intermission.

9:55 COLL 280. Estimation of crystal nucleation barriers in colloid-polymer mixtures. P. Virnau, A. Statt, K. Binder

10:25 COLL 281. Using smart polymers to regulate DNA-mediated nanoparticle assembly, crystal formation, and interparticle spatial properties. M.M. Maye, J. Tinklepaugh, K. Hamner, S. Pun

10:45 COLL 282. Directing the colloidal assembly of patchy spheres by capillary interactions. B. Bharti, D. Rutkowski, A. Kumar, K. Han, C.K. Hall, O.D. Velev

11:05 COLL 283. Membrane mediated assembly of chiral colloidal rafts. Z. Dogic

11:35 COLL 284. Directional self-assembly of polymeric colloids. E.A. Elacqua, X. Zheng, Y. Wang, M. Weck

Section F

Boston Convention & Exhibition Center
Room 109B

Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions

Cosponsored by CATL†

S. A. Morris, J. N. Russell, *Organizers*

C. J. Karwacki, *Organizer, Presiding*

J. R. Morris, *Presiding*

8:30 Introductory Remarks.

8:35 COLL 285. Probing the solid/gas and solid/liquid electrochemical interfaces using in situ/operando ambient pressure X-ray photoelectron spectroscopy. E. Crumlin

9:05 COLL 286. Structural evolution of an intermetallic Pd-Zn catalyst selective for propane dehydrogenation. J.R. Gallagher, D. Childers, H. Zhao, R.E. Winans, R. Meyer, J. Miller

9:35 COLL 287. Alloy catalysis across composition space: Elementary steps in hydrogenation reactions. A.J. Gellman, I. Sen, J. Liu

10:05 Intermission.

10:20 COLL 288. Unraveling the relationship between structure and activity using model catalysts under near-ambient pressures. A. Baber, K. Mudiyansele, S.D. Senanayake, F. Xu, P. Liu, J. Rodriguez, D.J. Stacchiola

10:50 COLL 289. Characterizing a new class of catalysts based on MOF node chemistry. J.T. Hupp

11:15 COLL 290. Ex situ and in situ characterization of plasmonic photocatalysts for solar fuel generation. N. Wu, D. Chu, S. Cushing, J. Li

ACS Scholars: Rising Stars in Academe

Sponsored by PRES, Cosponsored by AGRO, CARB, CMA, COLL, ENFL, ENVR, PROF, SCHB and YCC

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-resolved Spectroscopies

Liquid Environments

Sponsored by PHYS, Cosponsored by COLL

Complex Coacervation: Principles & Applications

Sponsored by AGFD, Cosponsored by COLL†

Memories of Henry Hill: His Legacy in Science and in Professional Service

Sponsored by HIST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES†, PROF and SCHB

True Stories from Entrepreneurs: BRIC Edition

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21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CINP, COLL, ENFL, PROF and SOCED

Protein-nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Applications and Consequences

Sponsored by PHYS, Cosponsored by COLL

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 107A

30 Years of Langmuir: Looking Back & Forward

R. M. Crooks, *Organizer, Presiding*

M. M. Santore, *Presiding*

2:00 COLL 291. Surface plasmon spectroscopy of nano sized metal particles. P. Mulvaney

2:30 COLL 292. Silica coating and other coating shells. L. Liz Marzan

3:00 COLL 293. Metal-organic frameworks for gas separations: Using fundamental experimental studies and molecular modeling to highlight features of interest and optimized material. P.L. Llewellyn, G. Maurin

3:30 Intermission.

3:45 COLL 294. Microgels: Simple matter where complexity matters. W. Richtering

4:15 COLL 295. Zwitter-surfaces and zwitter-solids. J.B. Schlenoff

4:45 COLL 296. Personal views on Langmuir as a reader, author, reviewer, editor, and EIC. F.M. Winnik

Section B

Boston Convention & Exhibition Center
Room 107B

Surface Modification to Control Cell/Surface Interactions

H. Moehwald, *Organizer*

A. M. Peterson, *Organizer, Presiding*

2:00 COLL 297. Impacts of gold nanoparticle charge and ligand type on surface binding and toxicity to gram-negative and gram-positive bacteria. V. Feng, I. Gunsolus, T. Qiu, H. Frew, L. Nyberg, K. Johnson, K. Hurley, A. Vartanian, L.M. Jacob, S.E. Lohse, M.D. Torelli, R.J. Hamers, C.J. Murphy, C.L. Haynes

2:20 COLL 298. Investigation of effects of adsorption and immobilization onto silica nanoparticles on antimicrobial activity of Cecropin P1 and Cecropin P1C. X. Wu, P. Wei, M.J. Wirth, A. Bhunia, X. Zhu, G. Narsimhan

2:40 COLL 299. Chitosan-based polymeric nitric oxides: Preparation, characterization, and antimicrobial effects. R. Tang, Y. Sun

3:00 COLL 300. Surface grafted polymers for microarray platforms and understanding biochemical interactions. C.I. Biggs, M. Gibson

3:20 COLL 301. Sequence-specific peptoids for the molecular design of antifouling brushes and biointerface. K. Lau, P.B. Messersmith, D. Palmer

3:40 Intermission.

4:00 COLL 302. Metal surface nanostructuring to guide cell behaviour. S. Ulasevich, O. Baidukova, E.V. Skorb

4:20 COLL 303. Silk macromolecules with amino acid-poly(ethylene glycol) grafts for controlling LbL encapsulation and aggregation of recombinant bacterial cells. I. Drachuk, R. Geryak, M. Chyashnavichyus, R. Calabrese, S. Harbaugh, N. Kelley-Loughnane, D.L. Kaplan, M.O. Stone, V.V. Tsukruk

4:40 COLL 304. Hydrogen-bonded polymer nanocoatings as mediators of T cell immunity. V.A. Kozlovskaya, L.E. Padgett, H. Tse, E.P. Kharlampieva

5:00 COLL 305. Surface charge density in PEMUs and its influence on cell adhesion. C.J. Arias Ramos, T.C. Keller, J.B. Schlenoff

5:20 COLL 306. Cancer cells/stromal cells co-culture on polyelectrolyte multilayer films: A template for studying cell-cell interaction in tumor progression. A. Daverey, O. Scheideler, K.M. Brown, S. Kidambi

Section C

Boston Convention & Exhibition Center
Room 107C

Biochemical Ligands at Interfaces: From Molecular Scale Characterization to Devices

Financially supported by JPK Instruments and NT MDT

G. Liu, T. Ye, *Organizers*

A. B. Subramaniam, *Presiding*

2:00 COLL 307. Protein structures at device interfaces. C. MacLaughlin, W. Shi, G.C. Walker

2:40 COLL 308. Characterization of protein and binding at model interfaces for optimization of activity. C.L. Berrie, J.K. Tucker, M.L. Richter

3:20 COLL 309. Self-assembly of polypeptides on metal surfaces in vacuum by soft-landing electrospray ion beam deposition. S. Rauschenbach, S. Abb, G. Rinke, L. Harnau, K. Kern

3:45 Intermission.

4:00 COLL 310. Improving in vivo brain neurotransmitter sensors. H. Cao, N. Nakatsuka, H. Yang, P.S. Weiss, A.M. Andrews

4:40 COLL 311. Force-based identification of single DNA bases with polymerase-tethered AFM tip. Y. Kim, Y. Lee, J. Park

Section D

Boston Convention & Exhibition Center
Room 108

Basic Research in Colloids, Surfactants & Nanomaterials

Nanoparticle Assembly

R. Nagarajan, *Organizer*

I. U. Arachchige, *Presiding*

2:00 COLL 312. Dynamic covalent control of nanoparticle properties and self-assembly. E.R. Kay

2:20 COLL 313. 2D Nanocrystals of molecular Janus particles. H. Liu, K. Yue, W. Zhang, S.Z. Cheng

2:40 COLL 314. Small angle scattering of anisotropic nanoparticles and their assemblies. A. Senesi, B. Lee

3:00 COLL 315. Withdrawn.

3:20 COLL 316. Withdrawn.

3:40 COLL 317. Dynamic self-assembly of nanoparticles: Achieving switchable materials. W. Lewandowski, D. Pocięcha, M. Fruhnert, C. Rockstuhl, E. Görecka

4:00 COLL 318. Sol-gel method: An advanced technique to obtain a 3D superstructure of metal-semiconductor hybrid nanoparticles. L. Nahar, I.U. Arachchige

4:20 COLL 319. Charge induced adsorption of string-like particles for omnidirectionally transparent superhydrophobic surface. G. Wu, Y. Zhao, D. Ge, S. Yang

4:40 COLL 320. Ultra-large-area SERS-active monolayers fabricated by assembly of anisotropic Au/Ag core/shell nanoparticles. T. Bai, Z. Guo, N. Gu

5:00 COLL 321. Sol-gel method for the assembly of noble metal nanoparticles into metallic aerogels. X. Gao, I.U. Arachchige

5:20 COLL 322. Porous conducting superstructures of metal colloids: Noble metal aerogels. X. Gao, L. Nahar, I.U. Arachchige

Section E

Boston Convention & Exhibition Center
Room 109A

Colloid-Polymer Architectures & Mixtures

Colloids at Interfaces and in Melts

S. M. Balko, *Organizer*

T. Kreer, *Organizer, Presiding*

2:00 COLL 323. Conformation, effective interactions, and assembly of polymer-coated nanoparticles at liquid interfaces. E. Del Gado, K. Schwenke

2:30 COLL 324. Withdrawn.

2:50 COLL 325. Withdrawn.

3:10 Intermission.

3:25 COLL 326. Motion of a nanoparticle in an unentangled polymer melt – passive and active micro-rheology. A. Kuhnhold, W. Paul

3:55 COLL 327. Floating superhydrophobic assemblies. M. Zhang, A.J. Crosby, T.J. McCarthy

4:15 COLL 328. Structure and dynamics in polymer melts mixed with compact stars. H. Meyer

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Section F

Boston Convention & Exhibition Center
Room 109B

Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions

Cosponsored by CATL†

S. A. Morris, J. N. Russell, *Organizers*

C. J. Karwacki, *Organizer, Presiding*

J. R. Morris, *Presiding*

2:00 COLL 329. Effects of defects and hydroxyl groups on adsorption and photoluminescence of zinc oxide. J.E. Whitten

2:30 COLL 330. AP-XPS and HERFD XAS as complementary operando probes in electrocatalysis AP-XPS and HERFD XAS as complementary operando probes in electrocatalysis. D. Friebe

3:00 COLL 331. In operando tracking of surface electrochemical redox activity in solid oxide electrochemical cells using near infrared radiation imaging. A. Geller, M.B. Pomfret, J. Owrutsky, B.W. Eichhorn

3:30 Intermission.

3:45 COLL 332. Vibrational sum frequency generation spectroscopy for probing the triple junction in heterogeneous catalysis. F. Geiger

4:15 COLL 333. In operando studies of CuO_x and MoO_x model surfaces for application as chemical warfare agent destruction catalysts. L. Trotochaud, A. Head, Y. Yu, O. Karslioglu, M. Hartl, B.W. Eichhorn, H. Bluhm

4:45 COLL 334. In-operando characterization of the structural dynamics of supported heterogeneous catalysts during transformations of C-C and C-H bonds. R.G. Nuzzo

5:15 COLL 335. Monitoring catalytic surface phenomena under reaction conditions and establishing structure-activity/selectivity relationships. I.E. Wachs, A. Chakrabarti, M. Zhu, S. Lwin, C. Keturakis, Y. Tang

ACS Scholars: Rising Stars in Industry

Sponsored by PRES, Cosponsored by AGRO, CARB, CMA†, COLL, ENFL, ENVR, PROF, SCHB and YCC

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-resolved Spectroscopies

Biological Interfaces and Interactions

Sponsored by PHYS, Cosponsored by COLL

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector

Sponsored by SCHB, Cosponsored by CMA, COLL, HIST, I&EC, POLY, PRES and PROF

Complex Coacervation: Principles & Applications

Sponsored by AGFD, Cosponsored by COLL†

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Protein-nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Applications and Consequences

Sponsored by PHYS, Cosponsored by COLL

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

R. Nagarajan, *Organizer*

8:00 - 10:00

92, 94, 98, 101, 103, 106-107, 110-111, 113-114, 116, 119, 121-122, 125-127, 130, 133-135, 137, 143-144, 146-148, 150-152, 155-157, 161, 166, 169-171, 179-180, 182-184, 187-188, 192, 195, 199, 205, 209, 214, 218, 220, 224, 226. See previous listings.

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 107A

Polymer & Biopolymer Based Nanomaterials

Nanomaterials for Drug Delivery

B. P. Chauhan, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL 336. Elevated inhibition effect of self-assembled nanohydrogel of curcumin-hyaluronic acid conjugates on amyloid β -protein aggregation and cytotoxicity. Z. Jiang, X. Dong, Y. Sun

8:55 COLL 337. Intravenously administered nanoparticles halt bleeding and protect the central nervous system after trauma. E.B. Lavik, A. Shoffstall, D. Hickman, M. Lashof-Sullivan, K. Bogle, P. VandeVord

9:15 COLL 338. pH-Responsive intracellular degradable hydrogel cubes for cancer therapy. V.A. Kozlovskaya, B. Xue, J. Chen, E.P. Kharlampieva

9:35 COLL 339. Self-assembled nanoparticles containing cyclodextrins and their application in targeted drug delivery. T. Loftsson

9:55 COLL 340. Cancer vaccine using crosslinked CpG oligonucleotide/ β -glucans nanoparticles. N. Miyamoto, S. Mochizuki, K. Sakurai

10:15 Intermission.

10:30 COLL 341. Silver nanoparticle-embedded polymersome nanocarriers for the treatment of antibiotic-resistant infections. B. Geilich, A. van de Ven, S. Sridhar, T. Webster

10:50 COLL 342. Poly(1,2-glycerol carbonate)-graft-succinic acid-paclitaxel conjugate polymer for tunable nanoparticle delivery of paclitaxel. I. Ekladios, H. Zhang, M.W. Grinstaff

11:10 COLL 343. Structural and micellar stability of nanoscale amphiphilic polymers: implications for atherosclerosis bioactivity. Y. Zhang, Q. Li, Y. Pines, P. Moghe, K.E. Uhrich

11:30 COLL 344. Design of hybrid poly(lactide co glycolic) nanoparticles and in vivo fate studies for the assessment of nanoparticle degradation. S. Moya

11:50 COLL 345. Biodegradable polymer multilayer capsules for delivery of mRNA. M. Kakran, M. Antipina

Section B

Boston Convention & Exhibition Center
Room 107B

Surface Modification to Control Cell/Surface Interactions

H. Moehwald, *Organizer*

A. M. Peterson, *Organizer, Presiding*

8:30 COLL 346. Cell surface engineering for translational medicine: From single cell modification to disease therapeutics. B. Wang

8:50 COLL 347. Investigating the impact of nanoconjugation on EGFR-induced apoptosis. L. Wu, B.M. Reinhard

9:10 COLL 348. Transferrin-modified single walled carbon nanohorns for selective uptake into cancer cells. A. Pekkanen, M.R. DeWitt, T.E. Long, M.N. Rylander

9:30 COLL 349. Differences between the surface properties of emerging aerogel biomaterials and planar substrates: Tuning cell/surface interactions on microporous materials for neuronal scaffolds using organic surface coating strategies. W.A. Alexander, I. Romines, N. van Kampen, F. Sabri

9:50 COLL 350. Impacts of surface modification induced by cold atmospheric plasma (CAP) on human mesenchymal stem cell (hMSC) differentiation. M. Wang, P. Favi, M. Keidar, T. Webster

10:10 Intermission.

10:30 COLL 351. Protein films fabricated via nanoimprint lithography and inkjet printing: A new scaffold for cell patterning. L. Wang, B. Duncan, E. Jeoung, R. Tang, B. Creran, K. Saha, Y. Yeh, C. Subramani, T. Kushida, Y. Engel, V.M. Rotello

10:50 COLL 352. Print surfaces with desired cell adhesion properties. Z. Zhao, X. He

11:10 COLL 353. Development of hyaluronic acid hydrogels for human neural stem cell engineering. W. Ma, G. Jin, W.H. Suh

11:30 COLL 354. Macromolecule solvent density distribution can be reconstructed from heteroatoms proximal radial distribution functions. B. Nguyen, B.M. Pettitt

Section C

Boston Convention & Exhibition Center
Room 107C

Experimental & Computational Approaches to Reactions at the Surface of Colloidal Nano Materials, Facilitated by Photo Excitation & Charge Transfer

R. Nagarajan, *Organizer*

S. Linic, *Presiding*

8:30 COLL 355. Enhancing supercapacitor energy-storage materials with sustainable, Earth-abundant metals via nanoplates and molecular spacers. J. Mitchell, D. Banks, C. McNeill, I. Shcherbakov, J.C. Poler

8:55 COLL 356. Probing the mechanistic of charge transfer from optically excited plasmonic metal nanoparticles and adsorbates leading to chemical transformations. S. Linic

9:20 COLL 357. Single molecule dynamics of a new class of altitudinal molecular rotors. N.A. Wasio, C.J. Murphy, M. Marcinkowski, M.L. Liriano, E.H. Sykes

9:45 COLL 358. Influence of metal vacancy of undoped anatase TiO₂ on p-type conductivity, room-temperature ferromagnetism, and remarkable photocatalytic performance. S. Wang, L. Pan, J. Zou, L. Wang, X. Zhang

10:10 COLL 359. Calculated photoinduced interfacial electron transfer of Fe(II) light harvesters on TiO₂ nanocrystals. L.A. Fredin, P. Persson

10:35 COLL 360. Photocatalytic CO₂ reduction under periodic illumination of ZnS colloids. M.I. Guzman, R. Zhou

11:00 COLL 361. Controlling surface deposition of gold nanoparticles for the fabrication of highly porous silicon membranes via metal-assisted chemical etching. B.D. Smith, D. Zhitomirsky, J.C. Grossman

11:25 COLL 362. Corona phase molecular recognition of fibrinogen. G. Bisker, H.D. Park, N. Iverson, J. Ahn, J.T. Nelson, M. Landry, S. Kruss, M. Strano

Section D

Boston Convention & Exhibition Center
Room 108

Basic Research in Colloids, Surfactants & Nanomaterials

Bio-Nano Interactions

R. Nagarajan, *Organizer*

R. A. Gross, *Presiding*

8:30 COLL 363. Adhesion of cerium oxide nanoparticles on supported lipid bilayers: Implications for nanoparticle-membrane interactions. P. Yi, W. Gu, K. Chen

8:50 COLL 364. Chemo-enzymatic routes to lipopeptides and their colloidal properties. R.A. Gross

9:10 COLL 365. Preparation of long (~7.2kb) DNA origami scaffold using PCR and lambda exonuclease digestion. W. Patterson, M. Rahman, H. Sizek, P. Sizek, H. Zhong, M.L. Norton

9:30 COLL 366. Design and synthesis of synthetic antibodies, *CoPhMoRe* and the *inverse CoPhMoRe* problem for helically wrapping polymers on single-wall carbon nanotubes. J. Ahn, G. Bisker, S. Kruss, Z. Ulissi, M. Strano

9:50 COLL 367. Nanopore entry of proteins and macromolecules. K. Lau, A.M. Sousa, T.D. Lazzara

10:10 COLL 368. New stimuli responsive lipid nanotube for protein transport and release: From molecular design to application. H. Unsal, N. Aydogan

10:30 COLL 369. Fibrinogen adsorption and relaxation kinetics and silica particle capture on graphene-modified glass. A. Chen, M.M. Santore

10:50 COLL 370. Multimodal nanobiocatalysis: Toward the synthesis of pharmaceutically relevant enantiopure drugs and drug intermediates. U.C. Banerjee, J. Bhamik, B. Dwivedee, J. Laha

11:10 COLL 371. Interaction of graphene oxide with bacterial cell membranes: Insights from AFM-based force spectroscopy. S. Romero-Vargas Castrillon, F. Perreault, A.F. de Faria, M. Elimelech

11:30 COLL 372. Noncovalent approach for developing hybrid mesoporous silica nanoparticle-peptide amphiphile system. M. Sardan, A. Yildirim, D. Mumcuoglu, A.B. Tekinay, M.O. Guler

11:50 COLL 373. Nanotribology of a catechol-functionalized alkane with terminal chain branching. M. Ruths, K. Persson

Section E

Boston Convention & Exhibition Center
Room 109A

Colloid-Polymer Architectures & Mixtures

Synthesis of Nanoparticles and Their Assemblies

T. Kreer, *Organizer*

S. M. Balko, *Organizer, Presiding*

8:30 COLL 374. Chiroplasmonic nanoparticles and their assemblies. J. Yeom, W. Ma, B. Yeom, L. Xu, W. Feng, C. Xu, N. Kotov

9:00 COLL 375. Nanoparticle synthesis, surface modification, and colloidal dispersion facilitated by polymer amphiphiles. P. Alexandridis

9:20 COLL 376. Click assembly of nanoparticles into colloidal polymers. W. Zheng, K. Haner, H. Liang

9:40 Intermission.

9:55 COLL 377. Polymer-induced lipid cluster formation: Effects of charge density, curvature, lipid composition and polymer concentration. C. Yu, H. Jiang, Y. Xia, N. Tennakoon, Y. Liu, M. Nieh

10:15 COLL 378. Synthesis and characterization of the structure and activity of gold nanoparticles when coated with poly (oxonorborene)-based synthetic mimics of antimicrobial peptides (SMAMPs). Z. Zheng, D. Boschert, K. Lienkamp, Z. Rosenzweig

10:35 COLL 379. Synthesis of nanobowls with a Janus template. A. Mo, P. Landon, C. Emerson, C. Zhang, P. Anzenberg, S. Akkiraj, R. Lal

10:55 COLL 380. Synthesis and investigation of thermoresponsive core shell nanoparticles. S. Kurzhals, R. Zirbs, T. Grünewald, H. Lichtenegger, E. Reimhult

Section F

Boston Convention & Exhibition Center
Room 109B

Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions

Cosponsored by CATL†

C. J. Karwacki, J. R. Morris, J. N. Russell, *Organizers, Presiding*

8:30 COLL 381. In-situ investigations of the interaction of small molecules with Fe²⁺-substituted MOF-5. M. Dinca, C. Brozek, S.A. Stojan

9:00 COLL 382. Core-shell nanoparticles: In situ surface monitoring by Synchrotron X-ray spectroscopy. S. Carenco, C. Wu, M. Salmeron

9:30 COLL 383. Probing cooperative phenomena in nanoscale metal catalysts by operando techniques. A. Frenkel

10:00 Intermission.

10:30 COLL 384. Structure of carbon supported bimetallic Pt-M catalysts during aqueous phase reforming of biomass derived oxygenates. A.M. Karim, Z. Wei, D.G. Vlachos, Y. Wang

11:00 COLL 385. Isolation of reactive chemical species in heme-containing metal-organic frameworks. J.S. Anderson, A. Gallagher, M. Kelly, J. Park, H. Phan, D. Harris

11:30 COLL 386. Multifunctional chemical sensors designed on 2D nanomaterials for detection and degradation of low-level contaminants. P.V. Kamat, R. Alam

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-resolved Spectroscopies

Photophysical Dynamics of Biological and Biomimetic Systems

Sponsored by PHYS, Cosponsored by COLL

Complex Coacervation: Principles & Applications

Sponsored by AGFD, Cosponsored by COLL†

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

Transforming University-Industry Partnerships for an Innovative Future

Envisioning, Enabling and Executing

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

Protein-nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Methods and Tools for Characterization

Sponsored by PHYS, Cosponsored by COLL

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 107B/C

Langmuir Lectures, NanoLetters Award Lecture, ACS Materials & Interfaces Award Lecture

R. Nagarajan, *Organizer*

R. J. Hamers, *Presiding*

2:00 Introduction of Professor Catherine Murphy.

2:05 COLL 387. Golden age of colloids and surfaces. C.J. Murphy

2:50 Introduction of Professor Buddy Ratner.

2:55 COLL 388. Biointerfaces: Beginnings, state-of-the-art, and horizons. B.D. Ratner

3:40 Introduction of Professor Xiaolin Zheng.

3:45 COLL 389. Bridging combustion and nanotechnology. X. Zheng

4:30 Introduction of Professor Alejandro L. Briseno.

4:35 COLL 390. Crystal chemistry at the molecule-substrate and molecule-molecule interface in organic electronic systems. A.L. Briseno

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

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Transforming University-Industry Partnerships for an Innovative Future

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Complex Coacervation: Principles & Applications

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WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 107A

Polymer & Biopolymer Based Nanomaterials

Biopolymer Based Nanomaterials

B. P. Chauhan, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL 391. Electrostatically assembled protein-polymer nanoparticles for cartilage repair. N. Shah, B. Geiger, M.A. Quadir, A. Goel Bajpayee, A.J. Grodzinsky, P.T. Hammond

9:15 COLL 392. Exploring the synthesis, structure, and biological activity of concatenated siRNA polymers. K. Shopsowitz, C. Wu, S. Morton, E. Dreaden, P.T. Hammond

9:35 Intermission.

9:50 COLL 393. Application of polysaccharide-based stabilizers in batch and microfluidic emulsification for preparing polylactide particles with drug delivery applications. A. Chebil, M. Leonard, C. Nouvel, J. Six, A. Durand

10:10 COLL 394. Photocrosslinked polymersomes as responsive and multifunctional synthetic bioanoreactors. B. Voit, D. Appelhans, J. Gaitzsch, D. Gräfe, M. Yassin, B. Ilysan

10:30 COLL 395. Nanocapillary binding of particles: A generic approach for assembling reconfigurable structures at nanoscale. B. Bharti, J. Meissner, A. Fameau, M. Rubinstein, G.H. Findenegg, O.D. Velev

10:50 COLL 396. Repeat-protein hierarchical self-assembly results in hierarchical and anisotropic mechanical properties. T. Zarkovic Grove, N. Carter

Section B

Boston Convention & Exhibition Center
Room 107B

Nanomaterials for Defense & Homeland Security Applications

R. Nagarajan, *Organizer*

E. Wilusz, *Presiding*

8:30 COLL 397. Development of agent-detecting nanofiber sensors for garments. L. Han, E. Wilusz, D. Ensor

9:00 COLL 398. Hybrid graphene oxide for trace level identification of explosives selectively using Raman fingerprint. P.C. Ray

9:30 COLL 399. Sensing, decontamination, and filtration by the multifunctional zirconium hydroxide. G.W. Peterson

10:00 COLL 400. Novel nanostructured colorimetric sensor for the detection of explosives. R. Anandakathir, M.J. Sobkowicz, B.M. Budhall

10:30 COLL 401. Detection of biological threats using gold nanoparticles in lateral flow immunoassays: Dengue hemorrhagic fever. H. de Puig Guixé, J. Tam, C. Yen, K. Hamad-Schifferli, L. Gehrke

11:00 COLL 402. Multicolored silver nanoparticles for multiplexed disease diagnostics: Distinguishing dengue, Yellow Fever, and Ebola viruses. C. Yen, H. de Puig Guixé, J.O. Tam, J. Gómez-Márquez, I. Bosch, K. Hamad-Schifferli, L. Gehrke

11:30 COLL 403. Sensing and imaging with isotropic and anisotropic metallic nanostructures. S. Hunyadi Murph

Section C

Boston Convention & Exhibition Center
Room 107C

Nanotheranostics for Cancer Applications

S. A. Morris, P. Rai, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COLL 404. Self-assembled peptide amphiphile nanoparticles for rational combination therapies against metastatic solid tumors. E.C. Dreaden, Y. Kong, M.B. Yaffe, P.T. Hammond

8:55 COLL 405. Functionalization of single walled carbon nanohorns for simultaneous fluorescence imaging and cisplatin delivery. A. Pekkanen, M.R. DeWitt, J. Sirrine, T.E. Long, M.N. Rylander

9:15 COLL 406. Etchable plasmonic and quantum dot probes to image and quantify cellular internalization in vivo. G.B. Braun, T. Friman, H. Pang, A. Pallaoro, T. Teesalu, E. Rtuoslahti

9:35 COLL 407. Rapid and quantitative multiplexed nanoparticle platform for the identification by surface-enhanced Raman spectroscopy of cells at low concentrations flowing in a microfluidic channel. A. Pallaoro, M.R. Hoonejani, G.B. Braun, C.D. Meinhardt, M. Moskovits

9:55 COLL 408. Nanoscience approach to the synthesis of novel radionuclide substrates. E.H. Sykes, A. Pronschinske

10:15 Intermission.

10:30 COLL 409. Stimuli-responsive reagents for improved cell isolations. B. Nehilla, M. Manganiello, S. Hussell, R. Salmon, R. Myers

10:50 COLL 410. Theranostic graphene quantum dots decorated magnetic nanoparticle for selective capture and two photon imaging of rare tumor cells in second biological window. P.C. Ray

11:10 COLL 411. Engineering remotely triggered liposomes to target triple-negative breast cancer. A. Sneider, F. Ekiz Kanik, C. Tsiros, P. Rai

11:30 COLL 412. Next generation magnetic lipid nanohybrids for theranostics. S. Biswas, J.A. Kulkarni, Y.Y. Tam, S. Chem, Y.K. Tam, P.R. Cullis

11:50 COLL 413. Enzyme-instructed self-assembly (EISA) for potential cancer therapy. X. Du, J. Zhou, B. Xu

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Section D

Boston Convention & Exhibition Center
Room 108

**Basic Research in Colloids,
Surfactants & Nanomaterials**
**Advanced Techniques
Probing Nanomaterials**

R. Nagarajan, *Organizer*

T. Guo, *Presiding*

8:30 COLL 414. EELS imaging analysis of silicon cluster superlattices. Y. Iwata, T. Uchida, N. Orita, H. Matsuhata

8:50 COLL 415. Advances in nanomaterial analysis using laboratory X-ray diffraction equipment. J.E. Quinn, J. Bolze

9:10 COLL 416. Fluorescence lifetime spectroscopy: A new addition to the toolkit used to monitor the formation and degradation of semiconductor quantum dots in solution. T. Curry, Z. Rosenzweig

9:30 COLL 417. Study nanomaterials using synchrotron X-ray scattering for structures and kinetics. X. Zuo, Y. Sun, V.P. Conicello

9:50 COLL 418. Latest developments in X-ray nanochemistry. T. Guo

10:10 COLL 419. Super-resolution imaging and spectroscopy of Au₂₅ nanoclusters using two-photon excited fluorescence near-field scanning optical microscopy. N. Abeyasinghe, S. Kumar, R. Ho Wu, R. Jin, T.G. Goodson

10:30 COLL 420. Withdrawn.

10:50 COLL 421. Investigating lipid corona formation onto nanoparticle surfaces through fluorescence correlation spectroscopy. L.M. Jacob, M.D. Torelli, A. Vartanian, E. Melby, T.F. Kuech, J. Troiano, L.L. Olenick, C.J. Murphy, R.J. Hamers, J.A. Pedersen, F. Geiger

11:10 COLL 422. Stable ferromagnetic nanoparticle dispersions: Surface modification of graphene coated nanomagnets allow stable dispersions of functionalizable ferromagnetic nanoparticles. C. Hofer, V. Zlateski, E.M. Schneider, R.N. Grass, M. Zeltner, W.J. Stark

11:30 COLL 423. Substrate-induced broken degeneration of plasmonic nanoparticles: Dependence on wavelength and polarization. V. Pini, P.M. Kosaka, J. Ruz, M. Encinar, D. Ramos, O. Malvar, J. Tamayo, M. Calleja

Section E

Boston Convention & Exhibition Center
Room 109A

**Metrology of Characterization,
Simulation & Theory of Biomembranes**

J. Katsaras, *Organizer*

M. Nieh, *Organizer, Presiding*

M. Dutt, *Presiding*

8:30 Introductory Remarks.

8:35 COLL 424. ³¹P CODEX NMR and phospholipid lateral diffusion in membranes. P.M. Macdonald, Q. Saleem, A. Lai

Technical program information
known at press time.

The official technical program
for the 250th ACS National
Meeting is available at:
www.acs.org/boston2015

9:05 COLL 425. Exploring the interactions of ions with fluid lipid bilayers. P.S. Cremer

9:35 COLL 426. Droplet interface bilayer: A model for biomembrane water permeability studies. S. Lee

10:05 Intermission.

10:15 COLL 427. Molecular dynamics study of pore formation by melittin in 1,2-Dioleoyl-sn-glycero-3-phosphocholine (DOPC) and 1,2-di-(9Z-octadecenoyle)-sn-glycero-3-phospho-(1'-rac-glycerol) (DOPG) mixed lipid bilayer. Y. Lyu, X. Zhu, N. Xiang, G. Narsimhan

10:45 COLL 428. Gold nanoparticle – lipid nanodisk self-assembly: Insights from computer modeling. E. Dormidontova, Z. Wang, H. Sharma

11:15 COLL 429. Novel scattering methods reveal structure of single supported lipid membranes. T. Kuhl, E. Watkins, J. Kurniawan, J. Majewski

Big Chemistry from Small Businesses

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**Structure & Dynamics in Complex
Chemical Systems: Gaining New
Insights through Recent Advances
in Time-resolved Spectroscopies**
**Structure, Dynamics, and
Behaviors of Material Systems**

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**Protein-nanomaterial Interfaces &
Protein Coronas: Physical Properties,
Biocompatibility, & Biological Impact**
Applications and Consequences

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WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 107A

**Polymer & Biopolymer
Based Nanomaterials**

B. P. Chauhan, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 COLL 430. Cyclic cyclosiloxane bound silver nanospheres. B.P. Chauhan, S. Chaudhry, A. Patel

2:25 COLL 431. Modulation of biomineral crystal growth and assembly by polymeric matrices. G. Mallam, M. Tsianou

2:45 COLL 432. Hyaluronic acid-based hydrogels with network-disruptive dangling ligands for the assembly of acinar spheroids. E.W. Fowler, T. Ozdemir, S. Pradhan-Bhatt, D. Harrington, R. Witt, M.C. Farach-Carson, X. Jia

3:05 COLL 433. Transglutaminase catalyzed PEGylation of alginate microgels for islet cell encapsulation. C.D. White, M. Pelletier, A.L. Garle, P. Gaines, B.M. Budhll

3:25 Intermission.

3:40 COLL 434. Copolymer nanoparticles via RAFT emulsion polymerization: Synthesis, characterization, and interfacial activity. V. Cunningham, A. Alswieleh, K.L. Thompson, M. Williams, G.J. Leggett, O.M. Musa, S.P. Armes

4:00 COLL 435. Light sensitive smart nanocontainer. Z. Chen, N. Li, A. Schlimme, J. Gassensmith

4:20 COLL 436. Encapsulation of upconversion materials by heterophase methods. K. Katta, D. Busko, R. Munoz-Espi, S. Balushev, K. Landfester

4:40 COLL 437. Chymotrypsin immobilized onto surface functionalized macro and nanoscale Nylon 6,6 solid supports. D.E. Wong, K. Senecal, J.M. Goddard

Section B

Boston Convention & Exhibition Center
Room 107B

**Nanomaterials for Defense &
Homeland Security Applications**

R. Nagarajan, *Organizer*

K. M. McCoy, *Presiding*

2:00 COLL 438. Seeding metal-organic frameworks on Nycoc fabric using atomic layer deposition: Opportunities for soldier uniforms with integrated chemical hazard mitigation. C.J. Oldham, J. Zhao, P.C. Lemaire, P.S. Williams, H.J. Walls, G.W. Peterson, G.N. Parsons

2:30 COLL 439. Water-soluble polyelectrolyte complexes as safe flame retardant nanocoating for woven fabric. J.C. Grunlan, M.M. Halle, A.B. Morgan, M. Leistner

3:00 COLL 440. Computationally aided design of self-decontaminating multicalyst polyelectrolyte membranes (MC-PEM). J. Landers, J. Colon, K. Zong, A. Vishnyakov, A.V. Neimark

3:30 COLL 441. Autonomous, adaptive, responsive, and modular second skin based on organohydrogels. E. Wilusz, R. Nagarajan, P. D'Angelo, M.E. Helgeson, B.D. Olsen, T. Hatton, L. Bromberg, J. Owens, D.J. McGarvey, W. Creasy

4:00 COLL 442. Water-based flame retardant multilayer nanocoating for polyester-cotton. M. Leistner, A.A. Abu-Odeh, S.C. Rohmer, J.C. Grunlan

4:30 COLL 443. Photocatalytic and gas sensor properties of metal oxide-decorated polypropylene swatches. I. Unlu, E.A. Welsh, R. Pang, J.W. Soares, D.M. Steeves, S.K. Sengupta, J.E. Whitten

Section C

Boston Convention & Exhibition Center
Room 107C

**Nanotheranostics for
Cancer Applications**

S. A. Morris, P. Rai, *Organizers, Presiding*

2:00 Introductory Remarks.

2:05 COLL 444. Delivery of chemically modified proteins to the nucleus of cells. R. Tang, M. Ray, Y. Jiang, Z. Jiang, V.M. Rotello

2:25 COLL 445. How nanoparticle design affects targeting selectivity: Insights from computer modeling. E. Dormidontova, S. Wang

2:45 COLL 446. DNA-conjugated silicon nanoparticles for the detection of MicroRNA-21. X. Su

3:05 COLL 447. Role of nanogold apoE reconstituted vehicles (NERVs) as potential drug delivery systems. S. Chuang, Y. Shon, V. Narayanaswami

3:25 COLL 448. Magnetization relaxation of magnetic nanoparticles for hyperthermia in live cells: Non-invasive monitoring. D. Soukup, S. Moise, E. Cespedes, J. Dobson, N. Telling

3:45 Intermission.

4:00 COLL 449. Boron- and gadolinium-rich nanoparticles for cancer treatment using neutron capture therapy. I. Zharov

4:20 COLL 450. Smart surfaces for distinguishing epithelial cells and lymphocytes in laminar flow. S. Kalasin, M.M. Santore

4:40 COLL 451. Synthesis of biocompatible thermoresponsive PEGMA nanoparticles for dual release. E. Yavuz, M. Ulasan, H. Cavusoglu, Y. Cengeloglu, M. Yavuz

5:00 COLL 452. Zwitterionic bio-interface: From cell membrane to protein mimic. J. Ji

5:20 COLL 453. Direct cytosolic delivery of siRNA using nanoparticle-stabilized nanocapsules. Y. Jiang, R. Tang, B. Duncan, Z. Jiang, B. Yan, R. Mout, V.M. Rotello

Section D

Boston Convention & Exhibition Center
Room 108

**Basic Research in Colloids,
Surfactants & Nanomaterials**
Applications to Nanomedicine

R. Nagarajan, *Organizer*

J. L. Liu, *Presiding*

2:00 COLL 454. Pulsed magnetic field induced fast drug release from magnetoliposomes via ultrasound generation. G. Podaru, R. Dani, H. Wang, M.T. Basel, P. Prakash, S.H. Bossmann, V. Chikan

2:20 COLL 455. Multifunctional drug carriers with programmable properties. S. Rahmani, S. Saha, H. Durmaz, A. Misra, A. Dishman, J. Lahann

2:40 COLL 456. Multichannel nanosensor for instantaneous readout of cancer drug mechanisms. N. Le, S. Rana, R. Mout, K. Saha, G. Tonga, C. Rotello, V.M. Rotello

3:00 COLL 457. Structural and biological characterization of Fe₃O₄-loaded spherical and tubular liposomes for magnetic drug targeting. M. Sakuragi, K. Taguchi, K. Sakurai, K. Kusakabe

3:20 COLL 458. Natural product functionalized nanomaterials applied in cancer therapeutics. E. Hernandez, P. Hanumandla, S. Bashir, J.L. Liu

3:40 COLL 459. Controlled cross-linking of nano- and micromaterials for biomedical applications. K. Rashwan, G. Sereda, D. Engebretson, G. Bertsch, E. Brakke, A. Fritza, S. Schwabe

4:00 COLL 460. Gold nanorods indirectly promote migration of metastatic human breast cancer cells in 3D cultures. E. Grzincic, C.J. Murphy

4:20 COLL 461. Quantitative detection of rapid nuclear protein trafficking using nanoparticle stabilized capsules. M. Ray, Z. Jiang, R. Tang, V.M. Rotello

4:40 COLL 462. Design of molecular gelator – solvent systems guided by solubility parameters. Y. Lan, M.A. Rogers, M. Corradini

Section E

Boston Convention & Exhibition Center
Room 109A

**Metrology of Characterization,
Simulation & Theory of Biomembranes**

J. Katsaras, M. Nieh, *Organizers*

P. S. Cremer, E. Dormidontova, *Presiding*

2:00 COLL 463. Quantifying tension effects on phase transitions and domain features in phospholipid membranes. M.M. Santore

2:30 COLL 464. Effect of membrane composition and protein lipidation on the free energy of binding of HIV-1 matrix to lipid membranes. M. Barros, F. Heinrich, S.A. Datta, A. Rein, M. Lösche, H. Nanda

3:00 COLL **465.** Monitoring the formation of Gram-positive bacterial membrane mimics using QCM-D. **K. Wang,** R. Nagarajan, T.A. Camesano

3:30 COLL **466.** Association of model neurotransmitters with lipid bilayer membranes. **B. Josey,** M. Lösche, F. Heinrich, R. Cantor

4:00 Intermission.

4:10 COLL **467.** Scattering and simulation studies identify molecular control mechanisms in cell signaling. **M. Lösche,** F. Heinrich, H. Nanda, A. Ross, A. Gericke, R. Harishchandra

4:40 COLL **468.** Modeling interactions between charged nanoparticles and multicomponent vesicles. **F. Aydin,** M. Dutt

5:10 COLL **469.** Direct probes of supported lipid bilayers interacting with 4-nm diameter gold nanoparticles. **F. Geiger**

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-resolved Spectroscopies

New Techniques

Sponsored by *PHYS*, Cosponsored by *COLL*

Protein-nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Applications and Consequences

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THURSDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 107A

Polymer & Biopolymer Based Nanomaterials

Characterization of Nanomaterials

B. P. Chauhan, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL **470.** Interphase effects on polymer and water dynamics in cellulose biocomposites — ²H and ¹³C NMR relaxometry. **C. Terenzi,** K. Prakobna, I. Furó, L. Berglund

8:55 COLL **471.** Quantitative tissue spectroscopy of near infrared fluorescent nanosensor implants. **G. Bisker,** N. Iverson, E. Farias, V. Ivanov, J. Ahn, G.N. Wogan, M. Strano

9:15 COLL **472.** Facile assembly enhanced spontaneous fluorescent response of Ag⁺ containing polyelectrolyte multilayer films. **X. Huang,** N. Zacharia

9:35 COLL **473.** Characterizing polymeric micelles employed for DDS by use of SAXS and FFF. **K. Sakurai,** Y. Sanada, I. Akiba, K. Shiraiishi, M. Yokoyama, Y. Shinohara, Y. Amemiya

9:55 Intermission.

10:10 COLL **474.** Controlling nanocomposite hydrogel mechanics via bioinspired interfacial bond dynamics. **N. Holten-Andersen,** Q. Li

10:30 COLL **475.** Micromechanical properties of nanostructured soft silicon hydrogel contact lenses. **M. Chyasnachyus,** S.L. Young, V.V. Tsukruk

10:50 COLL **476.** Nanostructured functional thin films through vapor phase deposition: A BIMREL's approach to bioinspiration. **G. Demirel**

11:10 COLL **477.** Design of multistimuli responsive films through LBL assembly for the control of protein adsorption. **A. Oस्पova,** C. Pradier, C. Jérôme, J. Landoulsi, S. Demoustier-Champagne

Section B

Boston Convention & Exhibition Center
Room 107B

Nanomaterials for Defense & Homeland Security Applications

R. Nagarajan, *Organizer*

K. M. McCoy, *Presiding*

8:00 COLL **478.** Remote giant multispectral plasmonic shifts of labile hinged nanorod array via magnetic field. **R. Geryak,** J. Geldmeier, V.V. Tsukruk

8:30 COLL **479.** Transparent superhydrophobic surfaces with enhanced mechanical abrasion resistance enabled by mesh structure. **S. Shiratori,** N. Yokoi, M. Tenjimbayashi, K. Manabe

9:00 COLL **480.** Lanthanide doped silica nanospheres: Surface sampling in deposition studies. **E.M. Durke,** A. Jenkins, W.O. Gordon

9:30 COLL **481.** Facile synthesis and surface modification of HfO₂ nanoparticles for nanocomposite γ -ray scintillators. **C. Liu,** T. Hajagos, D. Kishpaugh, Y. Jin, W. Hu, Q. Chen, Q. Pei

10:00 COLL **482.** Hydrophobic mesoporous silica discoids for effective sorption of oil substances. **I. Sokolov,** S. Palantavida

10:30 COLL **483.** Ultrabright fluorescent silica particles for multiplexing security tagging and labeling. **I. Sokolov,** S. Palantavida

11:00 COLL **484.** Self-assembly of quantum rods into controlled alignments using DNA origami and their use as energy acceptors in bioluminescence resonance energy transfer. **M.M. Maye,** T.L. Doane, L.M. Karam, Y. Chen

Section C

Boston Convention & Exhibition Center
Room 107C

Nanoparticles in Food, Agricultural, & Environmental Settings

Cosponsored by *AGFD*

C. M. Sabliov, *Organizer*

D. Britt, C. Dimkpa, J. M. Goddard, *Organizers, Presiding*

8:30 COLL **485.** Effect of capping agent on the interactions of zinc sulfide nanocrystals with a model environmental surface. **A.L. Marsh,** M.P. Schmidt

8:50 COLL **486.** Direct views of the nano-bio interface. **F. Geiger**

9:10 COLL **487.** Influence of a combined lecithin and Pluronic F127 surfactant on stability of lutein-loaded zein nanoparticles as a function of time and temperature. **T. Chuachareon**

9:30 COLL **488.** Effect of humic acid and fulvic acid on the aggregation and stability of TiO₂ nanoparticles. **M. Luo,** M. Zhu, J. Ren, Y. Tang, H. Duan, H. Wang

9:50 Intermission.

10:10 COLL **489.** Enhanced NOM removal from drinking water sources using stable dispersions of poly(vinylbenzyl trimethylammonium chloride) functionalized SWCNTs synthesized under ARGET-ATRP conditions: "Nano-resins" for water purification. **B.R. Johnson,** T.B. Eldred, J.C. Poler

10:30 COLL **490.** Stabilization of lipase (CaLb) through hierarchical interfacial assembly and performance in deep eutectic solvents. **S.M. Andler,** L. Wang, J. Talbert, B. Duncan, Y. Jeong, V.M. Rotello, J.M. Goddard

10:50 COLL **491.** Evidence for the use of nanoparticles for improving crop productivity. **C. Dimkpa,** P. Bindraban

Section D

Boston Convention & Exhibition Center
Room 108

Basic Research in Colloids, Surfactants & Nanomaterials

Optical Properties and Applications

R. Nagarajan, *Organizer*

A. Almutairi, *Presiding*

8:30 COLL **492.** Light management using nanophotonic organic materials. **R. Chandrasekar**

8:50 COLL **493.** Quarter-wave antireflective coatings produced through random packing of silicated cellulose nanocrystals. **P. Buskens,** N. Meulendijks, R. van Ee, M. Burghoorn, E. van Veldhoven, M. Mourad

9:10 COLL **494.** Optical gain engineering in colloidal quantum dot solids toward continuous wave lasing. **F. Fan,** M. Adachi, S. Hoogland, O. Voznyy, E. Sargent

9:30 COLL **495.** Effects of V doping and MCM-41 loading strategies on the fabrication of Ti³⁺-TiO₂ quantum dots and its photocatalytic applications. **L. Pan,** S. Wang, Z. Huang, J. Zou, X. Zhang

9:50 COLL **496.** Iron chalcogenide nanocolloids for spray-printed solar cells. **D.R. Radu**

10:10 COLL **497.** Sol-gel chemistry of self-assembled photonic crystals. **K. Phillips,** G. England, N. Vogel, J. Aizenberg

10:30 COLL **498.** Photocatalytic reduction of fumarate to succinate on ZnS mineral surfaces. **R. Zhou,** M.I. Guzman

10:50 COLL **499.** Enhanced photoreduction of nitro-aromatic compounds by hydrated electrons derived from indole on natural montmorillonite. **C. Gu**

11:10 COLL **500.** Enhanced multiwavelength upconversion through excitation energy trapping in NaErF₄ core-shell nanocrystals. **N. Johnson,** S. He, A. Almutairi

11:30 COLL **501.** Efficient tailoring of upconversion selectivity by engineering local structure of lanthanide nanocrystals. **L. Sun,** H. Dong, C. Yan

11:50 COLL **502.** Lighting-up carbon nanotubes with asymmetric cyanine dyes. **O. Cavuslar,** H. Unal

Section E

Boston Convention & Exhibition Center
Room 109A

Basic Research in Colloids, Surfactants & Nanomaterials

Surface Science

R. Nagarajan, *Organizer*

E. A. Jarvis, *Presiding*

8:30 COLL **503.** Investigation of the stability of silver halide films on the atomic scale. **J. Phillips,** A. Lee, H. Morgan, L. Jackson, E.V. Iski

8:50 COLL **504.** Oxygen deficient surfaces in metal oxide nanopowders. **E.A. Jarvis,** T. Whyte

9:10 COLL **505.** Semiconducting group IV quantum dots for tunable bandgaps. **R.J. Esteves,** I.U. Arachchige

9:30 COLL **506.** Surface chemistry of metal oxide nanoparticles. **M.C. Foster**

9:50 COLL **507.** Structural evolution in Ag-Ag₂S hybrid nanoprisms during sulfidation. **M.M. Shahjamali,** N. Zareae, N. Large, G.C. Schatz, C.A. Mirkin

10:10 COLL **508.** Withdrawn.

10:30 COLL **509.** Solvent effect on CO₂ electrochemical reduction on Pb(211) and Sn(112). **C. Cui,** H. Wang, X. Zhu, J. Han, Q. Ge

10:50 COLL **510.** Interfacial hydrogen bonding of substituted benzene derivatives on silica: The effects of electron withdrawing and donating groups. **J. Abelard,** A.R. Wilmsmeyer, A.C. Edwards, W.O. Gordon, E.M. Durke, C.J. Karwacki, D. Troya, J.R. Morris

11:10 COLL **511.** Effect of metal ions on the swelling performance of the hydrogel in enhancing salt resistance. **J. Pu,** B. Bai, T.P. Schuman

11:30 COLL **512.** On the intrinsic wettability of graphite. **H. Liu,** Z. Li

11:50 COLL **513.** Charge transfer effect of bimetallic nanostructures: Tuning SERS. **A. Chatterjee,** L. Whelan, E. Merschrod

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-resolved Spectroscopies

Structure, Dynamics, and Behaviors of Material Systems

Sponsored by *PHYS*, Cosponsored by *COLL*

Protein-nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Fundamentals and Applications

Sponsored by *PHYS*, Cosponsored by *COLL*

THURSDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 107A

Polymer & Biopolymer Based Nanomaterials

Design of Nanomaterials

B. P. Chauhan, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 COLL **514.** TMV-dendrimer bottle-brush conjugates. **M. Dharmarwardana,** S. Li, J. Gassensmith

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- 2:25 COLL 515.** Diblock copolymer worm-gels for cellular immobilization and storage. **N. Warren**, I. Canton, H.D. Moore, S.P. Armes
- 2:45 COLL 516.** Sugar-based surfactants utilizing low molecular weight, *atactic* poly(α -olefins) as tunable hydrophobic groups. **T.S. Thomas**, W. Hwang, L.R. Sita
- 3:05 COLL 517.** PEG decorated core-shell pNIPAm hierarchical microgels via host-guest interactions. **I. Antoniuik**, D. Kaczmarek, C. Amiel, I. Varga
- 3:25 Concluding Remarks.**

Section B

Boston Convention & Exhibition Center
Room 107B

Nanomaterials for Defense & Homeland Security Applications

R. Nagarajan, *Organizer*

E. Wilusz, *Presiding*

- 2:00 COLL 518.** Reactive amphiphilic polymer additives for self-decontamination of CWA simulants. **J. Lundin**, J.H. Wynne
- 2:30 COLL 519.** Chemical threat responsive carbon nanotube membranes. **M.B. Herbert**, C. Belger, J.G. Weis, T.M. Swager
- 3:00 COLL 520.** Metal-organic frameworks for the removal of G-agents and sulfur mustard. **J.B. DeCoste**, G.W. Peterson, J. Mondloch, M.J. Katz, O.K. Farha, J.T. Hupp
- 3:30 COLL 521.** Nanometric hydrogen bronze reagents for the detection and neutralization of explosives. **N.F. Materer**, A.W. Apblett
- 4:00 COLL 522.** Porous Co_3O_4 nano-array based monolithic catalysts for low temperature CO and hydrocarbon oxidation. **Z. Ren**, S. Wang, V. Botu, R. Ramprasad, P. Gao
- 4:20 COLL 523.** 3D ZnO/Perovskite core/shell nanorod array based catalysts: A promising PGM-free catalyst for low temperature hydrocarbons oxidation. **S. Wang**, Z. Ren, Y. Guo

Section C

Boston Convention & Exhibition Center
Room 107C

Nanoparticles in Food, Agricultural, & Environmental Settings

Cosponsored by AGFD†

C. M. Sabliov, *Organizer*

D. Britt, C. Dimkpa, J. M. Goddard, *Organizers*,
Presiding

- 2:00 COLL 524.** Probing silver nanoparticles in edible leaves and environmental waters by surface-enhanced Raman spectroscopy (SERS). **H. Guo**, B. Xing, L. He
- 2:20 COLL 525.** Silver nanoparticle loaded textile test materials: Impact of particle size and textile type on nanoparticle detection and characterization using multiple techniques. **J.M. Gorham**, K.E. Murphy, J. Liu, T. Nguyen, D. Holbrook, G. Stan, D. Tselenchuk, R.F. Cook, M.R. Winchester, R.I. Maccuspie, V.A. Hackley
- 2:40 COLL 526.** Computationally driven design of bioinspired cells interacting with antimicrobial mimetic nanoparticles. **X. Chu**, F. Aydin, M. Dutt
- 3:00 COLL 527.** Carvacrol loaded halloysite nanotubes as antibacterial nanoparticles for food-contact materials. **S. Hendessi**, B. Sevinis, S. Unal, F.C. Cebece, Y.Z. Menceoglu, **H. Unal**

3:20 Intermission.

- 3:40 COLL 528.** Rapid size and pH-dependent kinetics of silver nanoparticles in simulated gastric fluid to assess properties of ingested nanoparticles. **A.P. Ault**, J.L. Axson, D.I. Stark, A. Bondy, S. Capracotta, J. Keeney, A. Maynard, M.A. Philbert, I.L. Bergin
- 4:00 COLL 529.** Rhizosphere dissolution of CuO nanoparticles by wheat root exudates in a sand matrix. **P. McManus**, J. Stewart, D. Britt, D. Stevens, A.J. Anderson, J.E. McLean
- 4:20 COLL 530.** Nano delivery nutrient strategies to enhance crop nutrition. **C. Dimkpa**, P. Bindraban
- 4:40 COLL 531.** Monitoring bacterial metabolite production and response to nanoparticles using endogenous fluorescence. **D. Britt**, J. Adams, H. Wagner, J.E. McLean, A.J. Anderson
- 5:00 COLL 532.** Bio-inspired silica nanoparticles through biomolecular engineering. **C. Zhao**, D. Wibowo, A. Middelberg

Section D

Boston Convention & Exhibition Center
Room 108

Basic Research in Colloids, Surfactants & Nanomaterials

Biosensing and Biomedicine

R. Nagarajan, *Organizer*

M. Ruths, *Presiding*

- 2:00 COLL 533.** Novel strategy for ultrasensitive and highly selective detection of infectious pathogens with the help of chemiluminescent labels released from long spacer arm-functionalized magnetic nanoparticles. **N. He**, H. Yang, Z. Li, Y. Deng
- 2:20 COLL 534.** Hybrid platforms for improved bioassay detection limit. **E. Bonyi**, K. Aslan
- 2:40 COLL 535.** Withdrawn.
- 3:00 COLL 536.** Peptide loaded microgels as antimicrobial surface coatings. **L. Nyström**, R. Álvarez-Asencio, R. Nordström, M.W. Rutland, B. Saunders, M. Malmsten
- 3:20 COLL 537.** Water-based polymeric N-halamine biocides. **Z. Jing**, Y. Sun
- 3:40 COLL 538.** Controlling the colloidal aggregation of chemotherapeutics. **A.N. Ganesh**, C.K. McLaughlin, B. Shoichet, M.S. Shoichet
- 4:00 COLL 539.** De novo method for uric acid decrystallization using gold nanoparticles and medical microwaves. **Z. Boone-Kukoyi**, N. Thompson, C. Lansiquot, T.C. Clement, B. Kioko, T. Ogundolie, **K. Aslan**
- 4:20 COLL 540.** Pharmacokinetic model of a tissue implantable insulin sensor. **G. Bisker**, N. Iverson, J. Ahn, M. Strano
- 4:40 COLL 541.** Effects of functionalities on drug binding, drug releasing, and biofilm-controlling properties of PMMA based denture biomaterials. **J. Wen**, Y. Sun

Section E

Boston Convention & Exhibition Center
Room 109A

Basic Research in Colloids, Surfactants & Nanomaterials Applications

R. Nagarajan, *Organizer*

E. V. Iski, *Presiding*

- 2:00 COLL 542.** Withdrawn.

- 2:20 COLL 543.** Multifunctional nanostructures: Fundamentals and applications. **S. Hunyadi Murph**
- 2:40 COLL 544.** Surfactant ionic liquids with unusually high capacitances for high-temperature flexible supercapacitors. **X. Mao**, P. Brown, M. Costa Gomes, T. Hatton
- 3:00 COLL 545.** Aqueous-based fabrication of low-VOC nanostructured block copolymer films as effective marine antifouling coatings. **S. Kim**, N. Gunari, D. MacNeil, G.C. Walker
- 3:20 COLL 546.** Polyacrylamide microgels and pore modeled oil recovery performance. **Z. Chen**, T.P. Schuman, B. Bai
- 3:40 COLL 547.** Effects of clay surfaces on diethyl phthalate degradation in Fenton reactions. **J. Gao**
- 4:00 COLL 548.** Surface-modified $\text{Li}[\text{Li}_{0.2}\text{Ni}_{0.17}\text{Co}_{0.07}\text{Mn}_{0.56}\text{O}_2]$ nanoparticles with AlF_3 as cathode for Li-ion battery. **Y. Bai**, X. Lu, W. Zhang
- 4:20 COLL 549.** Highly efficient autonomous nanomotors in micromolar halogen media. **F. Wong**, A. Sen
- 4:40 COLL 550.** Spin coating polyelectrolyte coacervate thin films. **K.D. Kelly**

COMP

Division of Computers in Chemistry

H. L. Woodcock and W. Cornell, *Program Chairs*

BUSINESS MEETINGS:

Business Meeting, 3:00 PM: Saturday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 157A

Accelerated Discovery of Chemical Compounds: Design New Polymers & Inorganic Materials from Integration of Polymer Science, Materials Science, & Informatics

Polymer Structures

J. Cheng, Y. Tseng, *Organizers*

J. E. Rice, *Organizer, Presiding*

8:30 Introductory Remarks.

8:45 COMP 1. PolyName2Structure, mapping polymer names to structures. **Y. Tseng**, C. Lin, J. Cheng

9:15 COMP 2. Application of CurlySMILES to the encoding of polymer systems. **A. Drefahl**

9:45 Intermission.

10:05 COMP 3. HELM: An open standard for complex polymeric structures. **T. Zhang**

10:35 COMP 4. From discovery to deployment: Big data in materials R&D. **J.W. Pitera**

Section B

Boston Convention & Exhibition Center
Room 156A

Integrated Approaches in Structure-Based Drug Design

Cosponsored by CINF and MEDI

Financially supported by Pfizer

V. Shanmugasundaram, F. F. Vajdos, *Organizers*,
Presiding

8:00 Introductory Remarks.

8:05 COMP 5. Wscore: integration of active site water structure into an empirical scoring function for calculating protein-ligand binding affinity. **R.A. Friesner**

8:45 COMP 6. Water, thermodynamics, and drugs, oh my. **E.S. Manas**, A.P. Graves

9:20 COMP 7. Discovery and optimization of a series of potent and selective Pan-Trk ligands. **S. Skerratt**

9:55 Intermission.

10:10 COMP 8. In silico identification of Nav 1.7 inhibitors — building a homology model (Part I) and structure-based virtual screening (Part II). **D.S. La**

10:50 COMP 9. Using computational chemistry to drive design in the discovery of a potent, selective, brain penetrant and in vivo active LRRK2 kinase inhibitor. **B.L. Kormos**, J.L. Henderson, M.M. Hayward, K.J. Coffman, J. Jasti, R.G. Kurumbail, T.T. Wager, P.R. Verhoest, S. Noell, P. Galatsis

11:25 COMP 10. Decision support for drug discovery: Some recent advances. **M.A. Murcko**

Section C

Boston Convention & Exhibition Center
Room 156C

Calculating pKa's & Redox Potentials

Predicting pKa's

M. Coote, H. B. Schlegel, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 COMP 11. Rapid progress in the estimation of pK_a values. **G.C. Shields**

9:10 COMP 12. Calculating pK_a 's, reduction potentials, and reorganization energies for electrochemical proton-coupled electron transfer processes. **S. Hammes-Schiffer**

9:40 COMP 13. Predicting pK_a — beyond small, rigid molecules. **N. Haworth**, Q. Wang, M.L. Coote

10:00 Intermission.

10:20 COMP 14. Prediction of pK_a 's and acidities of metals ions in solution and of amino acids. **D.A. Dixon**, V.E. Jackson, M. Stover

10:50 COMP 15. Calculation of redox potentials, spin splittings, and pK_a 's in transition metal containing systems using the DFT-LOC methodology. **R.A. Friesner**

11:20 COMP 16. pK_a values in proteins determined by electrostatics applied to molecular dynamics trajectories. **E. Knapp**, T. Meyer

Section D

Boston Convention & Exhibition Center
Room 156B

Best in Class Computational Software by Integration

Cosponsored by CINF

A. Gobbi, P. Walters, *Organizers, Presiding*

8:00 COMP 17. Integrated suite of modeling tools that empower scientists in structure- and property-based drug design. **J. Feng**

8:30 COMP 18. AIDEAS: An integrated cheminformatics solution. **R.R. Gupta**

9:00 COMP 19. Autocorrelator v2.0: Adapting for a resource limited environment. **M.A. Lardy**

9:30 COMP 20. What's old is new again: Cheminformatics and the 'modern' web. P. Watson

10:00 Intermission.

10:15 COMP 21. Developing an integrated software ecosystem at Merck. S.A. Johnson

10:45 COMP 22. Pharmed: Bring virtual screening to your browser. D. Koes

11:15 COMP 23. Building an integrated information environment for drug discovery. J. Weiss, G. Bemis, C.H. Faerman, J. Feng, B. Goldman, X. Zhang, P. Walters

11:45 Panel Discussion.

Section E

Boston Convention & Exhibition Center
Room 157B

Molecular Mechanics

Applications

H. L. Woodcock, *Organizer*

S. K. Natesan, *Presiding*

8:30 COMP 24. Understanding the mechanism and product specificity of PRMT1 using theory and experiment. O. Acevedo, S.M. Gathniaka, B. Boykin, S. Gui, J. Qu, J.M. Hevel

9:00 COMP 25. Conformational analysis of nucleosides with 2'- and 3'-fluoro substituents: Quantum mechanical- and molecular mechanics-based evidence for a three-state equilibrium. S.M. Graham

9:30 COMP 26. Building and simulating periodic amorphous models for microporous polymer networks. P.C. Fayon

10:00 Intermission.

10:15 COMP 27. Rational approach to conjugated porous material design. P. Heasman, A. Trewin

10:45 COMP 28. Atomistic folding simulations of native and mimetic peptides. H. Mohammadlarani, H. Vashisth

11:15 COMP 29. Molecular dynamics simulations of water within homo-oligomeric bundles. P.B. Moore, T.H. Nguyen, Z. Liu

11:45 COMP 30. Lipid bilayer perturbations by homo-oligomeric transmembrane protein bundles: A molecular dynamics study. P.B. Moore, T.H. Nguyen, Z. Liu

Section F

Boston Convention & Exhibition Center
Room 157C

Designing Chemical Libraries for Screening: Past, Present & Future

S. Das, *Organizer*

A. Shelat, *Organizer, Presiding*

8:00 Introductory Remarks.

8:15 COMP 31. Smart, automated, generation of molecular libraries for high-throughput virtual screening. E.O. Pyzer-Knapp, J.M. Hernández-Lobato, R.P. Adams, A. Aspuru-Guzik

8:45 COMP 32. Molecular libraries in high throughput virtual screening (HTVS) for novel materials: OPVs, OLEDs, and flow batteries. J. Aguilera-Iparraguirre, R. Gomez Bombarelli, E. Pyzer-Knapp, T. Hirzel, A. Aspuru-Guzik

9:15 COMP 33. Development of property-biased diversity-oriented molecular libraries: Applications to organic light emitting diodes. C. Rupakheti, R. Al-Saadon, P. Zhang, A.M. Virshup, D. Beratan, W. Yang

9:45 Intermission.

10:00 COMP 34. Structural alerts for the annotation and filtering of chemical libraries. C. Lagner

10:30 COMP 35. Designing fragment libraries: Past, present, and future. E.R. Zartler

11:00 COMP 36. Library design in pharmacophore and shape space. M.M. von Behren, M. Rarey

11:30 Panel Discussion.

Electronic Structure Methods for Large Systems

Novel Architectures and Representations for Large-Scale Calculations

Sponsored by PHYs, Cosponsored by COMP

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Sponsored by PHYs, Cosponsored by COMP

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 157A

Accelerated Discovery of Chemical Compounds: Design New Polymers & Inorganic Materials from Integration of Polymer Science, Materials Science, & Informatics

Polyinformatics

J. Cheng, Y. Tseng, *Organizers*

J. E. Rice, *Organizer, Presiding*

1:30 COMP 37. Simulated syntheses for descriptors of polymer architecture. S.G. Arturo

2:00 COMP 38. Polymer informatics: A frustrating opportunity. J. Winter

2:30 COMP 39. Successes and challenges in polymer materials informatics: Where are we now, and where can we be? C.M. Breneman, K. Wu, L. Schadler, C. Brinson, R. Ramprasad, S. Kumar

3:00 Intermission.

3:20 COMP 40. Random walk through polymer information retrieval. D. Wrublewski, D.L. Roth

3:50 COMP 41. And you thought cheminformatics was hard? Challenges in polymer informatics. J.E. Rice, J.W. Pitera, R.L. Martin, W.C. Swope

Section B

Boston Convention & Exhibition Center
Room 156A

Integrated Approaches in Structure-Based Drug Design

Cosponsored by CINf and MEDI

Financially supported by Pfizer

V. Shanmugasundaram, F. F. Vajdos, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 COMP 42. Structure, enzymology, and biophysical characterization of a Jak3-Type II inhibitor complex. F.F. Vajdos

2:15 COMP 43. Structure and computationally guided design of potent non-nucleoside inhibitors with improved pharmacological properties that target HIV reverse transcriptase and drug-resistant variants. K.S. Anderson

2:50 COMP 44. The devil is in the detail — two short stories on using direct binding data in lead optimization. U. Schmitz, J. Chandrasekhar, A. Niedziela-Majka, R. Sakowicz, S. Boyce, C. Higgs, W. Sherman, E. Lansdon

3:25 Intermission.

3:40 COMP 45. Transition state structure in the design of drug candidates. P. Tyler, G. Evans, R.H. Furneaux, V.L. Schramm

4:20 COMP 46. Using Ensemble-Docking and NMR constraints to generate high quality models of antagonist-bound HDM2 complexes. X. Fradera

4:55 COMP 47. Structure activity relationships of nuclear receptor, GPCR and kinase modulators revealed with differential HDX. P. Griffin

Section C

Boston Convention & Exhibition Center
Room 156C

Calculating pKa's & Redox Potentials

Predicting Redox Potentials

M. Coote, H. B. Schlegel, *Organizers, Presiding*

1:30 COMP 48. Fascinating redox behaviour of nitroxide radicals. M.L. Coote, G. Gryn'ova

2:00 COMP 49. Computation of redox potentials of a broad range of organic structures. A.J. Fry

2:30 COMP 50. Exploring unusual features of Pourbaix diagrams of molecular catalysts for solar fuels production.

J.T. Muckerman, M.Z. Ertem, M. Kowalczyk, E. Fujita, D.E. Polyansky, A. Lewandowska-Andralojc, X. Zhao, R.P. Thummel

3:00 Intermission.

3:20 COMP 51. Are thermodynamic cycles necessary for continuum solvent calculation of pKas, reduction potentials, and solution phase energetics? J. Ho

3:50 COMP 52. Simulating electrochemistry in water. T.A. Van Voorhis, M. Mavros, V. Vassier, T. Tsuchimochi

4:20 COMP 53. Predictive calculations of redox potentials of solvated molecules: A combined QM/EF/PCM approach. R.N. Tazhigulov, K.B. Bravaya

Section D

Boston Convention & Exhibition Center
Room 156B

Measuring "Success" of Molecular Modeling Efforts

A. Rusinko, *Organizer*

E. C. Sherer, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 COMP 54. Our experience with 6 years of impact-oriented performance metrics. S. Johnson, B.L. Claus, D.A. Loughney

2:10 COMP 55. Modeling the modeler: Design effectiveness, project impact, and organization structure. R.A. Denny, J. McDonald, J. Mathias

2:40 COMP 56. Changing times: The role for metrics, objectives. B. Sherborne

3:10 Intermission.

3:30 COMP 57. Binding affinity calculations: Benefits and limitations in drug discovery. C. Velez Vega, R.A. Pearlstein, D. McKay, T.P. Kurtzman, J. Duca

4:00 COMP 58. What it takes to develop trust/worthy QSAR models. D. Fourches, E. Muratov, A. Tropsha

4:30 COMP 59. Computational Chemistry @GSK — how do we know we're successful? E.S. Manas

5:00 Panel Discussion.

Section E

Boston Convention & Exhibition Center
Room 157B

Molecular Mechanics

Methodology

H. L. Woodcock, *Organizer*

V. S. Somiseti, *Presiding*

1:30 COMP 60. Diffusion wavelet decomposition for coarse-graining of polymer chains. C.B. Rinderspacher, J. Bardhan, A.E. Ismail

2:00 COMP 61. Development of coarse grain models for protein-lipid interactions and dynamics. R.D. Hills

2:30 COMP 62. Pauli potential: A history and new developments. J. Herzfeld, S. Ekesan

3:00 Intermission.

3:15 COMP 63. Enhancing constant-pH simulation in explicit solvent with a two-dimensional replica exchange method. J. Lee, B.T. Miller, A. Damjanovic, B. Brooks

3:45 COMP 64. Molecular dynamics studies using GPU and AMBER CUDA implementation of an antifreeze protein. A. Peramo

4:15 COMP 65. Wavelet analysis of molecular dynamics simulations of nucleic acids. Z. Heidari, D.R. Roe, R. Galindo, T.E. Cheatham, J. Ghasemi, A. Jabbari

4:45 COMP 437. Dopamine D1 receptor-agonist interactions using site-directed mutagenesis, homology modeling and molecular dynamics simulations. S. Mente, E. Guilmette, M. Salafia, D.L. Gray

Section F

Boston Convention & Exhibition Center
Room 157C

Designing Chemical Libraries for Screening: Past, Present & Future

S. Das, *Organizer*

A. Shelat, *Organizer, Presiding*

1:30 Introductory Remarks.

1:45 COMP 66. De novo library design: A philosophy of chemical space. G. Schneider

2:15 COMP 67. Examining the diversity of large collections of building blocks in 3D. M.D. Mackey, T. Cheeseright, P. Tosco, W. Wade, S.T. Meyer

2:45 COMP 68. Characterization of chemical libraries using scaffolds and network models. R. Guha, D. Nguyen

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3:15 Intermission.

3:30 **COMP 69.** Quantifying the diversity of chemical libraries through network modeling. G. Prabhu, S. Sen, S. Bhattacharya, M.P. Krein, N. Sukumar

4:00 **COMP 70.** Application of 3-point protein pharmacophoric signatures to focused library design. S. Das, J. Bowling, A. Singh, R.E. Lee, A. Shelat

4:30 Panel Discussion.

Electronic Structure Methods for Large Systems

Massively Parallel Electronic Structure

Sponsored by *PHYS*, Cosponsored by *COMP*

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Proteins

Sponsored by *PHYS*, Cosponsored by *COMP*

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Sponsored by *PHYS*, Cosponsored by *COMP*

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 157A

Functional Polymers: Connecting Modeling and Experiment

Polymers for Energy and Environment

H. Ashbaugh, W. C. Swope, *Organizers*

S. W. Rick, *Organizer, Presiding*

J. K. Maranas, *Presiding*

8:30 Introductory Remarks.

8:40 **COMP 71.** Functional polymers for water desalination. M. Chaudhari, S.L. Rempe

9:10 **COMP 72.** Transport of ions and penetrants through structured polymeric matrices: Interplay of structure and dynamics of polymers. V. Ganesan

9:40 Intermission.

10:00 **COMP 73.** Simultaneous electron and ion conduction in block copolymers. N.P. Balsara, M. Bhatt

10:30 **COMP 74.** Ion clusters in neutral-charged polymer blends and copolymers. M. Olvera De La Cruz

11:00 **COMP 75.** Ionomer melt structure and dynamics: Connecting modeling and experiment. M.J. Stevens

Section B

Boston Convention & Exhibition Center
Room 156A

Molecular Dynamics Simulations in Drug Discovery

Free Energy of Binding

V. Hornak, *Organizer*

G. Cui, D. Shivakumar, *Organizers, Presiding*

8:30 **COMP 76.** Free energy sampling of protein-ligand recognition: Non-trivial conformational changes and water displacement. W. Yang

9:00 **COMP 77.** Free energy perturbation simulations: Methodology and application to drug discovery. R.A. Friesner

9:30 **COMP 78.** Using free energy calculations to test and improve force fields and guide lead optimization. D.L. Mobley

10:00 Intermission.

10:15 **COMP 79.** Molecular recognition of metabotropic glutamate receptor Type 1 (mGluR1): Synergistic understanding with free energy perturbation and linear response modeling. R. Zhou

10:45 **COMP 80.** Using the Movable Type sampling method to compute thermodynamic quantities for chemical and biological processes. K.M. Merz

11:15 **COMP 81.** Free energy perturbation: Retrospective and prospective application to potency prediction. F.E. Lovering

11:45 **COMP 82.** Rapid, accurate, and reproducible drug-protein binding affinity calculation. S. Wan, P.V. Coveney

Section C

Boston Convention & Exhibition Center
Room 156C

Quantum Chemistry

E. V. Patterson, *Organizer*

P. S. Hudson, *Presiding*

8:30 **COMP 83.** FLUKE: An open-source QMMM interface for simulations with polarizable force fields. E.G. Kratz, G.A. Cisneros

9:00 **COMP 84.** Polarizable QM/MM based on the AMOEBA force field and linear-scaling DFT. J. Dziedzic, M.P. Head-Gordon, T.L. Head-Gordon, C. Skylaris

9:30 **COMP 85.** Accurate and efficient implementation of TD-DFT analytical frequencies within QM/MM and condensed-phase methods. G. Scalmani, M.J. Frisch

10:00 Intermission.

10:15 **COMP 86.** QM/MM nonadiabatic dynamics of photoinduced proton-coupled electron transfer in solution. P. Goyal, C. Schwerdtfeger, A. Soudackov, S. Hammes-Schiffer

10:45 **COMP 87.** Proton solvation in protic and aprotic solvents. E. Rossini, E. Knapp

11:15 **COMP 88.** Charge-dependent many-body exchange and dispersion interactions in combined QM/MM simulations. E.R. Kuechler, T.J. Giese, D.M. York

11:45 **COMP 89.** Reaction path force matching: A multiscale QM/MM approach. J. Pu

Section D

Boston Convention & Exhibition Center
Room 156B

Calculating pKa's & Redox Potentials Methodological Advances

M. Coote, H. B. Schlegel, *Organizers, Presiding*

8:30 **COMP 90.** Pushing around protons and electrons: What could possibly go wrong? C.J. Cramer

9:00 **COMP 91.** Solution-phase prediction of properties: Routes to predictive pKa's. A.K. Wilson, A. Rijoias, P. Patel, J. Wang

9:30 **COMP 92.** Protic ionic liquids: Effect of environment and solvent on proton transfer. E. Izgorodina

10:00 Intermission.

10:20 **COMP 93.** Withdrawn.

10:50 **COMP 94.** Exploring chemistry at extreme high pressure with the polarizable continuum model: Basis of the method and perspectives of application to electron-transfer reactions. R. Cammi

11:20 **COMP 95.** Calculating aqueous hydricities of [Ir]⁺-H complexes. S. Bellows, T. Cundari, W.D. Jones

Section E

Boston Convention & Exhibition Center
Room 157B

Molecular Mechanics

Biological Applications

H. L. Woodcock, *Organizer*

G. M. Gray, *Presiding*

8:30 **COMP 96.** Multiscale modeling and simulations for structure-based GPCR drug discovery. J. Li

9:00 **COMP 97.** Flexible dynamics of proteins in water with refined AMBER force field (FUJI). H. Fujitani

9:30 **COMP 98.** Melittin aggregation mechanism in aqueous solutions by molecular dynamics simulations. C. Liao, J.L. Slomovitch, J. Li

10:00 Intermission.

10:15 **COMP 99.** Withdrawn.

10:45 **COMP 100.** Rapid computation of thermodynamic properties over a large multidimensional space of nonbonded parameters. L. Naden, M.R. Shirts

11:15 **COMP 101.** Withdrawn.

11:45 **COMP 102.** Molecular dynamics based studies of the mechanisms and limitations of biomolecular evolution resulting in drug resistance. B.N. Dominy, M. Singh, T. Han, Y. Liu, Z. Jia, V. Agrawal

Section F

Boston Convention & Exhibition Center
Room 157C

Emerging Technologies in Computational Chemistry

C. L. Simmerling, *Organizer*

T. E. Balius, *Presiding*

8:30 **COMP 103.** Next-generation technologies in computational chemistry. D. Fourches

9:00 **COMP 104.** Development and sharing of ADME/Tox and drug discovery machine learning models. A. Clark, K. Dole, A. Coulon-Spector, A. McNutt, G. Grass, J. Freundlich, R. Reynolds, S. Ekins

9:30 **COMP 105.** Analytic energy gradients for range-separated many-body dispersion. M.A. Blood-Forsythe, T. Markovich, R.A. DiStasio, A. Aspuru-Guzik

10:00 Intermission.

10:15 **COMP 106.** Prediction of peptide-protein interactions using motif-derived fragments. K. Porter, D. Beglov, N. Alam, O. Schueler-Furman, D. Kozakov

10:45 **COMP 107.** When less is more: How excluding experimentally ambiguous observations may enhance the sensitivity of a model. J. Ghosh, M. Lawless, R.D. Clark

11:15 **COMP 108.** Multi-agent approach for coupling molecular dynamics with continuum based simulation. L.E. Achenie

Electronic Structure Methods for Large Systems

Fragment-Based Approaches

Sponsored by *PHYS*, Cosponsored by *COMP*

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Membrane Proteins, Nano Systems, and Motors

Sponsored by *PHYS*, Cosponsored by *COMP*

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Sponsored by *PHYS*, Cosponsored by *COMP*

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 157A

Accelerated Discovery of Chemical Compounds: Design New Polymers & Inorganic Materials from Integration of Polymer Science, Materials Science, & Informatics

Applications of Polymer

J. Cheng, Y. Tseng, *Organizers*

J. E. Rice, *Organizer, Presiding*

1:30 **COMP 109.** So we made all these polymers, now what do we do with the data? D.C. Webster

2:00 **COMP 110.** Open source, semantically rich tools for polymer visualization and analytics. M.D. Hanwell

2:30 **COMP 111.** WebFF: A smart force-field repository for soft materials. F.R. Phelan, H. Sun

3:00 Intermission.

3:20 **COMP 112.** Virtual High Throughput Screening of Organic Photovoltaic Materials. M. Krompiec, L. Nanson, N. Blouin, O. Lozman

3:50 **COMP 113.** Simulation-enabled genetic algorithm for polymer glass formation. D.S. Simmons, T. Patra, J. Hung, V. Meenakshisundaram

Section B

Boston Convention & Exhibition Center
Room 156A

Molecular Dynamics Simulations in Drug Discovery

Drug Discovery and Development Related Applications

V. Hornak, *Organizer*

G. Cui, D. Shivakumar, *Organizers, Presiding*

1:30 **COMP 114.** Breaking the millisecond barrier in molecular dynamics simulations of protein-ligand unbinding. P. Tiwary, M. Parrinello

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

2:00 COMP 115. Rational modulation of the induced-fit conformational change for slow-onset inhibition. C.L. Simmerling, P.J. Tonge, M. Garcia-Diaz

2:30 COMP 116. Deciphering cryptic binding sites on proteins by molecular dynamics in mixed solvent. S.R. Kimura, H. Hu, A. Ruvinsky, W. Sherman, A. Favia

3:00 Intermission.

3:15 COMP 117. Molecular dynamics as a needed tool in pharmaceutical design. A.E. Roitberg

3:45 COMP 118. Active site structure and dynamics in designed and evolved enzymes. G. Jimenez-Oses, S. Osuna, K.N. Houk

4:15 COMP 119. Application of molecular dynamics simulations to understanding β -secretase dynamics. A.C. Cheng, D.W. Borhani, A. Kalenkiewicz, D. Whittington, M. Jensen, D.E. Shaw

4:45 COMP 120. Understanding permeation of antibiotics through porins in Gram-negative bacteria using MD simulations and SAR. I. Bodrenko, S. Acosta Gutierrez, D. Benkerrou, T. D'Agostino, G. Mallocci, S. Samanta, M. Scorciapino, M. Ceccarelli

Section C

Boston Convention & Exhibition Center
Room 156C

Quantum Chemistry

E. V. Patterson, *Organizer*

T. D. McGee, *Presiding*

1:30 COMP 121. Development of the explicitly correlated pair theory using integral R12-operator for accurate description of electron-electron correlation. M.G. Bayne, A. Chakraborty

2:00 COMP 122. Self-consistent second order Green's function theory: Quasiparticle spectra, strong correlations, and fractional electron behavior. J. Phillips

2:30 COMP 123. Using second order Green's function theory to calculate ionization potentials and electron affinities. A. Welden, J. Phillips, D. Zgid

3:00 Intermission.

3:15 COMP 124. Electron correlations in solids via the perturbative Green's function embedding. A.A. Rusakov, D. Zgid

3:45 COMP 125. Effect of impurities and grain boundaries on the electrical properties of MoS₂ devices. A. Stroud, G.M. Leuty, C. Muratore, P.A. Derosa, R. Berry

4:15 COMP 126. Density perturbation theory. M.C. Palenik, B.I. Dunlap

4:45 COMP 127. First principles united atom model for imidazolium based ionic liquids. C. Son, J.G. McDaniel, A. Yethiraj

Section D

Boston Convention & Exhibition Center
Room 156B

Calculating pKa's & Redox Potentials

Biological Applications

M. Coote, H. B. Schlegel, *Organizers, Presiding*

1:30 COMP 128. Coupling between conformations, dynamics and protonations in biological systems. A.E. Roitberg

2:00 COMP 129. Computational electrochemistry: From small molecules to metalloproteins. L. Rulisek, U. Ryde, M. Srnec, M. Kyvala

2:30 COMP 130. Quantum chemical approach to estimating the thermodynamics of metabolic reactions. A. Aspuru-Guzik

3:00 Intermission.

3:20 COMP 131. Modeling of electrostatics and polarization effects in biomolecular systems within quantum chemical approaches. B. Mennucci

3:50 COMP 132. Obtaining accurate QM/MM free energies using novel sampling and reweighting approaches. P.S. Hudson, G. Koenig, F.L. Kearns, S. Boresch, H.L. Woodcock

4:20 COMP 133. Ground state chromophore reduction in cryptochromes: An insight from electronic structure calculations. R.N. Tazhigulov, K.B. Bravaya

Section E

Boston Convention & Exhibition Center
Room 157B

Drug Discovery

Applications of Computer-aided Drug Design

Y. Tseng, *Organizer*

J. Guo, *Presiding*

1:30 COMP 134. Can you see it too? Computer-aided drug discovery in the 21st century. C. Detering

2:00 COMP 135. Computational and experimental insights into the spermine-vectorized F14512 poisoning of type II topoisomerase. G. Palermo, E. Minniti, M. Greco, L. Riccardi, E. Simoni, M. Convertino, C. Marchetti, M. Rosini, C. Sissi, A. Minarini, M. Devoio

2:30 COMP 136. In silico efforts toward development and optimization of anthrax toxin lethal factor (LF) inhibitors as potential therapeutics. E.A. Amin, B. Finsel, D.G. Truhlar, M.A. Walters, J. Hawkinson, T. Chiu, E.K. Kurbanov, K.M. Maize, J. Solberg

3:00 Intermission.

3:15 COMP 137. Application of computational chemistry techniques to the discovery of Tankyrase inhibitors. A. Macias, L. Baker, C. Graham, N. Matassova, J.B. Murray, S. Roughley, A.E. Surgenor, H. Simmonite

3:45 COMP 138. Theory assisted explorations of the small molecule universe to discover new inhibitors of coactivator-associated arginine methyltransferase1 (CARM1). C. Rupakheti, L. Du, D. Beratan, Q. Wang

4:15 COMP 139. Prospective applications of structure-based drug design methods: Comparing to intuition and other typical scoring methods. W. Sherman

Section F

Boston Convention & Exhibition Center
Room 157C

Molecular Mechanics

Force Fields

H. L. Woodcock, *Organizer*

T. R. Stouch, *Presiding*

1:30 COMP 140. Developing ReaxFF force field to study syngas combustion kinetics. C.M. Ashraf, A.C. Van Duin

2:00 COMP 141. Recapitulation of early quantum chemistry by a pointillist rendering of electron charge and spin density. S. Ekesan, J. Herzfeld

2:30 COMP 142. OPLS3 force field: An improved classical force field for the modeling of drug-like small molecules, proteins, RNA, and DNA. R. Abel, E. Harder, W. Damm, M. Reboul, J. Maple, C. Wu, J. Xiang, D.S. Cerutti, D. Lupyan, L. Wang, M. Dahlgren, D. LeBard

3:00 Intermission.

3:15 COMP 143. Parameterization of an effective potential for protein-ligand binding from host-guest affinity data. L.B. Wickstrom, N. Deng, P. He, C.N. Nguyen, A. Mentas, M.K. Gilson, T.P. Kurtzman, E. Gallicchio, R.M. Levy

3:45 COMP 144. Atomic partial charges for fixed-charge force fields: Dealing with conformational dependence. C.I. Bayly

4:15 COMP 145. Development and application of Mg²⁺, Mn²⁺, Zn²⁺ and Cd²⁺ ion models for balanced interactions with nucleic acids. M. Panteva, G.M. Giambasu, D.M. York

4:45 COMP 146. Conformational control of arylamide foldamers: Predicting oligomer structures in solution through molecular dynamics simulations. V. Pophristic, Z. Liu, A. Abramyan

Electronic Structure Methods for Large Systems

Embedding Methods

Sponsored by *PHYS*, Cosponsored by *COMP*

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Protein Stability, Folding, and Aggregation

Sponsored by *PHYS*, Cosponsored by *COMP*

Undergraduate Research Posters

Computational Chemistry

Sponsored by *CHED*, Cosponsored by *COMP* and *SOCED*

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Sponsored by *PHYS*, Cosponsored by *COMP*

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

W. D. Cornell, H. L. Woodcock, *Organizers*

8:00 - 10:00

208, 210, 216, 219, 222, 227, 231, 233, 237, 239, 241, 246, 248-251, 253-254, 257-259, 264-265, 270, 274, 277-278, 282, 285-286, 304, 307, 311, 314, 320-321, 323, 331, 333, 337, 341-342. See subsequent listings.

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 157A

Functional Polymers: Connecting Modeling and Experiment

Polymers for Drug Delivery and Sensors

S. W. Rick, *Organizer*

H. Ashbaugh, W. C. Swope, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 COMP 147. Synergistic experimental and multiscale modeling approaches for optimizing anticancer drug nanocarriers. W. Jiang, X. Wang, J. Luo, S. Nangia

9:10 COMP 148. Computational studies of diblock star polymers and polyelectrolyte membranes. T.L. Head-Gordon

9:40 COMP 149. Nanogel star polymers: A platform for programmable macromolecular self-assembly. V.A. Piunova, W.C. Swope, J.E. Rice, R.D. Miller

10:10 Intermission.

10:30 COMP 150. Peptide-containing conjugates for triggered assembly and controlled delivery from collagen scaffolds. K.L. Kiick

11:00 COMP 151. Coarse-grained simulations of star block co-polymer aggregation and drug encapsulation. J.W. Pitera, W.C. Swope

11:30 COMP 152. Protein stabilization in organic solvent via designed random copolymer. B. Panganiban, B. Qiao, M. Olvera De La Cruz, E. Drockenmuller, T. Xu

Section B

Boston Convention & Exhibition Center
Room 156A

Molecular Dynamics Simulations in Drug Discovery

Methodology Development

V. Hornak, *Organizer*

G. Cui, D. Shivakumar, *Organizers, Presiding*

8:30 COMP 153. HTMD: A complete software workspace for simulation-guided drug design. S. Doerr, M. Harvey, G. De Fabritiis

9:00 COMP 154. Molecular dynamics of crystals. P. Janowski, C. Liu, J. Holton, D.A. Case

9:30 COMP 155. Using molecular dynamics to test structural fidelity and NMR relaxation in a prototype RNA hairpin. G.M. Giambasu, D.M. York, D.A. Case

9:50 Intermission.

10:05 COMP 156. Quantum mechanical force fields: A new tool for drug discovery. D.M. York

10:25 COMP 157. SPXP: A new mixed-precision model for stable molecular dynamics. S. Le Grand

10:55 COMP 158. Exploring polymorph free energy landscapes with Hamiltonian reweighted molecular dynamics. E. Dybeck, B. Bruns, N.P. Schieber, G. Koenig, M.R. Shirts

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Section C

Boston Convention & Exhibition Center
Room 156C

Quantum Chemistry

E. V. Patterson, *Organizer*
K. R. Jorgensen, *Presiding*

8:30 COMP 159. New multireference excited state method with dynamical correlation that treats ground and excited states equally. S. Yost, N. Mayhall, M.P. Head-Gordon

9:00 COMP 160. Withdrawn.

9:30 COMP 161. Excited state density functional tight-binding for rapid exploration of excited state potential energy surfaces. T. Kowalczyk

10:00 Intermission.

10:15 COMP 162. Hypothesis generation tools for predictive reaction mechanism discovery. P.M. Zimmerman

10:45 COMP 163. Global potential energy surface of quintet O₂ and dynamics of high-energy O₂-O₂ collision-induced energy transfer and dissociation. Y. Paukku, Z. Varga, R. Meana-Pañeda, G. Song, J. Bender, G.V. Candler, D.G. Truhlar

Section D

Boston Convention & Exhibition Center
Room 156B

Calculating pKa's & Redox Potentials

Energy Applications

M. Coote, H. B. Schlegel, *Organizers, Presiding*

8:30 COMP 164. Oxidation-reduction at the cathode of a Li-ion battery. D.G. Truhlar, S. Huang, B. Wang, B. Wilson, Y. Fang, N. Tran, A. Stein

9:00 COMP 165. Redox potential and pK_a descriptors for exploring the catalysis of renewables. J.A. Keith

9:30 COMP 166. Covalency in the lanthanide series: Ce(III) vs. Ce(IV) — what a difference an electron makes. R.L. Martin

10:00 Intermission.

10:20 COMP 167. Regulation of redox potentials of W-alkylidene complexes by ligand design. B. Rudshteyn, V.S. Batista

10:50 COMP 168. Withdrawn.

Section E

Boston Convention & Exhibition Center
Room 151B

Drug Discovery

Applications of Computer-aided Drug Design

Y. Tseng, *Organizer*

Y. Zhou, *Presiding*

8:30 COMP 169. Computational design and first-in-human studies of a biased (functionally selective) Apelin GPCR agonist. R.C. Glen, A.P. Davenport

9:00 COMP 170. First cyclization of sesquiterpene cations is as (E)-(Z) as that. C.S. Hamann, M. Lodewyk, D.J. Tantillo

9:30 COMP 171. Pred-HERG 2: An updated web-accessible computational tool for predicting cardiac toxicity. R. Braga, V.M. Alves, M.F. Silva, E. Muratov, D. Fourches, L.M. Liao, A. Tropsha, C.H. Andrade

10:00 Intermission.

10:15 COMP 172. Understanding and solving ADME/Tox issues in peptide-based drug discovery using novel computation tools in CMDInventus. A.S. Bayden, J. Audie, J.T. Swanson, M.A. Jarosinski, D.J. Diller

10:45 COMP 173. Development, validation, and application of CMDInventus to enable structure-based peptide drug design and discovery. D.J. Diller, J.T. Swanson, A.S. Bayden, M.A. Jarosinski, J. Audie

11:15 COMP 174. Withdrawn.

11:45 COMP 175. Design of a catalytic scavenger for organophosphorous compounds. J. Chemelle, I. Farnery, F. Nachon, X. Brazzolotto, C. touvrey, R. Terreux

Herman Skolnik Award Symposium

Sponsored by CINF, Cosponsored by COMP and MEDI

Electronic Structure Methods for Large Systems

Excited States and Strongly Correlated Electrons

Sponsored by PHYS, Cosponsored by COMP

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Proton and Electron Transport

Sponsored by PHYS, Cosponsored by COMP

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Sponsored by PHYS, Cosponsored by COMP

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 157A

Functional Polymers: Connecting Modeling and Experiment

Biological and Bioinspired Polymers

W. C. Swope, *Organizer*

H. Ashbaugh, S. W. Rick, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 COMP 176. Tuning collector substrate chemistry to manipulate the motion signatures of adhering particles: Capture, rolling, and arrest. M.M. Santore, S. Kalasin

2:10 COMP 177. Effect of monovalent vs. divalent ions on structure and side-chain interactions in a biomimetic polymer. M.D. Baer, C.J. Mundy, M.D. Daily

2:40 COMP 178. PB-SAM: A novel solution to the Poisson-Boltzmann equation for applications in polymer membrane design. M. Soniat, L. Felberg, T.L. Head-Gordon

3:10 Intermission.

3:30 COMP 179. Computational assessment of heparin-chemokine binding. A. Singh, W. Kett, I. Severin, I. Agyekum, J. Duan, I. Amster, A.E. Proudfoot, D.R. Coombe, R.J. Woods

4:00 COMP 180. Computational investigations of functional arylamide foldamer. Z. Liu, A. Abramyan, V. Pophristic

4:30 COMP 181. Investigation on the microscopic structure of cyclic polymers from zwitterionic polymerization. X. Li, A. Li, G. Sternhagen, P. Du, R. Kumar, D. Zhang

Section B

Boston Convention & Exhibition Center
Room 156A

Molecular Dynamics Simulations in Drug Discovery

Drug Discovery and Development Related Applications

V. Hornak, *Organizer*

G. Cui, D. Shivakumar, *Organizers, Presiding*

1:30 COMP 182. May the (dual) force be with you: Polarizable AMOEBA free energies at the speed of fixed charge force fields. I. Nessler, J. Park, L.L. Stevens, M.J. Schnieders

2:00 COMP 183. Computational enzyme engineering and computer aided drug design: Similarities, challenges, and opportunities facilitated through Markov state models. G. Kiss, V.S. Pande

2:30 COMP 184. Uncoupling the structure-activity relationship of β_2 adrenergic receptor ligands from membrane binding. C. Dickson, V. Hornak

3:00 Intermission.

3:15 COMP 185. Withdrawn.

3:35 COMP 186. Combating drug resistance: Lessons from the viral proteases of HIV and HCV. C. Schiffer

4:05 COMP 187. Molecular dynamics simulation of drug-lipid membrane interaction. X. Cheng

4:35 COMP 188. Targeting the more "druggable" protein states of Bcl-x_L in a highly dynamic protein-protein interaction system. L. Xing, Z. Guo, A. Thorarensen, S. Thaisrivongs

5:05 Panel Discussion.

Section C

Boston Convention & Exhibition Center
Room 156C

Quantum Chemistry

E. V. Patterson, *Organizer*

Q. Jia, *Presiding*

1:30 COMP 189. DGDF: Massively parallel method for large scale density functional theory calculations. W. Hu, L. Lin, C. Yang

2:00 COMP 190. Linear scaling density functional theory based on local seamlessly interconnected orbital domains. R. Khaliullin

2:30 COMP 191. Reduced-cost sparsity-exploiting algorithm for solving coupled-cluster equations. J. Brabec, C. Yang, A. Krylow, E. Epifanovsky, E. Ng

3:00 Intermission.

3:15 COMP 192. Development of the multicomponent coupled-cluster theory for investigating non-adiabatic electron-nuclear interactions in confined chemical systems. B. Ellis, A. Chakraborty

3:45 COMP 193. Systematically improvable multiscale solver for correlated electron systems. A. Kananenka

4:15 COMP 194. Increasing the applicability of strong correlated methods: Parallel implementation of SplitGAS in NWChem. K.D. Vogiatzis, W. Dejong, L. Gagliardi

4:45 COMP 195. Excited states of molecules in bulk clusters using expectation-value equations-of-motion coupled-cluster theory applied to bulk limit DNA. J.N. Byrd, R. Molt, B. Sanders, R.J. Bartlett

Section D

Boston Convention & Exhibition Center
Room 156B

Calculating pKa's & Redox Potentials

Biological Applications

M. Coote, H. B. Schlegel, *Organizers, Presiding*

1:30 COMP 196. Is there sufficient accuracy in current redox potential calculations to predict which amino acid will reduce a DNA base lesion? D. Close

2:00 COMP 197. Redox properties of nucleic acids: From dielectric models to path integral-based molecular simulations. P. Slavicek

2:30 COMP 198. Virtual mixture approach to the study of multistate equilibrium: Application to constant pH simulation in explicit water. X. Wu, B. Brooks

2:50 Intermission.

3:10 COMP 199. Reduction potentials of one-electron oxidized DNA bases, base pairs, and their analogs: A DFT and electrochemical study. A. Kumar, A. Adhikary, L. Lin, M.D. Sevilla

3:40 COMP 200. Continuum solvation with cavity scaling for calculating pKa's and redox potentials of intermediates in DNA oxidation and in water splitting catalysis. H.B. Schlegel

Section E

Boston Convention & Exhibition Center
Room 151B

Drug Discovery

Free Energy Calculation

Y. Tseng, *Organizer*

B. C. Fochtman, *Presiding*

1:30 COMP 201. Single 3D-QSAR models from template CoMFA that predict all ChEMBL-tabulated affinities. R.D. Cramer

2:00 COMP 202. Fast structure-based scaffold hopping with Contour[®]. Z. Liu, Y. Zheng, K. fan, D.A. Claremon, R.E. Gregg, S.B. Singh

2:30 COMP 203. Ligand-protein binding and ligand-based virtual screening using maximum clique algorithm. D. Janezic, J. Konc

3:00 Intermission.

3:15 COMP 204. Predicting potential protein-protein binding sites as pattern generator for further biological experiments. C. Jaeger, A. Stephan, S. Schilling, M. Buchholz

3:45 COMP 205. Fast FTflex: Efficient computational solvent mapping with flexible sidechains. B. Xia, S. Vajda, D. Kozakov

4:15 COMP 206. Homology modeling of the mTOR kinase domain and application to inhibitor design and optimization. L. Xiao

Herman Skolnik Award Symposium

Sponsored by CINF, Cosponsored by COMP and MEDI

Electronic Structure Methods for Large Systems

Ab Initio Molecular Dynamics

Sponsored by PHYS, Cosponsored by COMP

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

TUESDAY EVENING

Section A

Westin Boston Waterfront
Galleria

NVIDIA GPU Award

M. Berger, *Organizer*

6:00 - 8:00

COMP 207. Unraveling protein-protein interactions at the blood-brain barrier tight junctions using GPU-accelerated software platform and libraries. **F. Irudayanathan**, S. Nangia

COMP 208. From natural systems to technological innovation: Studying excitonic systems of tens of thousands of molecules using GPUs. **N.P. Sawaya**, J. Huh, T. Fujita, S.K. Saikin, A. Aspuru-Guzik

COMP 209. Insights into the effect of metal ions and conformational change on binding between protective antigen and tumor endothelial marker 8. **Z. Jia**, C. Ackroyd, T. Han, V. Agrawal, Y. Liu, K.A. Christensen, B.N. Dorniny

COMP 210. GPU-enabled design of artificial histone-like nanoparticles for DNA wrapping. **J.A. Nash**, A. Kwansa, Y.G. Yingling

COMP 211. Acceleration of virtual screening using GPUs. **S. Sirimulla**, M. Koebel, G. Schmadeke

Section A

Westin Boston Waterfront
Galleria

Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:00

COMP 212. Computational lead discovery targeting botulinum neurotoxin serotype E. **Y. Zhou**, B.E. McGillick, Y. Teng, I. Ojima, S. Swaminathan, R.C. Rizzo

COMP 213. DFT calculation investigating the mechanism for the synthesis of nano gold. **S. Ghaoui**, H.B. Pham, T. Pham

COMP 214. DFT study of competitive pathways for reductive functionalization of methyl ligands by 3d metal catalysts. **H. Fallah**, T. Cundari, F. Horng

COMP 215. Rhodium catalyst for single-step styrene production. **S. Karbalaei Khani**, B.A. Vaughan, M.S. Webster-Gardiner, T. Gunnoe, T. Cundari

COMP 216. Glycoside hydrolases: Predicting the function of Structural Genomics proteins of unknown function. **S. Somasundaram**, R. Parasuram, Z. Wang, C.L. Mills, P.J. Beuning, M.J. Ondrechen

COMP 217. Function prediction for the Structural Genomics members of the Haloacid Dehalogenase (HAD) superfamily. **M. Touch**, E.M. Mozur, M.J. Ondrechen

COMP 218. Predictive model for polymer coating materials and their antifouling activity: Application of mixture-QSAR approach. **B. Rasulev**, **F. Jabeen**, S. Stafslin, B.J. Chisholm, J. Bahr, M. Ossowski, P.R. Boudjouk

COMP 219. Inhibition of glycolytic pathway enzymes: Analysis of plasmodium falciparum and human triosephosphate isomerase ligand interactions. **N.Y. Forlemu**, **N. Alexandriu**

COMP 220. Developing the benchmark for protein macrocycle docking. **Z. Sun**, D. Beglov, D. Kozakov, D. Hall, S. Vajda

COMP 221. Intrinsic effects of glycosylation on protein folding and stability. **S. McHugh**

COMP 222. Computational exploration of protein dynamics to optimise ligand interactions and binding kinetics. **M. Date**, N. O'Connell, A.D. Ferguson, J. Dowling, J. Manchester

COMP 223. Simulations of water-soluble, helical meta-poly(phenylene ethynylene) foldamers: Parameterization, structure, and function. **A. Booras**, B. Abrams

COMP 224. Design of novel drug-like molecules in the context of protein binding site using Contour[®] growth algorithm and CoreHop[™] function. **Z. Liu**, P. Lindblom, K. Fan, Y. Zheng, D.A. Claremon, R.E. Gregg, S.B. Singh

COMP 225. Investigation of the catalytic mechanism of beta lactamase as a function of low barrier hydrogen bonds through the use of molecular dynamics simulations and QM/MM calculations. **A. Parisi-Goldblatt**, M. Kemp, Y. Chen, H.L. Woodcock

COMP 226. Surface structures of Cu-Ni binary alloy and interactions with Ag cluster: Monte Carlo simulations with EAM potentials. **D. Chung**, D. Kim, H. Guk, K. Choi, S. Choi

COMP 227. Understanding the Comparative Molecular Field Analysis (CoMFA) within the framework of molecular quantum similarity and chemical reactivity descriptors using density function theory. **A. Morales-Bayuelo**

COMP 228. Structural and dynamical effects of plasma treatment on model cell membranes: Molecular dynamic simulations of oxidized DOPC lipid bilayer membrane systems. **S. Kim**, R. Chang

COMP 229. Understanding the mechanism of enzyme-catalyzed CO₂ reduction reaction: QM/MM studies of NAD-dependent formate dehydrogenase. **H. Kim**, R. Chang

COMP 230. Withdrawn.

COMP 231. Merging human-readable and computer-readable structure data representations into unified documents. **W. Ihlenfeldt**

COMP 232. Protein structure refinement promoted by Molecular Dynamics, physics-based force fields and implicit solvent. **H. Huang**, H. Nguyen, J. Maier, V. Perrone, C.L. Simmerling

COMP 233. Calculations of pK_a's and redox potentials of nucleobases with explicit waters and polarizable continuum solvation. **B. Thapa**, H. Schlegel

COMP 234. Modeling solution X-ray scattering of biomacromolecules using explicit-solvent simulations and fast Fourier transfer. **D. Tong**, L. Lu

COMP 235. Computational analysis of loops at protein-protein interfaces for macrocycle probe design. **M. Bird**, T.R. Siegert, J. Kritzer

COMP 236. Structure and thermodynamics of heparin bound to carbon nanotubes. **J.J. Janke**, A.E. Garcia, R.J. Linhardt

COMP 237. Docking of PPI inhibitors to the protein-bound structures. **S. Belkin**, P. Kundrotas, I. Vakser

COMP 238. Organic conversions: An aid in perspective. **L. Whitehead**, R. Lawrence, M.D. Mackey

COMP 239. Mitishamba; A database of natural products from Kenya for drug discovery. **S. Dereese**, A. Ndakala, M. Rogo, J. Oyim, S. Manyim, N. Dudnik, P. Ertl, L. Whitehead

COMP 240. LiveDesign — our evaluation: A progress report. **L. Whitehead**, N. Stieff, P. Gedeck, J. Dowling, M. Brewer, M.L. Hall, H. Huang, O.J. Ingham

COMP 241. Identifying mutation resistant ligands in high-throughput virtual screening with the substrate envelope hypothesis. **M. Repasky**, J.L. Banks, I. Tubert-Brohman, C. Schiffer, W. Sherman

COMP 242. Lead refinement using de novo design algorithms: Application to HIVgp41. **B.C. Fochtman**, R.C. Rizzo

COMP 243. Implementation of a genetic algorithm for DOCK to aid in de novo design. **C. Singleton**, W.J. Allen, R.C. Rizzo

COMP 244. Quantitative structure activity relations (QSARs) to identify liquid-liquid extraction solvents. **R.B. Ross**, M. Nakamura, D. Fanselow, J. Reed, J. Miller, B. Haislet

COMP 245. Quantum mechanical non-Boltzmann Bennett: A novel approach to ensure relevant sampling in free energy simulation based on energetic overlap between levels of theory. **P.S. Hudson**, G. Koening, F.L. Kearns, S. Borech, H.L. Woodcock

COMP 246. Open chemistry: A suite of tools for computational chemistry data, visualization, and analytics. **M.D. Hanwell**

COMP 247. Quantifying DNA sequence artifacts in encoded library technology data processing. **N.V. Prabhu**, A. Olszewski, K.E. Lind, N. Carlson, J. Messer

COMP 248. Integrated design environment: Toward data-driven compound design. **P. Iyer**, G.A. Bakken, C. Butler, J. Klug-Mcleod, C. Poss, A.M. Wassermann

COMP 249. Use of free energy calculations to assess small molecule binding poses in the HIVgp41 conserved hydrophobic pocket. **T.D. McGee**, W.J. Allen, R.C. Rizzo

COMP 250. Self-consistent charge-dependent interaction models for use in condensed phase molecular simulation. **E.R. Kuechler**, T.J. Giese, D.M. York

COMP 251. Developing monovalent ion parameters for the optimal point charge (OPC) water model. **J.C. Dood**, B.P. Krueger

COMP 252. First-principles density functional theory modeling study on the redox chemistry of graphene oxides affected by oxygen functional groups. **J. Park**, S. Kim, K. Kim, S.W. Lee, S.S. Jang

COMP 253. Active machine learning for the detection of novel bioactive molecules and efficient model building. **D. Reker**, T. Rodrigues, P. Schneider, G. Schneider

COMP 254. Metal organic frameworks as vehicles for drug delivery. **K. Taylor-Edinbyrd**, T. Li, R. Kumar

COMP 255. Computational method for studying the photophysical properties and photostability of BODIPY dyes. **K. Komoto**, T. Kowalczyk

COMP 256. Investigation of acene-containing covalent organic frameworks as candidates for singlet fission. **V. Laszlo**, T. Kowalczyk

COMP 257. Exploring the use of new internal coordinate classes in geometry optimization using a generalized internal coordinate engine. **N. Giddings**, J.L. Sonnenberg, A.V. Marenych, M.J. Frisch, H.P. Hratchian

COMP 258. Transition state analysis and kinetic isotope effects in Zn(II)-catalyzed RNA transphosphorylation reactions. **H. Chen**, M.E. Harris, D.M. York

COMP 259. Structure-based design, synthesis, and evaluation of non-zinc-chelating inhibitors selective for matrix metalloproteinase 13. **K.V. Mahasenan**, M. Bastian, M. Gao, D. Ding, E. Frost, M.F. Chang, S. Mobashery

COMP 260. Kinetic network models reveal non-native salt-bridge effects on alpha-helix folding. **G. Zhou**

COMP 261. Density functional theoretical study on benzotriazole-containing planar conjugated polymers for efficient polymer field-effect transistors. **S. Hwang**, H. Woo

COMP 262. Examining the role of pre-organization in the binding of cyclic RGD peptides to $\alpha_2\beta_2$ integrin using a free energy perturbation approach. **A. Wakefield**, V.A. Voelz

COMP 263. Seeking alpha-synuclein ligands by structure-based in silico screening. **R. Kiss**, F. Aigbirhio, G. Tóth

COMP 264. Theoretical study of mono- and bimetallic catalysts for small molecules activation. **S. Bernales Candia**, K.D. Vogiatzis, L.J. Clouston, R. Siedschlag, R. Carlson, C. Lu, L. Gagliardi

COMP 265. Examining the conformational dynamics of the N-terminal region of MDM2 using Markov State Model approaches. **G.A. Pantelopulos**, V.A. Voelz

COMP 266. Parameterization of density functional tight-binding for the lithium intercalated graphite. **D. Kim**, D. Chung, H. Guk, K. Choi, S. Choi

COMP 267. Augmented minimal basis sets with optimized diffuse functions for fast and accurate calculations of optical rotatory dispersion. **T. Aharon**, M. Caricato

COMP 268. QSPR for correlation and prediction of the refractive indices of diverse data set of polymers. **M. Chen**, F. Jabeen, B. Rasulev, M. Ossowski, P. Boudjouk

COMP 269. Quantitative structure-property relationship (QSPR) study of glass transition temperatures for diverse set of polymers. **M. Chen**, F. Jabeen, B. Rasulev, M. Ossowski, P. Boudjouk

COMP 270. Using SAR data to evaluate poses in multicopy docking. **D.W. Moreland**

COMP 271. Development of highly self-consistent and predictive CoMFA and CoMSIA models for anthrax toxin lethal factor (LF) inhibitors. **T. Chiu**, E.A. Amin

COMP 272. DFT studies of the vibrational spectra of salicylic acid and related compounds. **W. Bosma**, M. Appell

COMP 273. Withdrawn.

COMP 274. Mutually polarizable model for water and the calculation of binding affinities. **M.L. Laury**, J.W. Ponder

COMP 275. Theoretical comparative study of oxygen adsorption on neutral and anionic Ag_n and Au_n clusters (n = 2 - 25). **J.D. Watts**, M. Liao, M. Huang

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 276.** Reactive molecular dynamics simulations of water-assisted cation diffusion in Cu-SSZ-13 zeolite. O. Sainbayar, J. Dumel, J.F. McCleerey, E. Gutschmidt, **E. Jaramillo**
- COMP 277.** Computational study of domain registration of lipid rafts. **N. Chen**, P.B. Moore
- COMP 278.** Temperature replica exchange simulations of major ampullate spidroin 1. **G.M. Gray**, J.L. Yarger, A. Van Der Vaart
- COMP 279.** First principles studies of gold nanoparticles and end terminated thiolates. **J.K. Roy**, H.P. Pinto, E. Vasquez, K.B. Walters, J.R. Leszczynski
- COMP 280.** Fragment-based prediction of drug distribution across the head-group and core strata of a phospholipid bilayer: Hexadecane-diacetyl phosphatidyl choline as surrogate phases. **S.K. Natesan**, S.M. Lynch, R. Subramaniam, I. Mathew, Z. Wang, S. Balaz
- COMP 281.** Getting a grip: Computational screening of functional supramolecular systems. **O. Chaarawi**, A.H. Steeves
- COMP 282.** Multiscale and multistate extrapolation of UV-Vis spectra. **M. Caricato**, **S. Ren**
- COMP 283.** Theoretical investigation of the neutral, cationic, and anionic criegee biradicals in the Earth's atmosphere. **S. Alhowity**, S. Guha
- COMP 284.** Improved prediction of peptoid structure and dynamics. **S. Mukherjee**, G. Zhou, V.A. Volz
- COMP 285.** Creating focused libraries for protein engineering. **A. Ajamian**
- COMP 286.** Rationalizing nonstandard interactions in ligand design: The duality of halogens. **C. Williams**
- COMP 287.** mFES: A robust molecular finite element solver for electrostatic energy computations. **I. Sakalli**, **E. Knapp**
- COMP 288.** Withdrawn.
- COMP 289.** Scalable, linear-time dynamic cutoff algorithm for molecular dynamics. **P. Springer**, P. Bientinesi, **A.E. Ismail**
- COMP 290.** Fast Fourier Transform sampling on the manifolds for modeling protein-protein interactions. **D. Padhorny**, A. Kazennov, K. Porter, D. Hall, D. Ritchie, D. Kozakov
- COMP 291.** Withdrawn.
- COMP 292.** High throughput modeling of exposures to semi-volatile chemicals in articles of commerce. **C.I. Nicolas**, M. Goldsmith, R. Pearce, R. Setzer, J. Wambaugh
- COMP 293.** Novel, cell-trained approach to biological target-guided chemical tools and its application to *Mycobacterium tuberculosis*. **A.L. Perryman**, X. Wang, S. Li, S.D. Paget, T.P. Stratton, A.J. Olson, S. Ekins, J. Freundlich
- COMP 294.** Treatment of explicit electrons in the ReaxFF reactive molecular dynamics and applications to battery interfaces. **M. Islam**, G. Kolesov, E. Kaxiras, A.C. Van Duin
- COMP 295.** Finding complex ab-initio reaction pathways. **B. Schaefer**, S. Goedecker
- COMP 296.** Use de novo design to help optimize target specificity. **L. Wang**, B.B. Masek, B. Wendt, S. Nagy
- COMP 297.** Density-guided method for improving conformational sampling of linear, branched, and cyclic molecules. **A. Sepehri**, T. Loeffler, B. Chen
- COMP 298.** Leveraging fast, accurate macrocycle sampling for design and optimization. **D.J. Sindhikara**, T. Day, K. Borrelli
- COMP 299.** Withdrawn.
- COMP 300.** Using ligand-based methods in the absence of ligands: "Fake" ligands to the rescue. **I.J. Enyedy**, D. Hall, M.R. McGann
- COMP 301.** Protein Ligand derived conformational distributions: Analysis and use to drive docking input conformer generation. **P. Sanschagrin**, S. Gothe
- COMP 302.** Predictive sampling of long-timescale protein functional motions in explicit solvent. **X. Li**
- COMP 303.** In silico model for NaATM1 type ATP binding cassette transporter conformational transitions: Insights from targeted molecular dynamics simulations. **Y. Liu**, Z. Jia, T. Han, V. Agrawal, **B.N. Dominy**
- COMP 304.** Effect of accumulated mutations in plasmodium falciparum dihydrofolate reductase activity. **T. Han**, V. Agrawal, Y. Liu, Z. Jia, **B.N. Dominy**
- COMP 305.** Structure and dynamics of a model helix-junction-helix system at varying salt conditions using GPU-accelerated simulations. **M. Panteva**, G.M. Giambasu, D.M. York
- COMP 306.** Mechanism of water oxidation by a dimanganese molecular catalyst: DFT studies with implications for thermodynamic efficiency. **J.R. Buchwald**, P.H. Dinolfo
- COMP 307.** Withdrawn.
- COMP 308.** Inhibitor development targeting HER2 incorporating bridging water molecules. **J. Guo**, R.C. Rizzo
- COMP 309.** Withdrawn.
- COMP 310.** Understanding single stranded DNA: From structure and dynamics to physical adsorption on surfaces. **H. Kim**, Y.G. Yingling
- COMP 311.** Coarse-grained models of petrochemical solvents: Simultaneously capturing structure and thermodynamics. **N.J. Dunn**, W.G. Noid
- COMP 312.** Functional characterization of Structural Genomics proteins in the Crotonase Superfamily. **C.L. Mills**, P.J. Beuning, M. Ondrechen
- COMP 313.** Withdrawn.
- COMP 314.** Analytic gradients for many body dispersion interactions in condensed phase. **T. Markovich**, M.A. Blood-Forsythe, A. Aspuru-Guzik, R.A. DiStasio
- COMP 315.** Identifying protein conformational changes of agonist-induced PPAR- γ using molecular dynamics. **B. Boykin**
- COMP 316.** Protein slow conformational fluctuations play a pivotal role in protein-ligand binding: A case study on cyclooxygenase enzyme systems. **E.W. Aitchison**, L. Zheng, W. Yang
- COMP 317.** Computational studies on potential PET imaging ligands for Galectin-3 in pancreatic cancer tumors. **A. Walker**, G.A. Cisneros
- COMP 318.** GistPP (gist post processing): Tools for solvation structural and thermodynamic analysis and visualization. **S. Ramsey**
- COMP 319.** Strong tunable visible absorption predicted for silicenes using TDDFT calculations. **K.M. Weerawardene**, C.M. Aikens
- COMP 320.** Improving the reliability of predictions from classical molecular dynamics: The restrained electrostatic potential charge method and beyond. **H. Qi**, H.J. Kulik
- COMP 321.** Design of next-generation polymer electrolytes: A site network model for ion transport from mechanistic insight. **M.A. Webb**, B.M. Savoie, T.F. Miller
- COMP 322.** Unraveling the mechanism of RNase A with multiscale computational approach. **T.D. Dissanayake**
- COMP 323.** Building water models, a different approach. **S. Izadi**, R. Anandakrishnan, A.V. Onufriev
- COMP 324.** Polarisation induced electron localisation error. **S.G. Dale**, E.R. Johnson
- COMP 325.** Nature and strength of N---S and π ---S interactions. **V. Nziko**, S. Scheiner
- COMP 326.** Identifying allosteric modulation and evolution of dynamic networks in Muscarinic receptors. **V. Agrawal**, Z. Jia, T. Han, Y. Liu, **B.N. Dominy**
- COMP 327.** Charge penetration markedly improves the electrostatics of the AMOEBA force field model. **J. Rackers**, J.W. Ponder
- COMP 328.** Quantum chemistry in the cloud. **R.C. Fortenberry**
- COMP 329.** Lipid-protein interactions and transporter conformational change. **R.D. Hills**
- COMP 330.** Molecular dynamics to investigate metalloenzymes that process DNA and RNA. **V. Genna**, R. Gaspari, M. Dal Peraro, **M. De Vivo**
- COMP 331.** Computational investigation of monosubstituted boroxines(RH₂B₃O₃): Structure and formation. **N.Z. Rao**, J.D. Larkin, C.W. Bock
- COMP 332.** Electronic excitation dynamics in condensed phase systems under proton irradiation. **Y. Kanai**
- COMP 333.** Withdrawn.
- COMP 334.** Toward computational design of iron-based chromophores for solar energy conversion. **E. Jakubikova**
- COMP 335.** Sodium diffusion in Type I and Type II silicon clathrates. **J.G. Slingsby**, N.A. Rorrer, L. Krishna, E. Toberer, C.A. Koh, **C.M. Maupin**
- COMP 336.** Metalloproteins: Multiscale treatment and design, facilitated by new methodologies. **C.E. Valdez**, M.R. Nechay, **A. Alexandrova**
- COMP 337.** XBSF: Halogen bonding scoring function and its implementation into AutoDock Vina. **S. Sirimulla**
- COMP 338.** Valinomycin as a classical anionophore — mechanism and ion selectivity. **S.A. Kostina**
- COMP 339.** Investigating protein-ligand binding through the lens of local water structure. **K. Haider**, M.K. Gilson, T.P. Kurtzman
- COMP 340.** Structural characterization of the complex between the TRPV1 channel and the DkTx toxin. **C. Anselmi**, C. Bae, J. Kim, K.J. Swartz, J. Faraldo-Gomez

Section A

Westin Boston Waterfront
Galleria**The Chemical Computing Group Excellence Award for Graduate Students**C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP 338. Catalysis in metal organic frameworks: Ethylene oligomerization and methane to methanol conversion. **R. Carlson**, L. Gagliardi, V. Bernales**COMP 339.** Equation of motion coupled-cluster calculations of K-edge X-ray absorption spectra. **B. Peng**, P. LeStrange, J.J. Goings, X. Li**COMP 340.** Accurate, efficient, and insightful quantum chemistry calculations of non-covalent interactions for large systems. **K. Lao**, J. Herbert**COMP 341.** Multiscale simulation reveals a multifaceted mechanism of proton permeation through the influenza A M2 proton channel. **R. Liang**, H. Li, J.M. Swanson, G.A. Voth**COMP 342.** Psi4NumPy: A hybrid C++/python interpreted quantum chemistry programming environment. **D. Smith**, K. Patkowski

Section A

Westin Boston Waterfront
Galleria**The OpenEye Outstanding Junior Faculty Award**C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP 343. Insights into protein-lipidoid assembly from molecular dynamics simulations. **H. Yu**, D. Slough, Y. Lin**COMP 344.** Redefining the rules for ring closure through computations: Quantifying substrate and catalyst control with quantum chemistry. **R.S. Paton****COMP 345.** Design of multicomponent shape-tunable carriers. **M. Dutt****COMP 346.** Computational design of hepatitis C virus vaccine immunogens. **G. Hart**, A. Ferguson

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 157A**Functional Polymers: Connecting Modeling and Experiment****Responsive Polymers**H. Ashbaugh, *Organizer*S. W. Rick, W. C. Swope, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 COMP 347. Computational design of azobenzene-containing monomers for light-mediated ROMP. **Q. Zhou**, I. Fursule, B. Berron, M. Beck**9:10 COMP 348.** Predictive simulations of amorphous composites: Their ultimate thermomechanical properties. **A. Strachan****9:40 COMP 349.** Monitoring the onset and evolution of polymer stimuli responsiveness during synthesis. **C.A. McFaul**, Z. Zhu, M.F. Drenski, N. Soleimani, **W.F. Reed**

10:10 Intermission.

Technical program information known at press time.**The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015**

10:30 COMP 350. pH responsive polymers: Non-trivial coupling between molecular organization, physical interactions and chemical state. I. Szeifer

11:00 COMP 351. Molecular design of shape memory polymer fibers that are thermally responsive. M.A. Pasquinielli, S.S. Tallury, B. Pourdeyhimi, R. Spontak

11:30 COMP 352. Self-assembly and responsiveness in peptide-based block copolymers. G. Strange, I. Smith, C. Machado, D.A. Savin

Section B

Boston Convention & Exhibition Center
Room 156A

Computational Study of Water

Applications of Thermodynamics of "Small Water"

D. J. Sindhikara, *Organizer*

C. Dickson, *Presiding*

8:30 COMP 353. Quantifying the entropy of binding for water molecules in protein cavities by computing two-particle correlations. D.J. Huggins

9:00 COMP 354. Exploiting active-site solvation structure and thermodynamics for drug discovery and design. T.P. Kurtzman, K. Haider, M.K. Gilson

9:30 COMP 355. Role of waters in molecular recognition. W. Sherman

10:00 Intermission.

10:15 COMP 356. On the study of water oxygen-hydrogen correlations toward efficient calculation of solvation entropies and enthalpies in biomolecular systems. C. Velez Vega, D. Mckay, T. Kurtzman, V. Aravamuthan, R.A. Pearlstein, J. Duca

10:45 COMP 357. Discrete solvent based method for the prediction of protein hydration sites. P. Setny

11:15 COMP 358. Old dog, new tricks: Free energy calculations with grand canonical Monte Carlo. G. Ross, M. Bodnarchuk, J. Essex

Section C

Boston Convention & Exhibition Center
Room 156C

Quantum Chemistry

E. V. Patterson, *Organizer*

B. Boykin, N. Ippolito, *Presiding*

8:30 COMP 359. Overcoming spin contamination with approximate projection models. H.P. Hratchian

9:00 COMP 360. Application of absolutely localized molecular orbital based energy decomposition analysis for second-order Møller-Plesset perturbation theory to non-covalent interactions. J. Thirman, M.P. Head-Gordon

9:30 COMP 361. New and improved energy decomposition analysis: Well-defined physical contributions to intermolecular interactions from density functional theory calculations? P. Horn, M.P. Head-Gordon

10:00 Intermission.

10:15 COMP 362. Resolving multiple spin contaminants using approximate projection. L.M. Thompson, H.P. Hratchian

10:45 COMP 363. Orbital analysis of molecular optical activity based on configuration rotatory strength. M. Caricato

11:15 COMP 364. Versatile platform for the simulation of vibronic spectra. J. Bloino, A. Baiardi, V. Barone

11:45 COMP 365. Implicit matching pursuit method of quantum dynamics. V.S. Batista, A. Markmann

Section D

Boston Convention & Exhibition Center
Room 156B

Materials Science

M. Haranczyk, *Organizer*

R. S. Paton, *Presiding*

8:30 COMP 366. Natural gas and hydrogen storage in MOFs: The effect of geometry and charge distributions. E. Tsvion, M.P. Head-Gordon

9:00 COMP 367. Development of an improved molecular dynamics force field for surface-adsorption simulations of molybdenum disulfide (MoS₂). G.M. Leuty, R. Berry, C. Muratore, V. Varshney, C.H. Turner

9:30 COMP 368. Hybrid QM/MM simulation of bond scission in thermoset polymers. S.A. Barr, G. Kedziora, A. Ecker, R.J. Berry, J. Moller, T. Breitzman, G.M. Leuty

10:00 Intermission.

10:15 COMP 369. Tuning the electronic structure of anatase through fluorination. D. Corradini, D. Dambournet, M. Salanne

10:45 COMP 370. Non-equilibrium multiscale coarse-grained simulation of energetic molecular crystalline materials. S. Izvekov, M.S. Sellers, B.C. Barnes, J.P. Larentzos, J.K. Brennan, B.M. Rice

11:15 COMP 371. Computational nanoparticle screening for immune stimulation. A. Golius, L. Gorb, J.R. Leszczynski, O. Isayev

Section E

Boston Convention & Exhibition Center
Room 151B

Drug Discovery

Structure-based Approaches

Y. Tseng, *Organizer*

C. Singleton, *Presiding*

8:30 COMP 372. Free energy calculations in drug discovery. R. Abel, T. Lin, B. Kim, L. Wang, S. Mondal, Y. Deng, J. Knight

9:00 COMP 373. Practical assessment of evaluating free energy differences between classical and QM Hamiltonians. C.I. Cave-Ayland, C. Skylaris, J. Essex

9:30 COMP 374. Fast and accurate approach for binding free energy calculations for protein-ligand complexes: A Movable Type sampling method. H. Zhong, Z. Zheng, K.M. Merz

10:00 Intermission.

10:15 COMP 375. Molecular free energy calculation using the Movable Type method with conformer identification program. Z. Zheng, K.M. Merz

10:45 COMP 376. Free energy calculations with FEP+: Retrospective validation and prospective applications. W. Sherman

11:15 COMP 377. Testing the effects of including receptor desolvation in docking calculations. T.E. Balius, M. Fischer, C.N. Nguyen, A. Cruz-Balberdy, T.P. Kurtzman, M.K. Gilson, B. Shoichet

Electronic Structure Methods for Large Systems

Correlated Wavefunction Approaches

Sponsored by PHYS, Cosponsored by COMP

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by CINF, Cosponsored by AGRO, COMP, ENVR and MEDI

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Modeling pH and Water Dependent Properties

Sponsored by PHYS, Cosponsored by COMP

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Sponsored by PHYS, Cosponsored by COMP

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 157A

Functional Polymers: Connecting Modeling and Experiment

Polymer Self-assembly and Polymers at Interfaces

H. Ashbaugh, S. W. Rick, *Organizers*

W. C. Swope, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 COMP 378. Polydispersity dominates the self-assembly of polymer grafted nanoparticles. S. Kumar

2:10 COMP 379. Tapered block copolymers: Controlling segment sequence to improve materials properties. T.H. Epps

2:40 COMP 380. Computational investigations on the structure and dynamics of polyelectrolyte micelles using molecular dynamics simulation. X. Li, P. Du, S. Xuan, G. Sternhagen, D. Zhang, R. Kumar

3:10 Intermission.

3:30 COMP 381. Theory-informed design of functional soft matter for energy science and technology. B. Sumpter

4:00 COMP 382. Directed block polymer assembly: Equilibrium and non equilibrium considerations. A. Ramirez-Hernandez, J.J. De Pablo

4:30 COMP 383. Exploring the role of covalent architecture in the behavior of amphiphilic polymers. S.M. Grayson, B. Zhang, Y. Wang

Section B

Boston Convention & Exhibition Center
Room 156A

Computational Study of Water

Water Methods & Biological Phenomena

D. J. Sindhikara, *Organizer*

J. D. Gough, *Presiding*

1:30 COMP 384. Connecting free energy surfaces in implicit and explicit solvent: An efficient method to compute conformational and solvation free energies. N. Deng, B. Zhang, R.M. Levy

2:00 COMP 385. Study of protein-spanning water networks and implications for protein-protein interactions mediated through hydrophobic effects. D. Cui

2:30 COMP 386. Molecular dynamics studies of retroviral arginine-rich peptide-RNA recognition. M.C. Nagan

3:00 Intermission.

3:15 COMP 387. On the importance of water-protein and water-ligand interactions in opioid receptors. J.D. Gough, D.M. Kilburg, B. Olson

3:45 COMP 388. Water-choreography reveals intrinsic filtering mechanism: The antibiotic pathway through *E. Coli* porins. S. Acosta-Gutierrez, C. Matteo, M. Scorciapino, I. Bodrenko

4:15 COMP 389. Computational studies of the protonation of a strong base by carbonic acid in an aqueous solution. P.M. Kiefer, S. Daschakraborty, D. Pines, E. Pines, J.T. Hynes

Section C

Boston Convention & Exhibition Center
Room 156C

Quantum Chemistry

E. V. Patterson, *Organizer*

E. G. Kratz, *Presiding*

1:30 COMP 390. Understanding the origins of stereoselectivity in organic reactions: A quantum mechanical approach. V. Aviyente

2:00 COMP 391. Ab initio quantum mechanical calculations on Δ -9 THC and important neurotransmitters: Implications for potential receptor interactions. S.D. Baldwin

2:30 COMP 392. Withdrawn.

3:00 Intermission.

3:15 COMP 393. Solvation and primary structure effects on the deamidation of asparaginyl residues in peptides. J. Van der Mynsbrugge, S. Moors, V. Van Speybroeck, S. Catac

3:45 COMP 394. Environmental fate in organic contaminants: The role of quantum chemistry. N.J. Deyonker, W.A. Alexander, K.A. Charbonnet

4:15 COMP 395. Automatic generation of detailed chemical models for chlorinated hydrocarbons. F. Seyedzadeh, R.H. West, R. Low, A. Sharratt, C. Giddisb

4:45 COMP 396. Computational chemistry portal: Publishing results onto the semantic web. N.S. Ostlund, M. Sopek, B. Wang, S.J. Chalk

Section D

Boston Convention & Exhibition Center
Room 156B

Materials Science

M. Haranczyk, *Organizer*

L. Valenzano, *Presiding*

1:30 COMP 397. Computationally driven discovery of new generation blue OLEDs. R. Gomez Bombarelli, J. Aguilera-Iparraguirre, T. Hirzel, M.A. Forsythe, A. Aspuru-Guzik

2:00 COMP 398. Shape matters: 1D, 2D, and 3D quantum confinement in semiconducting nanocrystals. J.A. Scher, A. Chakraborty

2:30 COMP 399. Unraveling the coupling between demixing and crystallization in mixtures. C. Desgranges, J. Delhommelle

3:00 Intermission.

3:15 COMP 400. Trading certainty for speed: Extrapolating uncertainty due to coarse-graining of molecular dynamics simulations. T. Rosch, P. Patrone, F.R. Phelan

3:45 COMP 401. Development of negative stress-optical coefficient materials assisted by quantitative structure property relationship (QSPR) modeling. **H. Wang, W. Zhou, S. Chang, N. Pothayee, P. Agawal, J. Storer**

4:15 COMP 402. Computationally optimizing fullerenols as specific non-covalent drug carriers: Discriminating H-bond anchoring, van der Waals adhesion, and electrostatic interactions. **J.A. Mayer, S.W. Cranford**

Section E

Boston Convention & Exhibition Center
Room 151B

Drug Discovery

Ligand-based Approaches

Y. Tseng, *Organizer*

E. Gianti, *Presiding*

1:30 COMP 403. Ligand deconstruction: Why some fragment binding positions are conserved and others are not. **D. Kozakov, D. Hall, S. Jehle, L. Luo, S.O. Ochiana, E. Jones, M.P. Pollastri, K.N. Allen, A. Whitty, S. Vajda**

2:00 COMP 404. Mix-and-match (Q) SAR modelability. **A. Zakharov, O. Tarasova, V. Poroiikov, M.C. Nicklaus**

2:30 COMP 405. Exploring protein families with Profile-QSAR. **L. Tian, E.J. Martin, V.R. Polyakov**

3:00 Intermission.

3:15 COMP 406. Polypharmacology modeling using deep learning approaches. **O. Isayev, R. Politi, A. Tropsha**

3:45 COMP 407. New approach to identifying common pharmacophores using pharmacophore feature-based shape alignment. **M. Repasky, S. Dixon**

4:15 COMP 408. Significance of significance: Finding meaning in molecular similarity. **P.C. Hawkins**

Electronic Structure Methods for Large Systems

Novel Representations and New Contraction Schemes

Sponsored by PHYS, Cosponsored by COMP

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by CINF, Cosponsored by AGRO, COMP, ENVR and MED1

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Macromolecular Interactions

Sponsored by PHYS, Cosponsored by COMP

THURSDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 157A

Functional Polymers: Connecting Modeling and Experiment

Polymeric Properties and Polymer-Nanoparticle Mixtures

S. W. Rick, *Organizer*

H. Ashbaugh, W. C. Swope, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 COMP 409. Determining the molecular weight and molecular weight distribution of polymer brushes grown via surface-initiated polymerization from flat substrates. **J. Genzer**

9:10 COMP 410. Bridging length scales from the atomistic to the mesoscale with thermodynamically consistent coarse-grained models. **M. Guenza**

9:40 COMP 411. In silico design: Synthesis and characterization of functional polymeric materials. **C.M. Colina**

10:10 Intermission.

10:30 COMP 412. Computational insight into the polymerization of conjugated electroluminescent polymer PPV: Diradical character of monomers and dimers. **J. Durdevic, S. Wouters, J. Romanova, A. Shimizu, B. Champagne, T. Junkers, D.J. Vanderzande, D. Van Neck, M.E. Waroquier, V. Van Speybroeck, S. Catac**

11:00 COMP 413. Using simulations and experiments to connect the design of polymer functionalization on the nanoparticles to morphology and macroscopic properties of polymer nanocomposites. **A. Jayaraman, T.B. Martin, R. Krishnamoorti, K. Mongcopa**

11:30 COMP 414. Conformations and dynamics of molecular combs and bottle-brushes in melts. **M. Rubinstein, W. Daniel, J. Paturej, K. Matyjaszewski, S. Sheyko**

Section B

Boston Convention & Exhibition Center
Room 156A

Computational Study of Water

Water Models, Phenomena, & Applications

D. J. Sindhikara, *Organizer*

C. H. Andrade, *Presiding*

8:30 COMP 415. Donor-acceptor interactions in the hydrogen-bond networks of hexagonal ice and liquid water. **R. Khaliullin**

9:00 COMP 416. Determining melting temperature of ice with the Effective Fragment Potential. **C.H. Borca, L.V. Slipchenko**

9:30 COMP 417. Molecular dynamics investigation of deeply supercooled water using a direct polarization model. **L. Wang, C. Schwantes, T.J. Lane, J. Seilberg, A.R. Nilsson, T.J. Martinez, V.S. Pande**

10:00 Intermission.

10:15 COMP 418. Computational study of nucleation in acid catalyzed system. **T. Loeffler, A. Sapehri, R. Kumar, B. Chen**

10:45 COMP 419. Withdrawn.

Section C

Boston Convention & Exhibition Center
Room 156C

Quantum Chemistry

E. V. Patterson, *Organizer*

M. L. Laury, *Presiding*

8:30 COMP 420. Electronic structure of the cofacial, oxo-bridged dicobalt complex of a hexacarboxamide cryptand ligand. **K.D. Vogiatzis, J. Stauber, E.D. Bloch, C.C. Cummins, D.G. Nocera, L. Gagliardi**

9:00 COMP 421. Computational study of $\text{Cr}_3(\text{dpa})_3(\text{NCS})_2$: Electronic structure and potential energy surface along the chromium chain. **M. Spivak, X. López, C. de Graaf**

9:30 COMP 422. Functional mimic approach toward rational design of bioinspired iron molecular electrocatalyst for H_2 oxidation. **N. Kumar, J. Darmon, M. Helm, S. Raugai**

10:00 Intermission.

10:15 COMP 423. Establishing the zeolite SSZ-13 as test system for quantum chemical methods. **F. Goeltl, P. Sautet, I. Hermans**

10:45 COMP 424. Multiconfiguration pair-density functional theory: Applications for transition metal systems. **R. Carlson, G. Li Manni, L. Gagliardi, D.G. Truhlar**

11:15 COMP 425. Jahn-Teller dynamics in selected transition-metal compounds. **A.V. Marenich**

Section D

Boston Convention & Exhibition Center
Room 156B

Materials Science

M. Haranczyk, *Organizer*

L. E. Achenie, *Presiding*

8:30 COMP 426. Ab initio molecular dynamics study of a dye sensitized solar cell incorporating a room temperature ionic liquid as its electrolyte. **A. Byrne, D. Coker, N. English**

9:00 COMP 427. Controlling molecular rectification via symmetrical molecule-electrode coupling. **W. Ding, M. Koepf, C. Koenigsmann, A. Batra, C.F. Negre, L. Venkataraman, G.W. Brudvig, V.S. Batista, C.A. Schmuttenmaer, R.H. Crabtree**

9:30 COMP 428. Why is the mercury electrode so good for CO_2 reduction catalyzed by the $[\text{Ni}(\text{cyclam})]^{2+}$ complex? **W. Ding, J. Froehlich, C.P. Kubiak, V.S. Batista**

10:00 Intermission.

10:00 COMP 429. Reconciling the electronic and geometric corrugations of the h-BN/Rh(111) and graphene/Ru(0001) nanomeshes. **W. McKee, Y. Xu, V. Meunier**

10:30 COMP 430. Critical steps and structures in Pt(111) surface oxidation: A ReaxFF reactive forcefield study. **D. Fantauzzi, J.E. Mueller, T. Jacob**

Section E

Boston Convention & Exhibition Center
Room 151B

Drug Discovery

Ligand-based Approaches

Y. Tseng, *Organizer*

C. Velez Vega, *Presiding*

8:30 COMP 431. Is it worth making? Assessing the information content of new structures. **M.D. Mackey, T. Cheeseright, P. Tosco, S. Tomasio**

9:00 COMP 432. Analyzing the structural sensitivity of QSAR models using matched molecular pairs. **R.D. Clark, D. Miller**

9:30 COMP 433. Conformer generation for small organic molecules: Teaching distance geometry about experimental torsion-angle preferences. **S. Riniker**

10:00 Intermission.

10:15 COMP 434. Novel ligand conformational search algorithm using the "Movable Type" method. **L. Pan, Z. Zheng, K.M. Merz**

10:45 COMP 435. Where's the proton? How theory and data combine to study these elusive species. **L. Westerhoff, O. Borbulevych**

11:15 COMP 436. Impact of new features and current performance of DOCK6. **W.J. Allen, T.E. Balias, S. Mukherjee, S. Brozelli, D. Moustakas, T. Lang, D.A. Case, I.D. Kuntz, R.C. Rizzo**

Electronic Structure Methods for Large Systems

SCF Functionals and Algorithms

Sponsored by PHYS, Cosponsored by COMP

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Nucleic Acids

Sponsored by PHYS, Cosponsored by COMP

ENFL

Division of Energy and Fuels

A. Park and X. Wang, Program Chairs

SOCIAL EVENTS:

Dinner, 6:30 PM: Tuesday

BUSINESS MEETINGS:

Program Meeting, 12:00 PM: Sunday

Business Meeting, 5:00 PM: Monday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 258B

Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application

H2 Generation

Cosponsored by CATAL

S. W. Lee, Y. Shao, *Organizers*

F. Jiao, J. Sun, *Organizers, Presiding*

8:00 ENFL 1. Bimetallic Pt-M catalysts for aqueous phase reforming of glycerol. **A.M. Karim, Z. Wei, D.L. King, Y. Wang**

8:30 ENFL 2. Mechanistic studies and design descriptors for CO oxidation over transition-metal-substituted CeO_2 nanoparticles. **J.S. Elias, M. Risch, L. Giordano, M.N. Azzam, Y. Shao-Horn**

9:00 ENFL 3. Manipulation of photo-generated electrons and holes in semiconductor photocatalysts for solar water splitting. **J. Gong, P. Zhang**

9:30 Intermission.

9:40 ENFL 4. Catalysis in aqueous phase: Reforming of polyols for hydrogen production. **Y. Wang, A.M. Karim, Z. Wei, D.L. King**

10:10 ENFL 5. Mesoporous crystalline silicon and evaluation of its hydrogen evolution performance. **D. Wang**

10:40 ENFL 6. Hydrogen production by plasma-induced decomposition in the presence of metal sulfide semiconductor catalysts. **A. Wang, L. Zhao, Y. Wang**

11:00 ENFL 7. Isokinetic temperature and size-controlled activation of ruthenium-catalyzed ammonia borane hydrolysis. **C. Na, H. Ma**

11:20 ENFL 8. Analysis of carbon-hydrogen bond on the ball milled graphite. **Y. Zhang**

Section B

Boston Convention & Exhibition Center
Room 258C

Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization and Storage
CO₂ Capture Using Advanced Materials

Cosponsored by ENVR†

J. H. Lee, O. M. Yaghi, *Organizers*

S. P. Katikaneni, C. Petit, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENFL 9. Rotary wheel adsorber for carbon capture. M. Enzo, E. Shiko, A. Greenaway, A. Gibson, A. Gromov, M. Lozinska, E. Campbell, P.A. Wright, S. Brandani

9:15 ENFL 10. Thermodynamics of CO₂ capture in metal-organic framework. D. Wu, J.J. Gassensmith, T. McDonald, X. Guo, Z. Quan, S.V. Ushakov, P. Zhang, J.R. Long, A. Navrotsky

9:35 ENFL 11. Nanoporous polymers for efficient CO₂ capture and separation. A. Coskun

9:55 Intermission.

10:05 ENFL 12. Solid CO₂ adsorbent based on linear polyethyleneimine and nanosilica for improved desorption kinetics. H. Zhang, A. Goepfert, S.G. Prakash, G.A. Olah

10:25 ENFL 13. Amino-functionalization of soft-templated mesoporous carbon for anthropogenic CO₂ capture. S. Chai, Z. Liu, K. Huang, S. Dai

10:45 ENFL 14. Amine-based adsorbents for CO₂ capture from simulated flue gas. G. Xue

11:05 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 259A

Porous Materials for Energy & Sustainability from Discovery to Application

Financially supported by KAUST & Framergy

D. Jiang, S. Ma, *Organizers*

Y. Han, *Organizer, Presiding*

C. Tsung, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 15. Conjugated microporous polymers for photochemical water splitting. R.S. Sprick, J. Jiang, B. Bonillo, S. Ren, T. Ratvijitvech, p. guiglion, M. Zwiijnenburg, D. Adams, A.I. Cooper

8:50 ENFL 16. Functional organic frameworks in non-powdery forms. Y. Liu

9:20 ENFL 17. Porous polymers that rapidly remove organic contaminants from water. W. Dichtel, A. Alsaibee, B.J. Smith, L. Xiao

9:50 Intermission.

10:00 ENFL 18. Covalent organic frameworks for electric energy storage and power supply. D. Jiang

10:30 ENFL 19. Porous organic ligands as new platforms for preparing efficient heterogeneous catalysts. F. Xiao, Q. Sun, L. Wang, X. Meng

11:00 ENFL 20. Functional porous organic polymers through novel bottom-up design. W. Zhang, H. Yang, Y. Du, Y. Zhu, Y. Jin

11:30 ENFL 21. Porous organic frameworks as sustainable photocatalysts for organic synthesis. J. Zhang

Section D

Boston Convention & Exhibition Center
Room 259B

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Surface Science

Cosponsored by CATL

Z. Wu, *Organizer*

S. D. Senanayake, *Organizer, Presiding*

W. Huang, *Presiding*

8:05 Introductory Remarks.

8:10 ENFL 22. Structure and spectroscopy of clean and modified ceria surfaces. H. Freund

8:50 ENFL 23. Structure and reactivity of Ni nanoparticles supported on Ti-modified ceria. J. Zhou, E.W. Peterson

9:25 ENFL 24. Redox processes of ceria explored on a model inverse catalyst. G. Thornton

10:00 Intermission.

10:10 ENFL 25. Ceria at a closer look — reducibility traced down to the atomic scale. M. Reichling

10:45 ENFL 26. Bridging the pressure and materials gaps: Ambient pressure XPS experiments on CeO₂(100). D.R. Mullins

11:20 ENFL 27. In situ low-energy electron microscopy of ceria inverse model catalysts. J. Flege

Section E

Boston Convention & Exhibition Center
Room 260

Solar Energy and Solar Cells

R. T. Koodali, *Organizer*

Y. H. Hu, *Organizer, Presiding*

S. Kar, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL 28. Recent progress of perovskite solar cells at UCLA. Y. Yang

9:15 ENFL 29. Improved stability of mesoscopic perovskite solar cells with bifunctional molecules. H. Han

9:55 ENFL 30. Tailoring atomically thin materials with tunable composition and properties. S. Kar

10:35 Intermission.

10:50 ENFL 31. Inorganic-organic hybrid tin and lead based perovskites: From chemistry to solar cells. M.G. Kanatzidis

11:30 ENFL 32. Carbon nanosheets and nanofibers for dye-sensitized solar cells. W. Wei, Y.H. Hu

11:50 Concluding Remarks.

Section F

Boston Convention & Exhibition Center
Room 261

Biofuels for Powering the World: Discovery to Application

Catalytic Fast Pyrolysis

Cosponsored by CATL and ENVR

C. Mukarakate, M. R. Nimlos, *Organizers*

D. Robichaud, B. G. Trewyn, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENFL 33. Catalytic and noncatalytic pyrolysis of biomass in non-inert environments for production of deoxygenated bio-oil and chemicals. C.A. Mullen, A. Boateng, Y. Elkasabi, M. Schaffer

9:05 ENFL 34. In-situ and ex-situ catalytic pyrolysis of miscanthus x giganteus in PyGC-MS and comparison with bench-scale spouted-bed reactor. D.P. Gamliel, S. Du, G.M. Bollas, J. Valla

9:25 ENFL 35. Prevention of fast deactivation of zeolites in biomass upgrading by utilizing MFI type nanosheet catalyst. M. Xu, S. Budhi, C. Mukarakate, M.R. Nimlos, B.G. Trewyn, R.M. Richards

9:45 ENFL 36. Catalytic cracking of soybean oil by different hierarchical zeolite containing mesoporous SiO₂-Al₂O₃ using a Curie point pyrolyzer. A. Ishihara

10:05 Intermission.

10:20 ENFL 37. Reactions of water and coke precursors during vapor phase upgrading of biomass pyrolysis products with HZSM-5: Role of water on improving catalyst lifetime and formation of phenols and naphthols. C. Mukarakate, D. Robichaud, S. Budhi, T. Evans, J. McBrayer, K. Iisa, R. Baldwin, J. ten Dam, M. Watson, M.R. Nimlos

10:50 ENFL 38. Steam cofeeding during vapor phase upgrading of biomass — mechanistic understanding through model compounds. D. Robichaud, T. Evans, C. Mukarakate, M.R. Nimlos

11:10 ENFL 39. Hydrodeoxygenation (HDO) of bio-oil model compounds with synthesis gas using a Cu based water gas shift catalyst with a Mo/Ni/K catalyst. A.G. Karunanayake, M.L. Crowley, R. T. Wijayapala, T.E. Mlsna

11:30 Concluding Remarks.

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SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 258B

Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application

CO₂ & Solar

Cosponsored by CATL

S. W. Lee, J. Sun, *Organizers*

F. Jiao, Y. Shao, *Organizers, Presiding*

1:30 ENFL 40. Recycling CO₂ via C-H carboxylation. M. Kanan

2:00 ENFL 41. Electrocatalytic reduction of CO₂ over Pd nanoparticles. G. Wang

2:30 ENFL 42. Nanostructured metals for electrochemical carbon dioxide reduction. F. Jiao, J. Rosen, Q. Lu, G.S. Hutchings

2:50 ENFL 43. Withdrawn.

3:10 Intermission.

3:20 ENFL 44. Important role of electrocatalysis in dye-sensitized solar cells (DSSCs). Y.H. Hu

3:50 ENFL 45. Deterministic modeling of carbon nanotube near-infrared solar cells. D.O. Bellisario, J.A. Paulson, M. Strano, Z. Ulissi

4:10 ENFL 46. Templating intermolecular reactivity on nanostructured surfaces for solar CO₂ reduction. M.E. Louis, T. Jin, T. Fenton, G. Li

4:30 ENFL 47. Electrochemical CO₂ conversion catalysts for integrated monolithic solar-fuel generators. J. Koh, H. Jeon, Y. Hwang, B. Min

Section B

Boston Convention & Exhibition Center
Room 258C

Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization and Storage
Prospects on CO₂ Capture and Conversion

Cosponsored by ENVR

C. Petit, O. M. Yaghi, *Organizers*

S. P. Katikaneni, J. H. Lee, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENFL 48. Optimal CO₂ reduction strategy for a refinery via CO₂ capture and conversion technologies. K. Roh, J.H. Lee

2:15 ENFL 49. Toward 2030: Bridging the knowledge gap for solvent development for post-combustion CO₂ separations. D.J. Heldebrant, P.K. Koech, R. Rousseau, V. Glezakou, D.C. Cantu, D. Malhotra, F. Zheng, C. Freeman, M. Bearden

2:45 ENFL 50. CO₂ capture chemistry of azolide-based ionic liquids: Interplay between CO₂, ions, and water. T.B. Lee, S. Seo, T. Gohdrone, Q. Sheridan, E. Maginn, J.F. Brennecke, W.F. Schneider

3:05 Intermission.

3:15 ENFL 51. Developing transformational solvents for flue gas clean up: Synthesis and characterization of energetically viable carbon dioxide binding organic liquids. D. Malhotra, P. Koech, D.J. Heldebrant, D. Cantu, V. Glezakou, R. Rousseau

3:35 ENFL 52. Chemical and physical characterizations of liquid-like nanoparticle organic hybrid materials (NOHMs) designed for CO₂ capture and conversion. A. Park, M. Gao, C. Petit

3:55 ENFL 53. Thermo- and pH-responsive nanogel particles for reversible carbon dioxide capture and burst release. P. Werz, B. Rieger

4:15 ENFL 54. Carbonate eutectic promoted MgO based adsorbents for CO₂ removal at 300-400 °C. X.S. Li, R. Xing, K. Zhang, R. Dagle, D.L. King

4:35 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 C

Boston Convention & Exhibition Center
Room 259A

Porous Materials for Energy & Sustainability from Discovery to Application

Financially supported by KAUST & Framergy
Y. Han, D. Jiang, *Organizers*

S. Ma, *Organizer, Presiding*

P. McGrier, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 55. MOFs and COFs for carbon capture and conversion. O.M. Yaghi

1:50 ENFL 56. Metal-organic framework materials for energy related applications. P. Feng

2:20 ENFL 57. Catalysts prepared by confining metal nanoclusters in metal organic frameworks. W. Huang, X. Li, C. Xiao

2:50 ENFL 58. Photo-functional zwitterionic metal-organic frameworks with tunable adsorption properties. M. Wriedt, D. Aulakh, W. An, H.K. Bilal

3:10 Intermission.

3:20 ENFL 59. Metal-organic frameworks from design strategies to applications. M. Eddaoudi

3:50 ENFL 60. Nanopore controlled catalysis: Syntheses of core-shell MOF catalysts. C. Tsung

4:20 ENFL 61. Acetylene adsorption on metal organic frameworks (MOFs). P. Cheng, Y.H. Hu

4:40 ENFL 62. Nanoporous materials for adsorption cooling applications. R. Motkuri, J. Jenks, L.X. Dang, S. Ma, P.B. McGrail

5:00 ENFL 63. Water-stable, ultrahigh surface area zirconium MOFs based on ftw topology. T. Wang, W. Bury, D. Gomez-Gualdron, N. Vermeulen, J. Mondloch, P. Deria, K. Zhang, P. Moghadam, A. Sarjeant, R. Snurr, J.F. Stoddart, J.T. Hupp, O.K. Farha

Section D

Boston Convention & Exhibition Center
Room 259B

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Powder Catalysts

Cosponsored by CATL

S. D. Senanayake, *Organizer*

Z. Wu, *Organizer, Presiding*

W. Huang, *Presiding*

1:20 ENFL 64. Some key issues in the development of ceria-based soot oxidation catalysts. A. Trovarelli, E. Aneggi, C. de Leitenburg, J. Llorca

2:00 ENFL 65. Methane catalytic combustion over hierarchical Pd@CeO₂/Si-Al₂O₃: Effect of the presence of water. P. Fornasiero, M. Carnello, C. Chen, J. Delgado, E. Fonda, R.J. Gorte, V. Matolin, M. Monai, T. Montini, K.C. Prince, N. Tsud

2:35 ENFL 66. Hydrogen production from water over doped CeO₂. H. Idriss, Y. Al-Salik, D. Anjum, T. Ahmed

3:10 Intermission.

3:20 ENFL 67. Noble metal/ceria catalysts for the WGS reaction. Why Au and Pt behave differently? M. Gonzalez-Castaño, T. Ramirez-Reina, V. Lopez-Flores, S. Ivanova, L. Martinez, J.A. Odriozola

3:55 ENFL 68. Low temperature water gas shift: TPR-XANES investigation of Pt/ceria catalysts doped with calcium. L. Linganiso, G. Jacobs, B.H. Davis, D.C. Cronauer, A.J. Kropf, C.L. Marshall

4:30 ENFL 69. Taking advantage of oxygen transfer from ceria to metal catalysts. C. Chen, T.M. Onn, P. Fornasiero, R.J. Gorte

4:50 ENFL 70. In situ spectroscopic study of the effect of surface structure on the interaction of SO₂ with CeO₂. U. Tumulari, M. Li, S. Dai, G. Rothen, Z. Wu

Section E

Boston Convention & Exhibition Center
Room 260

Solar Energy and Solar Cells

Y. H. Hu, *Organizer*

R. T. Koodali, *Organizer, Presiding*

N. Wu, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 71. Control growth of large grained hybrid perovskite thin films for solar cell applications. H. Tsai, W. Nie, A. Mohite, H. Yen, J.J. Crochet, J.C. Blancon, S. Tretiak, H. Wang

1:45 ENFL 72. What are the most important properties of the hybrid lead halide perovskites? G. Hodes

2:25 ENFL 73. High efficiency millimeter-scale crystalline perovskite solar cells. A. Mohite

3:05 Intermission.

3:20 ENFL 74. Nanostructure and interface engineering for low-cost and high-performance solar energy devices. S. Yang

4:00 ENFL 75. Controlled preparation and electrode applications of manganese-based oxides with micro/nano structures. J. Chen

4:40 ENFL 76. Band structures and charge processes in solar energy materials. N. Wu

5:20 Concluding Remarks.

Section F

Boston Convention & Exhibition Center
Room 261

Biofuels for Powering the World: Discovery to Application

Pyrolysis

Cosponsored by CATL and ENVR

C. Mukarakate, M. R. Nimlos, *Organizers*

D. Robichaud, B. G. Trewyn, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENFL 77. Novel thermo-chemical biomass conversion with the reciprocating biomass conversion reactor (RBCR). N. Parziale

2:05 ENFL 78. Hydrodeoxygenation of phenol over bulk nickel phosphides. Y. Wang, Z. Yu, T. Dong

2:25 ENFL 79. Exploring mechanisms of fast pyrolysis of lignin via high resolution and tandem mass spectrometry and quantum chemical calculations: A synthetic model compound study. P. Murria, J.C. Degenstein, J. Gao, H. Sheng, J.J. Nash, R. Agrawal, W. Delgass, F. Ribeiro, H.I. Kenttamaa

2:45 ENFL 80. Mechanistic study of ethanol dehydrogenation to ethoxy on Cu-based catalysts: A key step in Ethyl acetate synthesis from bio-ethanol. Y. Chen, K. Sun, Z. Wu, R. Wu, M. Zhang, L. Wang

3:05 Intermission.

3:20 ENFL 81. Integrated biofuel and nanomaterial production via pyrolysis of silver nitrate impregnated biomass. J. Xue, E. Ziade, J.L. Goldfarb

3:50 ENFL 82. Characterization of municipal solid waste bio-oil by FT-ICR mass spectrometry. R. Beasley, R.P. Rodgers, A.G. Marshall

4:10 ENFL 83. Production of hydrocarbon-rich fuels by two-step hydrous pyrolysis of *Scenedesmus/Desmodesmus* sp. algae. W. Obeid, P. Hatcher

4:30 Concluding Remarks.

National Science Foundation's Centers for Chemical Innovation

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21st Century Chemistry Education: Formal and Informal

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MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 258B

Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application

Fuel Cells & ORR

Cosponsored by CATL

Y. Shao, J. Sun, *Organizers*

F. Jiao, S. W. Lee, *Organizers, Presiding*

8:00 ENFL 84. Rational design of oxygen reduction reaction and hydrogen peroxide catalysts: From surface science to nanoparticles. I. Chorkendorff

8:30 ENFL 85. New strategies for the development of Pt-based catalysts toward oxygen reduction. Y. Xia

9:00 ENFL 86. Recent development of platinum and non-platinum oxygen reduction and evolution catalysts. H. Yang

9:30 ENFL 87. Oxygen reduction reaction on carbon-based catalysts. U.S. Ozkan, D. Singh, K. Mamtani, J. Tian

10:00 Intermission.

10:10 ENFL 88. Synthesis and assembly of nanocatalysts for efficient electrochemical reduction reactions. S. Sun

10:40 ENFL 89. First principles studies of electrocatalysis at oxide/metal interfaces. J. Greeley, Z. Zeng, J. Kubal, H. Chun

11:10 ENFL 90. Porous structure based high performance electrocatalysts for low temperature fuel cells. J. Lee

11:40 ENFL 91. Design and fabrication of Pt nanoclusters on poly(benzimidazole)-wrapped carbon nanotubes and evaluation for oxygen reduction reaction activity. Y. Hamasaki, T. Fujigaya, N. Nakashima

Section B

Boston Convention & Exhibition Center
Room 258C

Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization and Storage

CO₂ Conversion, Utilization and Storage

Cosponsored by ENVR†

J. H. Lee, O. M. Yaghi, *Organizers*

S. P. Katikaneni, C. Petit, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENFL 92. Experimental and theoretical examination of the catalytic reduction of CO₂ by renewable organo hydrides based on heterocyclic aromatic amines. C. Musgrave, C. Lim, A. Holder, J.T. Hynes, Y. Kuo

9:15 ENFL 93. Using catalysis to add value to waste CO₂ and to prepare polymers. C.K. Williams

9:55 ENFL 94. Computational investigations into CO₂ and bicarbonate reduction in protic conditions. M.C. Groenenboom, K.A. Grice, J.A. Keith

10:15 Intermission.

10:25 ENFL 95. Conversion of CO₂ into 3D graphene for efficient counter electrodes of dye-sensitized solar cells. W. Wei, K. Sun, Y.H. Hu

10:45 ENFL 96. CO₂ hydrogenation to methanol over Cu/ZnO/ZrO₂ catalysts prepared by chemical reduction. X. Dong

11:05 ENFL 97. Advanced electrocatalysis (ED) system for CO₂ mineralization with chemical absorbents. J. Han, J. Chung, J. Son, D. Song

11:25 ENFL 98. Impact of CO₂ dissolution in water on interfacial properties of CO₂/water/quartz systems. G. Javanbakht, M. Sedghi, W. Welch, L. Goual

11:45 Concluding Remarks.

Section C

Boston Convention & Exhibition Center
Room 259A

Porous Materials for Energy & Sustainability from Discovery to Application

Financially supported by KAUST & Framergy
Y. Han, S. Ma, *Organizers*

D. Jiang, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 99. Separation of carbon dioxide based on porous membranes. S. Dai

8:50 ENFL 100. Novel triptycene-based polymers of intrinsic microporosity for membrane gas separation applications. B. Ghanem, R. Swaidan, E. Litwiller, I. Pinnau

9:20 ENFL 101. Advanced molecular sieve membranes. Q. Song

9:50 Intermission.

10:00 ENFL 102. Tailoring the separation performance of zeolitic imidazolate frameworks (ZIFs)-enabled membranes and sorbents. W. Koros, C. Zhang

10:30 ENFL 103. Nanofluidic transport across nanoporous monolayer graphene membranes. R. Karnik

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

- 11:00 ENFL 104.** Materials for capture of CO₂ and acid gases studied via in situ and ex situ solid-state NMR. C. Chen, J.K. Moore, R. Marti, M.S. Conradi, M. Sakwa-Novak, C.W. Jones, S.E. Hayes
- 11:20 ENFL 105.** Versatile fabrication of nanostructured platinum films with enhanced catalytic response to the ethanol oxidation reaction. S.J. Richardson, N.J. Terrill, J.M. Elliott, A.M. Squires
- 11:40 ENFL 106.** Proton and lithium conducting pore-filled nanoporous silica colloidal membranes. I. Zharov

Section D

Boston Convention & Exhibition Center
Room 259B

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Theory

Cosponsored by CATL

S. D. Senanayake, Z. Wu, *Organizers*

A. Bruix, Y. Xu, *Presiding*

- 8:10 ENFL 107.** Modeling the structure and reactivity of ceria electrodes from ideal to realistic reaction environments. S. Fabris
- 8:50 ENFL 108.** Density functional theory examination of active sites of transition metal-doped ceria surfaces. M.J. Janik
- 9:25 ENFL 109.** Multiscale modeling of cerium oxide. K. Hermansson
- 10:00** Intermission.
- 10:10 ENFL 110.** Acid-base properties of adsorbates on oxides. H. Metiu
- 10:50 ENFL 111.** Ni/CeO₂ for hydrogen production: The role of metal support interactions. M. Ganduglia-Pirovano, D. López-Durán, J. Carrasco, Z. Liu, T. Duchon, J. Evans, S.D. Senanayake, E. Crumlin, V. Matolin, J. Rodriguez
- 11:25 ENFL 112.** Roles of oxygen vacancy in the surface reactivity of CeO₂(111). C. Zhao, Y. Xu

Section E

Boston Convention & Exhibition Center
Room 260

Solar Energy and Solar Cells

Y. H. Hu, R. T. Koodali, *Organizers*

D. Ma, S. Yang, *Presiding*

- 8:30** Introductory Remarks.
- 8:35 ENFL 113.** Ultrafast exciton dynamics in semiconductor nanowires and implications in solar energy conversion. J.Z. Zhang
- 9:15 ENFL 114.** Plasmonic enhancement mechanisms in solar energy harvesting. S. Cushing, J. Li, A.D. Bristow, D. Chu, N. Wu
- 9:55 ENFL 115.** Developing plasmonic nanostructures to harvest more photons for photovoltaic and photocatalytic applications. D. Ma
- 10:35** Intermission.
- 10:50 ENFL 116.** Novel photocatalytic processes. B. Han, Y.H. Hu
- 11:30 ENFL 117.** Effect of hydrothermal treatment temperature on the pore sizes of titanium dioxide. R.T. Koodali, S. Rasalingam
- 12:10** Concluding Remarks.

Section F

Boston Convention & Exhibition Center
Room 261

Biofuels for Powering the World: Discovery to Application

Hydrotreating, Upgrading and Gasification

Cosponsored by CATL and ENVR

C. Mukarakate, M. R. Nimlos, *Organizers*

D. Robichaud, B. G. Trewyn, *Organizers, Presiding*

8:30 Introductory Remarks.

- 8:35 ENFL 118.** Hydrogenation of catalytically upgraded biomass pyrolysis oils. R.J. French, K. Iisa
- 9:05 ENFL 119.** Removal of metals from pyrolysis oil at ambient temperature with ion-exchange resins. G. Zhou, S.H. Roby
- 9:25 ENFL 120.** Dry fractionation of straw prior to biofuels production. S. Chuetor, A. Barakat, T. Ruiz, X. Rouau
- 9:45 ENFL 121.** Process monitoring and analysis of biodiesel by bench-top NMR spectroscopy. S. Riegel
- 10:05** Intermission.
- 10:20 ENFL 122.** Impact of ethanol addition on vapor pressure and water tolerance of gasoline blending components. D. Karonis, V. Botsis, D. Chilari
- 10:40 ENFL 123.** Aspects of biomass gasification optimization: Feedstock blending and air-steam gasification for better product yields. W.S. Jablonski, J. Olstad, D. Carpenter
- 11:00 ENFL 124.** Mechanisms of formaldehyde generation from wood and implications to biomass treatment. G. Wan, C.E. Frazier
- 11:20 ENFL 125.** Production of gaseous fuels using biomass residues. S. Peres
- 11:40** Concluding Remarks.

ACS Scholars: Rising Stars in Academe

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Memories of Henry Hill: His Legacy in Science and in Professional Service

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21st Century Chemistry Education: Formal and Informal

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MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 258B

Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application

Fuel Cells

Cosponsored by CATL

F. Jiao, J. Sun, *Organizers*

S. W. Lee, Y. Shao, *Organizers, Presiding*

- 1:30 ENFL 126.** Designing porous structures in carbon-based electrocatalysts. X. Feng

- 2:00 ENFL 127.** Advanced non-precious metal nanocatalysts for fuel cells and hydrogen production. D. Deng

- 2:30 ENFL 128.** Electrocatalysts for hydrogen/bromine energy conversion systems. N. Singh, R. Liu, D.C. Upham, V. Yarlaga, S. Mubeen, T.V. Nguyen, M. Moskovits, H. Metiu, E.W. McFarland

- 3:00 ENFL 129.** Metal-free, carbon-based materials as catalysts for PEM fuel cells. Z. Wu, M. Benchaïfa, Z. Iqbal, X. Wang

- 3:20 ENFL 130.** Nanostructured carbons as electrode materials in solid acid fuel cells. A. Papandrew, R.A. Elgammal, O.E. Dyck, G.J. Duscher, W.D. Tennyson, G.M. Veith, D.B. Geohegan, T.A. Zawodzinski

3:40 Intermission.

- 3:50 ENFL 131.** Molybdenum dioxide (MoO₃)-based anode for hydrocarbon-fed solid oxide fuel cell (SOFC). S. Ha, M. Norton, B. Kwon

- 4:20 ENFL 132.** Routes to nanoconfined and high surface area solid acid electrolyte CsH₂PO₄. R.A. Elgammal, O.E. Dyck, A. Papandrew, I.N. Ivanov, G.J. Duscher, T.A. Zawodzinski

- 4:40 ENFL 133.** Alternative energy: Build effective cathode catalyst composed of nanocomposite. J.L. Liu, S. Bashir

- 5:00 ENFL 134.** Using vapor-grown Ru₃Pt₂ and Ru₂Pd₃ nanotubes to investigate the hydrogen oxidation reaction mechanisms in alkaline electrolyte. S. St. John, R. Atkinson, R.R. Unocic, A. Papandrew, T.A. Zawodzinski

Section B

Boston Convention & Exhibition Center
Room 258C

Innovative Electrochemical Energy Storage

Capacitive Energy Storage

J. Lu, *Organizer*

X. Ji, *Organizer, Presiding*

D. Jiang, *Presiding*

1:00 Introductory Remarks.

- 1:05 ENFL 135.** Understanding supercapacitors. D. Jiang
- 1:35 ENFL 136.** Preparation of 3D graphene by the baking bread method and its supercapacitive behavior. D. Shu
- 1:55 ENFL 137.** One-step-synthesis of 3D graphene for aqueous double-layer capacitors. L. Chang, W. Wei, Y.H. Hu
- 2:15 ENFL 138.** Graphene-based nanomaterials for highly efficient energy storage. H. Yen, H. Tsai, A. Chen, G. Wu, H. Wang

2:35 ENFL 139. Withdrawn.

2:55 Intermission.

- 3:00 ENFL 140.** Pseudocapacitive charge storage with transition metal oxides: Lessons from multifunctional electrode nanoarchitectures. J.W. Long, M.B. Sassin, C.N. Chervin, J.M. Wallace, D.R. Rolison

- 3:30 ENFL 141.** Aqueous redox-enhanced electrochemical capacitors: Design principles for high specific energies and slow self-discharge. S.W. Boettcher, S. Chun, B. Evanko, X. Wang, D. Vonlanthen, X. Ji, G.D. Stucky

- 4:00 ENFL 142.** High capacity supercapacitors with conducting polymer/redox biopolymer composite electrodes. S. Leguizamón, K.P. Diaz Orellana, J. Velez, M.C. Thies, M.E. Roberts

- 4:20 ENFL 143.** Supercapacitors electrodes prepared with vapor-phase polymerized poly(3,4-ethylenedioxythiophene) (PEDOT). L. Tong, K.H. Skorenko, A. Faucett, S.M. Boyer, J. Liu, J. Mativetsky, W.E. Bernier, W.E. Jones

- 4:40 ENFL 144.** Alternatively stacked Ni-Al LDH/rGO superlattice for electrochemical energy storage. X. Ge, C. Gu, J. Li

Section C

Boston Convention & Exhibition Center
Room 259A

Porous Materials for Energy & Sustainability from Discovery to Application

Financially supported by KAUST & Framergy

D. Jiang, S. Ma, *Organizers*

Y. Han, *Organizer, Presiding*

W. Zhang, *Presiding*

1:00 Introductory Remarks.

- 1:05 ENFL 145.** Electron crystallography as an important technique for discovery of novel porous materials. X. Zou
- 1:50 ENFL 146.** Shape selectivity and selectivity in methanol-to-hydrocarbons conversion. A. Bhan
- 2:20 ENFL 147.** Methane to acetic acid over Cu-exchanged zeolites: Mechanistic insights from a site-specific carbonylation reaction. K. Narsimhan, V. Michaelis, G. Mathies, W. Gunther, R.G. Griffin, Y. Roman-Leshkov

- 2:40 ENFL 148.** Catalytic cracking of heavy oils by hierarchical zeolite containing mesoporous silica-aluminas with large mesopore using Curie point pyrolyzer. A. Ishihara

3:00 Intermission.

- 3:10 ENFL 149.** Small molecule chemistry at the MOF secondary building units enabled by cation exchange. M. Dinca, C. Brozek, R.J. Comito, E. Metzger, A.W. Stubbs, Y. Tulchinsky

- 3:40 ENFL 150.** Electrochemically nanostructured polymer hybrids with remarkable synergy for energy storage. W. Tian, X. Mao, P. Brown, G.C. Rutledge, T. Hatton

- 4:00 ENFL 151.** Exploiting the structure-function relationships in porous hyperbranched polymer systems for energy storage applications. P. Bhattacharya, M.I. Nandiasiri, D. Lu, A. Dutta, Q. Dicken, D.A. Tomalia, W.A. Henderson, J. Xiao

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- 4:20 ENFL 152.** MIL-101(Fe) as a lithium-ion battery electrode material: a relaxation and intercalation mechanism during lithium insertion. **J. Shin, M. Kim, J. Cirera Fernandez, S. Chen, G.J. Halder, T.A. Yersak, F. Paesani, S. Cohen, S. Meng**
- 4:40 ENFL 153.** Bioinspired interconnected nitrogen-doping carbon nanoplatelets for high-performance hybrid supercapacitors. **W. Tian, Q. Gao**
- 5:00 ENFL 154.** Structure and surface chemistry of carbide-derived carbon supercapacitors. **B. Dyatkin, E. Mamontov, H. Wang, Y. Gogotsi**

Section D

Boston Convention & Exhibition Center
Room 259B

Advances in Ceria Based Catalysts: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Surface Science

Cosponsored by CATL

Z. Wu, *Organizer*

S. D. Senanayake, *Organizer, Presiding*

J. Zhou, *Presiding*

- 1:20 ENFL 155.** Adsorption and adhesion energetics of Au, Cu, and Ag atoms and nanoparticles onto CeO₂(111) by calorimetry: Comparison to other oxides. **C.T. Campbell, T. James, S.L. Hemmingson**
- 2:00 ENFL 156.** Pt₂ - CeO_x novel thin film catalyst as PEMFC anode. **V. Matolin**
- 2:35 ENFL 157.** Interpreting atomically resolved STM images of CeO₂(111) ultrathin films. **D. Grinter, B. Shaw, C.L. Pang, M. Wolf, J. Kullgren, K. Hermansson, G. Thornton**
- 2:55 Intermission.**
- 3:05 ENFL 158.** Growth of epitaxial CeO₂(111) film on Ru(0001) and its reduction by hydrogen. **T. Komeda**
- 3:45 ENFL 159.** Chemical activity of oxygen vacancies on ceria: A combined experimental and theoretical study on single crystal CeO₂(111). **C. Woell**
- 4:20 ENFL 160.** Hierarchical heterogeneity at the CeO₂-TiO₂ interface: Growth, electronic and geometric structure, and the photocatalytic water splitting activity of oxide on oxide nanostructures. **S. Luo, T. Nguyen Phan, A.C. Johnston-Peck, L. Barrio, S. Sallis, D.A. Arena, S. Kundu, W. Xu, L.F. Piper, E. Stach, D.E. Polyansky, E. Fujita, S.D. Senanayake, J. Rodriguez**
- 4:40 ENFL 161.** Faceting transition at the oxide-metal interface: The case of ceria on copper. **M. Aulická, T. Duchon, F. Dvorak, V. Stetsovych, J. Beran, K. Veltruska, J. Myslivecek, K. Masek, V. Matolin**

Section E

Boston Convention & Exhibition Center
Room 260

Energy & Fuels Joint Award for Excellence in Publication: Symposium in Honor of Phillip E. Savage

D. Dadyburjor, *Organizer*

E. B. Fox, M. Kidder, *Organizers, Presiding*

1:30 Introductory Remarks.

- 1:35 ENFL 162.** Hydrothermal processes for energy and fuels from algal biomass. **P.E. Savage**
- 2:15 ENFL 163.** Decade of algae bio-process engineering: The neglected importance of operational strategy and control. **W.R. Curtis**

- 2:45 ENFL 164.** Pilot-scale demonstration of hydrothermal liquefaction to produce bio-fuels from an algal feedstock. **P. Valdez**
- 3:15** Intermission.
- 3:30 ENFL 165.** Towards a model for predicting hydrothermal liquefaction of microalgae of varying composition. **T.J. Strathmann, S. Leow, Y. Li, J. Guest**
- 4:00 ENFL 166.** Algae biofuel production strategies: What have we learned from LCA and TEA and what does it mean? **L.M. Colosi, E. Connelly, A.F. Clarens, J.H. Lambert**
- 4:30 ENFL 167.** Opportunities for advanced biofuels to support advanced combustion. **C. Sun, S. Bohac, A.L. Boehman**
- 5:00** Concluding Remarks.

Section F

Boston Convention & Exhibition Center
Room 261

Chemical Looping Innovation for Low-Carbon Energy

J. Zhang, *Organizer*

P. Fennell, F. Li, *Organizers, Presiding*

1:30 Introductory Remarks.

- 1:35 ENFL 169.** Integrated computational and experimental investigation of the oxidation of glucose to gluconic acid on CuO nanoleaves: Insights into the role of lattice oxygen. **Y. Yang**
- 2:15 ENFL 172.** FeNi bimetallic carriers in chemical looping processes. **A. More, S. Bhavsar, G. Vesper**
- 2:55 ENFL 312.** Pressurized carbonation experiments in the presence of steam in a spouted-bed reactor. **J. Yao, Z. Zhang, M. Seats, P. Fennell**
- 3:15 ENFL 307.** Development of CuO-Fe₂O₃ mixed metal oxide oxygen carrier from lab scale to commercial scale: Bench scale fluidized bed tests and pilot scale (50 Kw_{th}) chemical looping combustion tests with methane/air. **R.V. Siriwardane, H. Tian, D. Straub, J. Weber, G. Richards, J. Riley**
- 3:35** Intermission.
- 3:40 ENFL 413.** Chemical looping combustion: What can we learn by comparing micro- and macro-scale models? **R. Porrazzo, G. White, R. Ocone**
- 4:10 ENFL 308.** Redox catalysts for partial oxidation of light paraffins under a chemical-looping scheme. **L. Neal, A. Shafiefarhood, J. Sofranko, F. Li**
- 4:40 ENFL 313.** Cold and hot study of the hydrodynamics of dual-CFB looping system. **L. Duan, S. Haider, K. Patchigolla, E. Anthony**
- 5:00 ENFL 170.** Withdrawn.
- 5:20** Concluding Remarks.

ACS Scholars: Rising Stars in Industry

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What's in Your Chemical Toolbox?

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MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

A. Park, X. Wang, *Organizers*

8:00 - 10:00

50, 62, 71, 85, 88, 131, 157.

See previous listings.

ENFL 174. Withdrawn.

180, 191, 279, 311, 314, 333, 353, 355, 396, 405, 410. See subsequent listings.

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 261

Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application

OER & HER

Cosponsored by CATL

F. Jiao, J. Sun, *Organizers*

S. W. Lee, Y. Shao, *Organizers, Presiding*

- 8:00 ENFL 175.** Activity trends and design principles for multitransition-metal (oxy)hydroxide oxygen evolution catalysts. **S.W. Boettcher, M. Burke, L. Trotochaud, S. Zou, L. Enman, A. Smith, A. Batchellor, M. Kast**

- 8:30 ENFL 176.** From bulk to nanoscale: δ -MnO₂ as a water oxidation catalyst. **I.G. McKendry, S.K. Kondaveeti, S.L. Shumlas, A.C. Thenuwara, Q. Kang, N.H. Attanayake, M. Zdilla, D.R. Strongin**

- 8:50 ENFL 177.** Controlled preparation and electrode applications of manganese-based oxides with micro/nanostructures. **J. Chen**

9:20 Intermission.

- 9:30 ENFL 178.** Self-healing oxygen evolving catalysts. **D.G. Nocera**

- 10:00 ENFL 179.** Advanced oxygen evolution catalysts for water electrolysis. **H. Xu**

- 10:30 ENFL 180.** Ultra-active water electrolysis with Ni-based catalysts. **M. Gong, W. Zhou, H. Dai**

- 10:50 ENFL 181.** Improved efficiency of water and zinc oxide electrolysis systems through the application of a heterogeneous water oxidation catalyst prepared from dicobalt octacarbonyl and 1,2-bis(diphenylphosphino)ethane. **A. Bloomfield, S.W. Sheehan, S.L. Collom, P.T. Anastas**

- 11:10 ENFL 182.** Electro- and photolytic hydrogen production by mononuclear cobalt complexes with pentadentate ligands. **X. Zhao, M. Yanney, M. Vennampalli, G. Liang, C.E. Webster**

Section B

Boston Convention & Exhibition Center
Room 258C

Innovative Electrochemical Energy Storage

Na-ion Batteries

J. Lu, *Organizer*

X. Ji, *Organizer, Presiding*

L. Mai, *Presiding*

8:00 Introductory Remarks.

- 8:05 ENFL 183.** Several strategies enhancing the electrochemical performance of organic Li and Na batteries. **J. Chen**

- 8:35 ENFL 184.** Advanced Na-ion batteries based on porous nanocarbon composites and hybrids. **Y. Yu, C. Zhu, J. Liu**

- 9:05 ENFL 185.** Structure-property relationship in layered cathode materials for sodium-ion batteries. **E. Lee, A. Gutierrez, M.D. Slater, J. Lu, Y. Kim, C.S. Johnson**

- 9:35 ENFL 186.** Olivine NaFePO₄ cathode synthesized by a green aqueous electrochemical conversion route for sodium ion batteries. **Y. Fang, L. Xiao, X. Ai, H. Yang, Y. Cao**

9:55 Intermission.

- 10:05 ENFL 187.** Recent progress for room-temperature stationary sodium-ion batteries. **Y. Hu**

- 10:35 ENFL 188.** Rational design of vanadium-based electrode materials for high performance sodium-ion batteries. **L. Mai, Y. Dong, S. Li, B. Wang, K. Zhao, L. Zhang**

- 11:05 ENFL 189.** Chemical modification approaches for metal-ion battery electrode materials with advanced performance. **E. Pomerantseva**

- 11:35 ENFL 190.** Continuum-scale electrochemical modeling of a Na/O₂ battery. **S. Khaleghi Rahimian, J. Liu, C.W. Monroe**

Section C

Boston Convention & Exhibition Center
Room 259A

Porous Materials for Energy & Sustainability from Discovery to Application

Financially supported by KAUST & Framergy

Y. Han, D. Jiang, *Organizers*

S. Ma, *Organizer, Presiding*

R. Motkuri, *Presiding*

8:00 Introductory Remarks.

- 8:05 ENFL 191.** Preparation of stable metal-organic frameworks for potential applications. **H. Zhou, S. Yuan, T. Liu, D. Feng**

- 8:50 ENFL 192.** Metal-organic framework nodes as nearly ideal supports for molecular catalysts: NU-1000- and UiO-66-supported iridium complexes for ethylene hydrogenation and dimerization. **S.O. Odoh, D. Yang, T. Wang, O.K. Farha, J.T. Hupp, C.J. Cramer, B.C. Gates, L. Gagliardi**

- 9:20 ENFL 193.** Structural studies of small molecule adsorption in MOFs. **Z. Hulvey, M.R. Hudson, C.M. Brown**

9:50 Intermission.

- 10:00 ENFL 194.** Porous coordination polymer heterostructures as battery cathode materials: Prussian blue analog core-shell particles. **D.R. Talham, C.H. Li, D. Asakura, M. Okubo**

- 10:30 ENFL 195.** Heterogenization of chiral metallosalen catalysts over frameworks. **Y. Liu, C. Zhu, Y. Cui**

- 11:00 ENFL 196.** Multifunctional metal-organic frameworks for next-generation dye sensitized solar cells. **M. Allendorf, M.E. Foster, S.M. George, D.K. Lancaster, K. Laong, L. Small, E. Spörke, V. Stavila, J. Wheeler**

- 11:30 ENFL 197.** Synthesis and design of functional covalent organic frameworks. **P. McGrier**

Section D

Boston Convention & Exhibition Center
Room 259B

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Theory & Powder Catalysts

Cosponsored by CATL

S. D. Senanayake, Z. Wu, *Organizers, Presiding*

8:10 ENFL 198. Insights into the chemistry of Ce oxides from the theoretical analysis of core-level spectra. **P.S. Bagus**, H. Idriss, C.J. Neelin

8:50 ENFL 199. Computational modeling of nanostructured ceria for the rational design of catalytic materials. **A. Bruix**

9:25 ENFL 200. Understanding ceria-based nanostructured catalysts: Water gas shift and methanol synthesis reactions example. **J. Graciani**

10:00 ENFL 201. How does thermal motion influence lattice atoms? Challenges on the (100) facet of ceria. **M. Capdevila-Cortada**, N. Lopez

10:20 Intermission.

10:30 ENFL 202. Crystal plane-dependent oxygen vacancy structures and catalytic surface chemistry of CeO₂. **W. Huang**

11:05 ENFL 203. Mesoporous ceria for water gas shift catalysis. **C. Guild**, D. Kriz, D. Vovchok, J. Llorca, W. Xu, A. Bruix, A. El-Sawy, S. Biswas, **S.L. Suib**, S.D. Senanayake

11:40 ENFL 204. Extremely porous Pt-CeO₂ structures grown on carbon films for fuel cells applications. **I. Matolinova**, J. Lavkova, M. Dubau, V. Potin, R. Fiala, V. Matolin

Section E

Boston Convention & Exhibition Center
Room 260

Energy & Fuels Storch Award in Fuel Science: Symposium in Honor of Ripudaman Malhotra

A. Park, *Organizer*

R. T. Koodali, X. Wang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENFL 205. Biomass economy: Challenges and opportunities. **M.A. Serio**, M.A. Wojtowicz

9:10 ENFL 206. Molecular-level kinetic modeling in thermochemical conversions: Software tools and their applications. **M.T. Klein**

9:45 ENFL 207. Polycyclic aromatic mixtures, tars, and their phase behaviors: Their importance in fuel conversion processes. **E. Suuberg**

10:20 Intermission.

10:35 ENFL 208. High temperature, high temperature gasification of coal chars prepared at high heating rates. **T.H. Fletcher**

11:10 ENFL 209. Catalytic pyrolysis and gasification of biomass and brown coal using natural products. **T. Takarada**

11:45 Concluding Remarks.

Section F

Boston Convention & Exhibition Center
Room 261

Chemical Looping Innovation for Low-Carbon Energy

P. Fennell, *Organizer*

F. Li, J. Zhang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 414. Hybrid chemical looping hydrogen process using mixed metal oxides. **V.J. Aston**, C. Muhich, C. Musgrave, **A.W. Weimer**

8:35 ENFL 173. Nanostructured metal oxides for chemical looping processes. **Q. Song**, W. Liu, S. Cao, Z. Zhang, P. Fennell, A. Cheetham, S. Scott, J. Dennis

9:05 ENFL 311. Investigation of multicycle performance of chemical looping gasification of biomass char using Fe-Ni bimetallic oxygen carrier under different atmospheres. **Z. Huang**, F. He, D. Chen, S. Liu, K. Zhao, G. Wei, A. Zheng, Z. Zhao, H. Li

9:25 ENFL 309. Withdrawn.

9:45 ENFL 415. Perovskite-structured redox catalyst for methane partial oxidation with lattice oxygen. **A. Mishra**, N. Galinsky, F. Li

10:05 Intermission.

10:10 ENFL 310. Modelling the reduction of Fe-based oxygen carriers for pressurized chemical-looping combustion of gaseous fuels. **Z. Zhang**, J. Yao, M. Boot-Handford, S. Scott, P. Fennell

10:40 ENFL 171. Model-based design of chemical-looping experiments for kinetic validation. **L. Han**, Z. Zhou, **G.M. Bollas**

11:10 ENFL 168. Studies on ethanol conversion for clean fuels. **J. Zhang**, X. Cao, P. Hu, Z. Zhong, J. Zhang, F. Li

11:30 ENFL 416. Carbon-hydrogen bond on the surface of nanosized hydrogenated graphite. **Y. Zhang**

11:50 Concluding Remarks.

Transforming University-Industry Partnerships for an Innovative Future Envisioning, Enabling and Executing

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Electron and Energy Transfer: From Molecular to Device Engineering for Minimizing Environmental Impacts

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Next Generation Nanomaterials: Advances and Perspectives for Biomedicine, Energy, and Environmental Protection

Biomedicine/Energy

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TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Halls A/B1

Advances in Chemistry of Energy & Fuels

A. Park, X. Wang, *Organizers*

2:00 - 4:00

ENFL 210. Separation, determination, and composition profile of lipids in biodiesel using hyphenation of gradient-HPTLC with fluorescence detection by intensity changes and mass spectrometry. **V.L. Cebolla**, C. Jarne, L. Membrado, M. Lapieza, M. Savi n, J. Orduna

ENFL 211. Amine borane assisted synthesis of ternary CoAgPd nanoparticles as efficient catalyst for dehydrogenation of formic acid. **W. Luo**

ENFL 212. Asphaltene used for enhancing polymer properties. **M.N. Siddiqui**

ENFL 213. Highly porous activated carbons prepared from single source precursor: Application to gas storage and separation. **B. Ashourirad**, P. Arab, H.M. El-Kaderi

ENFL 214. Withdrawn.

ENFL 215. Electronic conductivity of potassium-oxygen battery discharging product KO₂. **L. Ma**, X. Ren

ENFL 216. (13 13 1) Facets on Cu(110) induced by carpet-like ceria overlayer. **M. Aulick **, T. Duchon, F. Dvorak, V. Stetsovych, J. Beran, K. Veltruska, J. Myslivecek, K. Masek, V. Matolin

ENFL 217. Thermally stable, nonflammable, high lithium salt soluble phosphonium based ionic liquid electrolytes. **X. Lin**, M.W. Grinstaff

ENFL 218. Fabrication of carbon papers incorporating PEDOT:PSS with high electrical conductivity and gas permeability. **H. Kim**, Y. Lee, G. Park, S. Park, Y. Choi, Y. Yoo

ENFL 219. Ni doped VOx Nanotubes as a Na-ion battery applications. **H. Kim**, R. Kim, D. Kim, Y. Kim, S. Lee, K. Park

ENFL 220. Oxidative desulfurization in a film-shear reactor. **D.T. Seidenkranz**, B.R. Fox, M.N. Siddiqui, T. Saleh, B. Chanbasha, D. Tyler

ENFL 221. Withdrawn.

ENFL 222. Cu_{1.5}Mn_{1.5}O₄-CuO-Cu₂O nanomaterial with core-shell structure for lithium ion battery anode. **P. Liu**, L. Lu, Y. Xu, Q. Hao, X. Wang

ENFL 223. Evolution of hydrogen fluoride during coal pyrolysis and subsequent char combustion. **N. Tsubouchi**, Y. Mochizuki, N. Iwabuchi, Y. Akama, Y. Ohtsuka

ENFL 224. Nitrogen-doped graphene supported Fe₃O₃ nanoparticles as stable, efficient electrocatalyst for the oxygen reduction reaction. **L. Lu**, Y. Xu, P. Liu, Q. Hao

ENFL 225. Synthesis, characterization, and catalytic performance of NiMo/Al-SBA-15 catalysts in the hydrodesulfurization of dibenzothiophene. **D. Gao**, A. Duan, X. Zhang, Z. Li, Y. Qin

ENFL 226. Facile synthesis of MoS₂/N-rGO nanosheets hybrids with excellent hydrogen evolution reaction properties. **Z. Li**

ENFL 227. Facile route fabrication of manganese oxide/carbon nanofiber composite electrode materials with high capacitive performance. **H. Zhao**

ENFL 228. Ge-TiN nanocomposite thin-film electrode as an anode for lithium-ion batteries. **S. Kim**, M. Kim, D. Kim, D. Kwak, K. Park

ENFL 229. Facile synthesis of reduced graphene oxide/α-Fe₂O₃ hybrid films as supercapacitor electrodes. **Z. Yue**

ENFL 230. Insight into V-doping in Li₂FeSiO₄ cathode material for lithium-ion battery. **L. Zhang**, H. Sun, Y. Wen, X. Yang, Y. Huang, G. Liang

ENFL 231. Self-humidifying PFSA-zeolite proton exchange membrane effects of Nafion confinement and zeolite thickness. **V. Sim**, W. Han, **Z. Liu**, K.L. Yeung

ENFL 232. Effect of digestate supplemented with minerals on the growth and lipid production of *Scenedesmus dimorphus*. **S. Avula**, J. He, J.V. Blargan, Y. Xu, J. Belovich

ENFL 233. Direct observation of methane hydrate occurrence in natural sands using microfocus X-ray computed tomography. **L. Yang**, **J. Zhao**, W. Liu, Y. Li, Y. Song

ENFL 234. Numerical analysis of methane hydrate dissociation in porous media induced by microwave stimulation. **J. Zhao**, Z. Fan, Y. Song, J. Wang, D. Liu

ENFL 235. Roles of hollow silica and activated carbon on methane hydrate formation. **R. Suesuan**, **P. Rangsunvigit**, S. Kulprathipanja

ENFL 236. Aluminum-based MOF composite for microextraction of sulfonamides. **Y. Shih**, K. Wang, H. Huang

ENFL 237. Preparation and photocatalytic activity of porous Bi₂O₃. **A. Ishihara**

ENFL 238. Modeling and optimization of electro dialysis desalination and electrically driven molecule transport within a series of novel ionomers. **D. Wang**, C.J. Cornelius

ENFL 239. Predicting the enthalpy and entropy of vaporization of gasoline using an enhanced vapor pressure acquisition system. **S. Abernathy**

ENFL 240. Novel large-scale synthesis of C/S nanocomposite with mixed conducting networks through spray drying approach for Li-S batteries. **J. Ma**, Z. Fang, Y. Yan, Z. Yang, L. Gu, Y. Hu, H. Li, Z. Wang, X. Huang

ENFL 241. Sulfur speciation and extraction in Jet A. **K. Greeson**, A.J. Guentherer, J. Reams, C. Lee, J.M. Mabry

ENFL 242. Shale gas fracturing fluids using polymer grafted silica with enhanced suspendability. **M.H. Bell**, A. Viswanath, B.C. Benicewicz

ENFL 243. Enhanced oxygen reduction activity of nitride Pt-M (M = Fe, Co and Ni) core-shell nano-electrocatalysts: An experimental and computational study. **G. Park**, K.A. Kuttiyiel, Y. Choi, S. Hwang, T. Yang, D. Su, K. Sasaki, P. Liu, R.R. Adzic

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- ENFL 244.** Chemoselective catalytic conversion of glycerol to methyl lactate in methanol over Sn- β zeolites prepared by three synthesis methods. **W. Dong**
- ENFL 245.** Graphene oxide as dual-function conductive binder for PEEK-derived microporous carbons in high performance supercapacitors. **C. Kim, H. Zhang, J. Liu**
- ENFL 246.** Withdrawn.
- ENFL 247.** Poly(ethylene oxide)-*b*-poly(4-vinylbenzyl methoxytrisoxyethylene ether) diblock copolymer electrolytes for lithium batteries. **X. Jiang, Y. Fang, X. Sun, S. Dai**
- ENFL 248.** Discovery of a novel endophytic fungi that produces volatile organic compounds with fuel potentials. **Y. Wang**
- ENFL 249.** Extractants for adjacent rare earth ion separation with ionic liquid-based solvent extraction. **C. Do-Thanh, J. Stankovich, N.J. Williams, H. Luo, S. Dai**
- ENFL 250.** Data-driven approach to the discovery of new molecules for organic aqueous redox flow batteries. **S. Kim, E.O. Pyzer-Knapp, C. Suh, A. Aspuru-Guzik**
- ENFL 251.** TiO₂@ carbon nanostructure for improved lithium ion properties. **M. Kim, S. Han, S. Kim, D. Kwak, K. Park**
- ENFL 252.** Enhanced photovoltaic performance of inverted polymer solar cells utilizing multifunctional CdSe quantum dots monolayer. **B. Moon, S. Bae, S. Lee, J. Hwang, Y. Yi, D. Son**
- ENFL 253.** Abatement of CO₂ emission in the Chinese petroleum refining industry. **M. Du**
- ENFL 254.** PtSn alloy catalyst for ethanol electro-oxidation reaction. **D. Kwak, S. Han, M. Kim, J. Lee, K. Park**
- ENFL 255.** Understanding preignition peroxy chemistry for alkanes and alcohols. **M.J. Goldman, N.W. Yee, S.S. Merchant, W.H. Green**
- ENFL 256.** Detailed type analysis of petroleum samples by using comprehensive 2D gas chromatography/high-resolution mass spectrometry with field ionization. **M. Ubukata, S.E. Reichenbach, Q. Tao, Z. Wu, A.J. Dane, R.B. Cody**
- ENFL 257.** Borate chemistry in the transformation of biomass. **M. McCray, D.M. Schubert**
- ENFL 258.** Honeycomb-alumina supported garnet membrane: Composite electrolyte with low resistance and high strength for lithium metal batteries. **K. Liu, J. Li**
- ENFL 259.** Simple and scalable Si@TiO₂ yolk-shell anode design for high-capacity and long-cycle-life lithium-ion batteries. **Y. Jin, S. Li, Z. Zhu, J. Li**
- ENFL 260.** Investigating lignocellulosic biomass as renewable, non-food source of biofuel and the quest for an efficient pretreatment system. **B. Gikonyo**
- ENFL 261.** Probing changes in porosity and connectivity in Si nano particle electrodes. **L. Wang, Y. Mao**

- ENFL 262.** Renewable fuel production via mild biomass liquefaction process. **K. Mastro, J. Meng, K. McCabe, E. Larson, S. Gangwal**
- ENFL 263.** Evaluation on the potential with channel-type and cage-type metal-organic frameworks as absorbents in solid-phase microextraction. **H. Huang**
- ENFL 264.** Assembly and optimization of paper based microfluidic fuel cells(MFCs) in an alkaline environment. **V. Galvan, K. Domalaon, S. Sotex, C. Tang, F.A. Gomez, J. Haan, M. Jalali Heravi**
- ENFL 265.** Lignin deconstruction by oxidation: Model studies in conventional and ionic liquid solvents. **S.G. Yao, M.S. Meier, R. Pace, M. Crocker**
- ENFL 266.** Surface modification of activated carbon for the improvement of methane adsorption. **K. Nimprayoon**
- ENFL 267.** Impact of municipal solid waste paper mix as a blending agent on enzymatic hydrolysis and acidolysis. **F. Xu**
- ENFL 268.** Comparative study of OMC, MWCNT, and Vulcan Xc-72 as carbonaceous supports of Pt catalysts for direct alcohol fuel cells applications. **D. Morales, F.J. Rodriguez**
- ENFL 269.** Halogenation of natural gas components under mild conditions. **A. Leichtfuss, J. Baltrusaitis, J.D. Schuttlerfeld, Christos, B. Nothem, I. Jansen**
- ENFL 270.** Ligand-assisted co-assembly approach towards mesoporous transition metal oxide/noble metal hybrid catalysts for photochemical water oxidations. **B. Liu, C. Kuo, Z. Luo, S. Thanneeru, W. Li, W. Song, S. Biswas, S.L. Suib, J. He**
- ENFL 271.** Development of nitrogen-containing polymers-graphene oxide for oxygen reduction reaction. **M. Zhou, H. Yen, H. Wang**
- ENFL 272.** Evaluation of hierarchical pore structure zeolites for adsorptive desulfurization of model fuels. **K.X. Lee, C. Martino, J.A. Valla**
- ENFL 273.** Withdrawn.
- ENFL 274.** Preparation of electrochemically exfoliated graphene/MnO₂ nanocomposites by an electrostatic self-assembly process for supercapacitor application. **D. Shu**
- ENFL 275.** Odd-symmetric memristor from asymmetric switches. **P. Cheng, Y.H. Hu**

Section B

Boston Convention & Exhibition Center
Room 258C

Innovative Electrochemical Energy Storage

Future Li Batteries

X. Ji, Organizer

J. Lu, Organizer, Presiding

L. Yu, Presiding

1:00 Introductory Remarks.

1:05 ENFL 276. Advanced high energy and high power battery systems for automotive applications. **K. Amine, J. Lu**

1:45 ENFL 277. Solvent effects on oxygen redox reactions in lithium-air batteries. **D.G. Kwabi, V. Bryantsev, T. Batcho, Y. Shao-Horn**

2:15 ENFL 278. Rechargeable quasi-solid-state lithium air batteries. **H. Kim, T. Kim, V. Roev, H. Kwon, S. Kwon, H. Lee, D. Im**

2:35 ENFL 279. Investigation of confined lithia as cathode for high-energy lithium ion battery. **Z. Zhu, J. Li**

2:55 Intermission.

3:10 ENFL 280. Lithium-oxygen batteries: Computational studies of growth and nucleation mechanisms and effect on cell performance. **L.A. Curtiss**

3:40 ENFL 281. Nanostructured electrocatalysts synthesized using atomic layer deposition for lithium-oxygen batteries. **Y. Lei**

4:10 ENFL 282. Solid state lithiation and delithiation of sulfur: A new concept of lithium-sulfur batteries. **C. Fu, J. Guo**

4:30 ENFL 283. PMMA-based gel polymer electrolyte for lithium-air batteries. **C. Amanchukwu, Y. Shao-Horn, P.T. Hammond**

4:50 ENFL 284. Insights into the absorption mechanism of carbon nanotube paper-titanium dioxide as a multifunctional barrier for lithium-sulfur batteries. **G. Xu, B. Ding, H. Dou, P. Nie, J. Pan, X. Zhang**

5:10 ENFL 285. Several strategies enhancing the electrochemical performance of organic Li and Na batteries. **J. Chen**

Section C

Boston Convention & Exhibition Center
Room 259A

Porous Materials for Energy & Sustainability from Discovery to Application

Financially supported by KAUST & Framergy

Y. Han, S. Ma, Organizers

D. Jiang, Organizer, Presiding

D. Jiang, Presiding

1:00 Introductory Remarks.

1:05 ENFL 286. Nanomaterials with controlled porosity for energy applications. **F. Schueth**

1:50 ENFL 287. Porous colloidal Pt superparticles. **Y. Sun, Y. Hu, Y. Liu**

2:20 ENFL 288. Synthesis of SAPO-18, SAPO-18/34 and SAPO-34 molecular sieves and their catalytic performance for methanol-to-olefins reaction. **Y. Wang, S. Chen, Y. Jiang, Y. Gao, Q. Zhang, F. Chen**

2:40 ENFL 289. Nanoporous bimetallic catalyst for hydrogen evolution reaction. **F. Jiao**

3:00 Intermission.

3:10 ENFL 290. Synthesis and assembly of 1D inorganic semiconductor for solar energy conversion. **X. Feng**

3:30 ENFL 291. Nanoparticle prepared porous silica granulates and their application as oxygen carrier supports for chemical looping process. **Y. Liu, P. Kirchesch, F. Clemens**

3:50 ENFL 292. Low-temperature nitrogen-doping and activation of soft-templated mesoporous carbon for CO₂ capture. **K. Huang, S. Chai, R.T. Mayes, S. Dai**

4:10 ENFL 293. Nanosheet-like silica nanoparticles for CO₂ capture. **C. Lai, N. Pizzi, D.R. Radu**

4:30 ENFL 294. Oxidation Cu-SSZ-13 and active site characterization for methane conversion. **B. Ipek, M.J. Wulfers, J.P. Smith, K.S. Booksh, C.M. Brown, R.F. Lobo**

4:50 ENFL 295. Enhancement of catalytic performance in butene cracking by hierarchied ZSM-5 after chemical liquid deposition. **T. Wu, S. Chen, G. Yuan, S. Li**

5:10 ENFL 296. Waste-to-byproduct conversion of oil shale semicoke and ash to sorbent materials and zeolite precursors. **A. Vyas, J.L. Goldfarb**

Section D

Boston Convention & Exhibition Center
Room 259B

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion

Powder Catalysts

Cosponsored by CATL

S. D. Senanayake, Organizer

Z. Wu, Organizer, Presiding

H. Idriss, Presiding

1:30 ENFL 297. Novel ceria-based catalysts for the water-gas shift reaction. **J. Rodriguez, P. Liu, S.D. Senanayake, D.J. Stacchiola**

2:10 ENFL 298. Size and shape effects in nanostructured catalysts based on combinations of copper and cerium oxides for preferential oxidation of CO in H₂-rich streams. **A. Martinez-Arias**

2:45 ENFL 299. Dopants effect on the adsorption of CO₂ on CeO₂ surfaces. **M. Li, U. Tumulari, Z. Wu, S. Dai**

3:05 Intermission.

3:15 ENFL 300. Ceria-based nanomaterials toward bioapplication. **C. Yan**

3:55 ENFL 301. Dynamics of ionic and polaronic points defects on ceria surface. **W. Chueh**

4:30 Concluding Remarks.

Section E

Boston Convention & Exhibition Center
Room 260

Energy & Fuels Storch Award in Fuel Science: Symposium in Honor of Ripudaman Malhotra

A. Park, Organizer

R. T. Koodali, X. Wang, Organizers, Presiding

1:00 Introductory Remarks.

1:05 ENFL 302. Role of oxygen functional groups in retrogressive reactions. **P.F. Britt, A.C. Buchanan**

1:40 ENFL 303. Extreme catalysis: SAXS studies of endothermic fuel for scram jets. **R.E. Winans, S. Lee, S. Lee, S.L. Anderson**

2:15 ENFL 304. New asphaltene nanoscience and its impact on reservoir characterization. **O.C. Mullins**

2:50 Intermission.

3:05 ENFL 305. Beyond oil and gas: The methanol economy. **S.G. Prakash**

3:40 ENFL 306. Coal to liquids: Seeking cubic miles of oil. **R. Malhotra**

4:15 Concluding Remarks.

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Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Designs: From Molecules to Functional Materials

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Next Generation Nanomaterials: Advances and Perspectives for Biomedicine, Energy, and Environmental Protection

Energy/General

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WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 258B

Advances in Chemistry of Energy & Fuels

A. Park, *Organizer*

D. J. Heldebrant, X. Wang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 314. Electrochemically-mediated Li⁺ chelation by 1,2,3,4-tetrahydro-6,7-dimethoxy-1,1,4,4-tetramethylnaphthalene: In situ structural characterization and energy storage applications. E.V. Carino, J. Staszak-Jirkovsky, R.S. Assary, L.A. Curtiss, N. Markovic, F. Brushett

8:25 ENFL 315. Novel solid state superprotonic conductors and their application as fuel cell electrolytes. I. Santana Klein, S.K. Davidowski, T.G. Tucker, C. Angell

8:45 ENFL 316. Electrically driven molecule transport modeling and optimization of electrodialysis desalination within a series of novel ionomers. D. Wang, C.J. Cornelius

9:05 ENFL 317. Limited layered MoS₂ nanosheets as novel photocatalyst for solar hydrogen production from the splitting of water. R. Peng, Z. Wu

9:25 ENFL 318. CdS-CdTe P-N junction nanotubes for solar cell applications. W.P. Liyanage

9:45 ENFL 319. Free radical-based grafting reactions for the synthesis of lithium cage-based fluoropolymers. S. Xu, R. Jiang, Y. Gao

10:05 Intermission.

10:15 ENFL 320. Improve the performance of FCC catalyst by vanadium trapping components. F. Ren, Q. Liu, Y. Zhu

10:35 ENFL 321. Catalytic behavior of synthesized solid catalyst on magnesium sulfite oxidation. L. Wang, J. Wang, J. Guo

10:55 ENFL 322. Mechanistic insight into coke formation by catalytic pyrolysis of biomass pyrolysis relevant model compounds. S. Du, D.P. Gamliel, J. Valla, G.M. Bollas

11:15 ENFL 323. Palladium catalyzed, hydrogen free lignin depolymerization. M.V. Galkin, S. Sawadjoon, M. Dawange, V. Rohde, C. Dahlstrand, J.S. Samec

11:35 ENFL 324. Coal pyrolysis under the atmosphere generated in situ from methanol decomposition. X. He, L. Yang, H. Wu, Y. Zhang, A. Zhou

Section B

Boston Convention & Exhibition Center
Room 258C

Innovative Electrochemical Energy Storage

Advanced Characterizations & Electrolytes

J. Lu, *Organizer*

X. Ji, *Organizer, Presiding*

E. Pomerantseva, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL 325. In situ electrochemistry in transmission electron microscope. J. Li

8:35 ENFL 326. Exploring batteries at APS beamline 9-BM. T. Wu

9:05 ENFL 327. Ex-situ and in-situ characterizations of the Li removal from the anti-fluorite Li₂FeO₄. C. Zhan, J. Lu, K. Amine

9:25 ENFL 328. In situ transmission electron microscopy observation of lithium hair growth. A. Kushima, K. So, J. Li

9:45 ENFL 329. Investigation of ether-based electrolytes for nonaqueous redox flow batteries via high-throughput screening. L. Su, M. Ferrandon, J. Barton, N. Upia, J.T. Vaughney, F. Brushett

10:05 Intermission.

10:15 ENFL 330. Understanding the interaction, correlation, and frustration in battery materials at the electronic and atomic level using in-situ synchrotron X-ray probes. Y. Ren, Q. Liu, B. Aoun, C. Sun, J. Xie, W. Lu, Z. Chen

10:45 ENFL 331. Glyceryl triester as co-solvent in Li-battery electrolyte for high voltage application. B. Roy, D. Kim, Y. Kang, J. Park, S. Doo

11:05 ENFL 332. Preparation and properties of proton and lithium conducting membranes from polymer brush nanoparticles. I. Zharov

11:25 ENFL 333. Evaporation induced self-assembly of nanoflaky Li₃PS₄ for ultrathin solid electrolyte membrane. H. Wang, C. Liang

11:45 ENFL 334. Boron nitride-based study for energy storage application. W. Luo, H. Zhu, B. Yang, L. Hu

Section C

Boston Convention & Exhibition Center
Room 259A

International Symposium on Mesoporous Zeolites

Cosponsored by CATL, I&EC and INOR

Financially supported by Rive Technology, Zeolyst International, Chevron, Quantachrome Instruments, W. R. Grace

J. Garcia Martinez, K. Li, *Organizers*

F. Schueth, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL 335. Hierarchical zeolites: Increase in mesosurface via "bottom-up" or "top-down" methods and its influence in catalytic cracking. E. Falabella Sousa-Aguar

9:15 ENFL 336. Efficient catalyst design by NH₄OH treatment of USY zeolite. J. Van Aelst, A. Philippaerts, N. Nuttens, D. Verboeckend, M. Kurttepelii, E. Gobechevia, M. Haouas, S.P. Sree, J. Denayer, J. Martens, C. Kirschhook, F. Taulelle, S. Bals, G. Baron, P. Jacobs, B.F. Sels

9:45 ENFL 337. Investigation of enhanced mass transport and surface barrier in hierarchical zeolites. C. Chang, A.R. Teixeira, C. Li, P. Dauenhauer, W. Fan

10:15 Intermission.

10:25 ENFL 338. Mesoporous Y zeolite prepared by combining acid leaching and base treatment of a non-uniform aluminum-silicon distribution architecture. D. Yuan, C. Kang, P. Zeng, S. Ren, Q. Guo, B. Shen

11:05 ENFL 339. Effect of zeolite mesoporosity and acidity on the hydroconversion of *n*-hexadecane over Pt/based catalysts. E.F. Iliopoulou, E. Heracleous, A. Lappas, K. Triantafyllidis, N. Linares, J. Garcia Martinez

11:35 ENFL 340. Hydrodenitrogenation of *o*-ethylaniline over NiMo/SBA-15 catalysts promoted by citric acid. S. Jiang, Y. Zhou, Q. Wei

Section D

Boston Convention & Exhibition Center
Room 259B

Advances in Analytical Methods for Petroleum Upstream Applications

C. F. Ovalles, C. E. Rechsteiner, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 ENFL 341. Metallurgical considerations for petroleum sampling applications. T. Dudley

9:10 ENFL 342. Modular fluidic control hardware applications for process and laboratory analytics. M. Cost

9:40 ENFL 343. Ultrafast GC performance in the real world: Multi lab studies for repeatability and reproducibility. C.E. Rechsteiner, J. Crandall, N. Roques

10:10 Intermission.

10:20 ENFL 344. Frequently asked questions (FAQs) on high temperature simulated distillation. L.A. Carbognani, J. Carbognani, P.R. Pereira-Alamao

10:50 ENFL 345. Modern petroleomics. R.P. Rodgers, Y. Corilo, D.C. Podgorski, V. Lobodin, S.M. Rowland, P. Lalli, J.C. Putman, A. Clingenpeel, W.K. Robbins, J. Lu

11:20 ENFL 346. Application of microwave plasma atomic emission spectroscopy in crude oil analysis. J. Nelson, G. Greg, L. Poirier, D. Leong, P. Hajdu, F.A. Lopez-Linares

11:50 Concluding Remarks.

Section E

Boston Convention & Exhibition Center
Room 260

Energy & Fuels Storch Award in Fuel Science: Symposium in Honor of Ripudaman Malhotra

A. Park, *Organizer*

R. T. Koodali, X. Wang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 347. Fischer-Tropsch synthesis: Effect of CO conversion on product selectivities during deactivation by oxidation or by changing space velocity at stable conditions over unpromoted and Ru promoted 25% Co/Al₂O₃ catalysts. W. Ma, U. Graham, G. Jacobs, B. Todic, D.B. Bukur, B.H. Davis

8:40 ENFL 348. Withdrawn.

9:15 ENFL 349. Withdrawn.

9:50 Intermission.

10:05 ENFL 350. Study of the gas and solid phase catalytic behaviors of low loading metal catalysts in the alkaline thermal treatment of cellulose to H₂ with Ca(OH)₂. A. Park, M. Stonor, J.G. Chen

10:40 ENFL 351. Design and synthesis of materials for energy conversion and storage. Y.H. Hu

11:15 Concluding Remarks.

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Energy Storage, Solar Fuels, and Biofuels: Satisfying the Energy Needs While Decreasing the Carbon Footprint

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 258B

Advances in Chemistry of Energy & Fuels

D. J. Heldebrant, A. Park, *Organizers*

X. Wang, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 352. Cobalt-based chalcogenides nanostructure arrays as highly efficient bifunctional catalyst for oxygen reduction and evolution reactions. J. Masud, A. Swesi, W.P. Liyanage, N. Ashokaan, M. Nath

1:25 ENFL 353. Pyrolysis of fuels to absorb heat before use in combustion. P.R. Westmoreland, S.D. Crymble, S.J. Taylor

1:45 ENFL 354. Effect of Cs on product selectivity for the conversion of glycerol using a supported heteropolyacid catalyst. C. Mai, F.T. Ng

2:05 ENFL 355. Band-edge modulation of p-Si(111) and integration of H₂ catalyst with p-Si(111). J. Seo

2:25 ENFL 356. Glycerol hydrogenolysis to 1,2-propanediol with in situ hydrogen produced from methanol steam reforming. Y. Liu, F.T. Ng, G. Rempel

2:45 ENFL 357. In-situ FTIR investigation on semiconductor catalyst reduction. B. Han, Y.H. Hu

3:05 Intermission.

3:20 ENFL 358. Engineering nanocrystals for oxygen reduction. S. Guo

3:40 ENFL 359. Ruthenium PNP-pincer complex-catalyzed amine-free reversible hydrogen storage in formate salts without pH control or solvent change. J. Kothandaraman, M. Czaun, A. Goeppert, R.M. Haiges, J. Jones, R. May, S.G. Prakash, G.A. Olah

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4:00 ENFL 360. CO₂ absorption in 1-butyl-3-methylimidazole glycine ionic liquid. Q. Li, Y. Zhao, L. Wang, L. Yang

4:20 ENFL 361. Withdrawn.

4:40 ENFL 362. Withdrawn.

Section B

Boston Convention & Exhibition Center
Room 258C

Innovative Electrochemical Energy Storage

Advanced Li-Ion Batteries

X. Ji, *Organizer*

J. Lu, *Organizer, Presiding*

W. Luo, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 363. Research and development overview of new technologies and related materials for rechargeable batteries. F. Wu, L. Li

1:45 ENFL 364. Modification of interlayer distances of titanates by changing pH and their use as a lithium-ion battery anode with high capacity and rate capability. A. Yurum, M. Yarali, E. Bicer, S. Alkan Gursesl

2:15 ENFL 365. Voltage fading mechanism of Li-rich layered oxide cathode materials for lithium-ion batteries. A. Choi, H. Lim, K. Lee

2:45 ENFL 366. First principles study for site-selective Al or Ga doped Li₂MnO₃ phases. D. Yeon, J. Song, J. Park

3:05 ENFL 367. Antiperovskite Li₂OCl solid-state electrolyte films for Li-ion batteries. X. Lu, Y. Zhao, H. Xu, Q. Jia

3:25 Intermission.

3:35 ENFL 368. New high energy and power chemistries in 3D meso-structured electrodes for rechargeable batteries. P.V. Braun

4:05 ENFL 369. Design of metal-organic framework composite materials for energy conversion. F. Huo

4:35 ENFL 370. Yolk-shell nanomaterials for efficient lithium ion storage. S. Guo

4:55 ENFL 371. Monolithic lithium/sulfur-poly(acrylonitrile) composite-based batteries: Synthesis and structure-related electrochemistry. M. Buchmeiser, M. Frey, A. Hintennach

Section C

Boston Convention & Exhibition Center
Room 259A

International Symposium on Mesoporous Zeolites

Cosponsored by CATL, I&EC and INOR

Financially supported by Rive Technology, Zeolyst International, Chevron, Quantachrome Instruments, W. R. Grace

J. Garcia Martinez, K. Li, *Organizers*

E. Falabella Sousa-Aguirre, *Presiding*

1:30 Introductory Remarks.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

1:35 ENFL 372. Mesoporous zeolites and related materials for the conversion of biomass-based feedstocks. F. Schueth

2:15 ENFL 373. Investigation of hierarchical pore structure zeolites for biomass catalytic fast pyrolysis. D.P. Gamliel, L. Wilcox, N. Nguyen, J. Valla

2:45 ENFL 374. Modern view on zeolite stability: Integrity and application of zeolite catalysts in condensed aqueous phase. T. Ennaert, P. Jacobs, B.F. Sels

3:15 Intermission.

3:25 ENFL 375. On the rational design of zeolite clusters.

A.N. Migués, S.M. Auerbach, W. Sherman, S. Vaitheeswaran, A.N. Muskat

3:55 ENFL 376. Functionalization and mesoporosity control of zeolitic metal-organic frameworks. H. Zeng

4:25 ENFL 377. Extracrystalline siting of ruthenium-dioxide nanoparticles on NaY zeolites: Effective, atom-efficient dispersed electrocatalytic nanoelectrodes. V.M. Cepak, D.R. Rolison

4:55 Concluding Remarks.

Section D

Boston Convention & Exhibition Center
Room 259B

Advances in Analytical Methods for Petroleum Upstream Applications

C. F. Ovalles, C. E. Rechsteiner, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL 378. Bulk and spatially-resolved measurements of kerogen composition. A.E. Pomerantz, J. Yang, R. Kleinberg

1:35 ENFL 379. Studies on asphaltene-wax association in crude oils. E. Rogel, C.F. Ovalles, J. Vien, M. Morazan, M. Moir

2:05 ENFL 380. ¹³C-NMR analysis of low olefin contents in upgraded bitumen. M.I. Trujillo, Q. Wu, L. Carboognani Ortega, P.R. Pereira-Alamao

2:35 Intermission.

2:45 ENFL 381. Characterization of asphaltene solubility fractions from a deposit using atmospheric pressure photoionization coupled to Fourier transform ion cyclotron resonance mass. E. Rogel, M. Witt

3:15 ENFL 382. Gradient-based high performance thin-layer chromatography for an expanded SARA analysis of heavy petroleum products. V.L. Cebolla, C. Jarne, L. Membrado

3:45 Intermission.

3:50 ENFL 383. Quantitative analysis of olefins in motor fuels by Raman spectroscopy: Methodology and structural dependence of scattering intensity. M. Trygstad, Y. Bismilla, M. Kemper

4:20 ENFL 384. Molecular modeling for hydrogenation of light cycle oil. H. Fujinaga

4:50 Concluding Remarks.

Section E

Boston Convention & Exhibition Center
Room 260

Innovative Utilization Pathways for Natural Gas

Cosponsored by CATL

A. L. Boehman, A. Marchese, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENFL 385. Refining opportunity crudes and dealing with a high iron environment in FCC. M. Clough

2:05 ENFL 386. Effect of N₂ species on selective acetylene hydrogenation over Pd/SAC catalysts. M. Hu, X. Wang

2:35 ENFL 387. New reduced chemical kinetic mechanism for CFD simulations of natural gas/diesel dual fuel engines. A. Hockett, G. Hampson, A. Marchese

3:05 Intermission.

3:25 ENFL 388. Study on the autoignition characteristics of a HCCI engine fueled with natural gas. O. Lim

3:55 ENFL 389. Corn ethanol: The surprisingly effective route for natural gas consumption in the transportation sector. J.P. Szybist, S. Curran

4:25 ENFL 390. Dimethyl ether as a transportation fuel: Current status and research challenges. A.L. Boehman

4:55 Concluding Remarks.

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

WEDNESDAY EVENING

Advances in Chemistry for Carbon Capture, Utilization and Sequestration

Sponsored by ENVR, Cosponsored by ENFL

THURSDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 258B

Advances in Chemistry of Energy & Fuels

A. Park, *Organizer*

D. J. Heldebrant, X. Wang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL 391. Design and syntheses of highly stable mesoporous porphyrinic zirconium MOFs for gas storage. T. Liu

8:25 ENFL 392. Polymorphous alumina materials and HDS performance of FCC diesel. X. Wang, M. Zhang, H. Fang, A. Duan, C. Xu, Z. Zhao

8:45 ENFL 393. Upgrading inferior residue to produce light oil in a pretreating process. N. Jin, G. Wang, C. Wang, J. Gao, C. Xu

9:05 ENFL 394. Core structures analysis of heavy oils by using of CID FT-ICR-MS. K. Katano, T. Suzuki, R. Tanaka

9:25 ENFL 395. Measurement and analysis of release gas in oil tank. Z. Tang, Y. Deng, Y. Wang, Y. Luo, X. Guo, A. Liu, W. Lan, Q. Sun

9:45 ENFL 396. Compressed liquid density and the bulk modulus of conventional jet fuels and jet fuel surrogates. T. Kim, D. Kang, A.L. Boehman

10:05 Intermission.

10:15 ENFL 397. Indigenous algal growth on municipal sludge centrate and measuring lipid productivity using fluorospectroscopy and gravimetric analyses. T.C. Halfhide, S. Ergas

10:35 ENFL 398. Analysis of microbial diversity in bioaugmentation for biological treatment of petroleum refinery wastewater. H. Dong, H. Dong, M. Zhang, J. Li, S. Sun, J. Guo, M. KE, Z. Song, Z. Zhang

10:55 ENFL 399. Comparison of the reduction products: Vinylene carbonate vs. fluoroethylene carbonate. B.S. Subramanian Parimalam, M. Nie, B.L. Lucht

11:15 ENFL 400. Kinetics and thermal degradation of powder-free laboratory examination gloves by thermogravimetric analysis at 313°C and 408°C. N. Hamidi, M. Marcanikova

11:35 ENFL 401. Rational design of ultrathin graphene-protein supercapacitors for implantable biomedical devices. I.M. Mosa, A. Pattammattel, K. Kadimisetty, P. Pande, M.F. El-Kady, G. Bishop, M.J. Novak, A.K. Basu, C.V. Kumar, J. Rusling

Advances in Chemistry for Carbon Capture, Utilization and Sequestration

Sponsored by ENVR, Cosponsored by ENFL

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Designs: From Molecules to Functional Materials

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

THURSDAY AFTERNOON

Section B

Boston Convention & Exhibition Center
Room 258B

Innovative Electrochemical Energy Storage

Beyond Alkali Metal Ion Batteries

X. Ji, J. Lu, *Organizers*

J. Guo, Y. Shao, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL 402. Development of transformational electrochemical energy storage and conversion. G. Soloveichik

1:35 ENFL 403. Organic aqueous redox flow batteries. M.J. Aziz

2:05 ENFL 404. Rechargeable magnesium batteries: Electrolytes, cathodes, and beyond. G. Li

2:35 ENFL 405. Withdrawn.

2:55 ENFL 406. Optimized surface chemistry of dual-intercalation batteries. B. Dyatkin, J.A. Read

3:15 Intermission.

3:20 ENFL 407. Rechargeable Mg battery: Material and interface study. Y. Shao

3:50 ENFL 408. Prototype rechargeable aluminum battery. J. Guo, L. Geng

4:10 ENFL 409. Activation of MnO₂ cathode by water-stimulated Mg²⁺ insertion for magnesium battery. J. Song, M. Noked, E. Gillette, J. Duay, G. Rubloff, S. Lee

4:30 ENFL 410. Lewis acid-free and high anodically stable electrolytes for nonaqueous rechargeable magnesium-ion batteries. B. Pan, A.K. Burrell, Z. Zhang, C. Liao

4:50 ENFL 411. Size selective strategy for high-performance nonaqueous redox flow batteries. E. Montoto, E. Chenard, J. Hui, N. Gavvalapalli, K. Cheng, T. Lichtenstein, J. Moore, J. Rodriguez Lopez

5:10 ENFL 412. Multielectron electrochemical charge storage in 2D transition metal compounds.

C.P. Rhodes, A. Zaleski, C. Ly, G. Cruz

Division of Environmental Chemistry

D. Dionysiou, Program Chair

OTHER SYMPOSIA OF INTEREST:

National Science Foundation's Centers for Chemical Innovation (see PRES, Sunday)

Lab Safety 25 Years After Promulgation of the OSHA Laboratory Standard (see CHAS, Sunday, Monday)

Environmental and Energy-Related Inorganic Chemistry (see INOR, Sunday, Tuesday)

Transformation & Transport of Radionuclides in the Environment (see NUCL, Tuesday)

Transforming University-Industry Partnerships for an Innovative Future (see PRES, Tuesday)

Subsurface Geochemistry for Energy & the Environment (see GEOC, Tuesday, Wednesday)

SOCIAL EVENTS:

Reception, 6:30 PM: Tuesday

Dinner, 8:00 PM: Tuesday

BUSINESS MEETINGS:

Program Planning Meeting, 2:00 PM: Sunday

Long Range Planning Meeting, 3:00 PM: Sunday

Business Meeting, 7:00 PM: Sunday

Executive Committee Meeting, 7:30 PM: Sunday

SUNDAY MORNING

Section A

Boston Park Plaza Hotel and Towers Statler Room

New Challenges in Water Quality, Treatment, Reuse and Sustainability: Chemistry and Application of Advanced Oxidation Processes for Removal of Contaminants of Concern and Transformation Products

Processes

Cosponsored by CEI

R. de Fatima Peraita Muniz Moriera, D. Minakata, K. E. O'Shea, *Organizers*

D. D. Dionysiou, G. Li Puma, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 1. Fundamental understanding of radical transformation in UV-AOPs with different parent compounds: Implication on treatability. H. Liu, T. Jain, W. Li

8:30 ENVR 2. Utilizing chlorine atom reactivity in UV-based advanced oxidation processes: Kinetics and efficiencies of Cl atom reactions. K. Couch, S.P. Mezyk, K.P. Ishida

8:55 ENVR 3. Discovery of new fate of transformation products in aqueous phase advanced oxidation processes using ab initio quantum mechanical calculations. D. Minakata, D. Kamath, M. Rouleau

9:20 ENVR 4. Withdrawn.

9:45 Intermission.

10:00 ENVR 5. High-precision measurement of oxygen and hydrogen isotope ratios in water vapor using diode laser spectroscopy in the IR wavelength of 1.39 μm . W. Al-Basheer, A. Aljalal, K. Gasmi

10:25 ENVR 6. Enhanced anti-Stokes emission and photocatalytic activity in a dual-sensitizer triplet-triplet annihilation upconversion system. A. Hagstrom, F. Deng, C. Li, H. Kim, J. Kim

10:50 ENVR 7. Standard heats of oxidation for characterized soils. S.P. Mezyk, N. Moulton, M. Becker

11:15 ENVR 8. Photocatalytic oxidation of bisphenols (A, F and AF) in BR and CSTR. B. Erjavec, P. Hudoklin, K. Perc, T. Tisler, M. Sollner, A. Pintar

Section B

Boston Park Plaza Hotel and Towers St. James Room

Designing Safer Chemicals

Cosponsored by CEI

A. Voutchkova, *Organizer*

P. T. Anastas, J. B. Zimmerman, *Organizers, Presiding*

8:00 ENVR 9. On the design of safer commercial chemicals: Past, present, and future perspectives. S. DeVito

8:30 ENVR 10. Predicting cytotoxicity based on EPA ToxCast data and designing safer chemicals. L. Shen, F. Melnikov, R. Judson, A. Voutchkova, J. Kostal, J.B. Zimmerman, P.T. Anastas

9:00 ENVR 11. Framework to guide selection of chemical alternatives. D. Dorman, E.J. Beckman, P. Beak, J. Cura, A. Fairbrother, N. Greene, C. Henry, H. Holder, J.R. Hutchison, G. Paoli, J. Quint, I. Rusyn, K. Shelton, J. Tickner, A. Voutchkova, M.H. Wolf, M. Shelton-Davenport, K. Hughes

9:20 ENVR 12. Designing safer chemicals: Application of the principles of green chemistry in a chemical company. C. Rowlands

9:40 ENVR 13. Predictive tools for bioavailability and oxidative stress based on spectroscopic data. N. An, A. Voutchkova-Kostal

10:00 Intermission.

10:15 ENVR 14. Exploiting enhanced non-testing approaches to meet the needs for sustainable chemistry. G. Patlewicz, A. Richard, K. Houck, R. Judson

10:35 ENVR 15. Advancing safety assessments of chemicals through biological read across using multidimensional in vitro toxicity testing. F. Grimm, I. Rusyn

10:55 ENVR 16. Need for safer chemicals and rapid screening tools: The 2014 Freedom Industries chemical spill, West Virginia, USA. A.J. Whelton

11:15 ENVR 17. No substitutes allowed: Chemical processes that have thus far eluded a green alternative. C. Kashat, S. Anderson, J. Payne, S. Maurice, M.A. Benvenuto

Section C

Boston Park Plaza Hotel and Towers Berkeley/Ciarendon Room

Nano-Enabled Environmental Technologies

Technologies for Treatment of Microbial and Carbon-Based Contaminants

Financially supported by Boston University, Division

of Materials Science & Engineering

J. L. Goldfarb, *Organizer*

K. Doudrik, K. D. Hristovski, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 18. Fullerene-based multifunctional antimicrobial composites via block copolymer templates. K. Moor, C.O. Osuji, J. Kim

8:30 ENVR 19. Effects of rhamnolipid and carboxymethylcellulose coatings on reactivity of palladium-doped nanoscale zerovalent iron particles to trichloroethylene. S. Bhattacharjee, M. Basnet, N. Tufenkji, S. Ghoshal

8:55 ENVR 20. Removal of carbamazepine and tetracycline from water by magnetic carbonaceous nano-adsorbents prepared by ball-milling. D. Shan, S. Deng, W. Bin, Y. Wang, Y. Huang, G. Yu

9:20 ENVR 21. Drinkable book — a novel nano-enabled antibacterial paper filter for water purification in developing countries. T.A. Dankovich

9:45 Intermission.

10:00 ENVR 22. Nanoscale colloidal manganese oxides formation and their implications for drinking water treatment. M.E. Vargas-Vallejo, G. Hinds, W.R. Knocke, M.F. Hochella, F.M. Michel, M. Murayama

10:25 ENVR 23. Functional biodegradable nanoparticles for the remediation of environmentally relevant aldehyde and carboxylic acid contaminants in the gas phase. D.C. Whitehead

10:50 ENVR 24. Investigation of the kinetics and diffusion of carbon dioxide capture in amine modified MCM-36. C.F. Cogswell, H. Jiang, T. Nigl, S. Choi

11:15 ENVR 25. Arsenic, cadmium, lead, nickel, and thallium removal by copper based metal organic framework and investigation of their adsorption kinetics and thermodynamics. A. Yurdusen, Y. Yurum

Section D

Boston Park Plaza Hotel and Towers Beacon Hill Room

Advances in Drinking Water Disinfection: Byproducts Occurrence, Formation, Treatment, Health Effects, Epidemiology and Regulation

E. Sahle-Demessie, G. Sorial, *Organizers, Presiding*

8:00 ENVR 26. Control of bromate formation in UV/peroxymonosulfate, UV/persulfate and Co/peroxymonosulfate processes by ammonia, chlorine-ammonia, and ammonia-chlorine processes. L. Ling, Z. Li, J. Fang, C. Shang

8:25 ENVR 27. Withdrawn.

8:50 ENVR 28. Withdrawn.

9:15 ENVR 29. Withdrawn.

9:40 ENVR 30. Withdrawn.

10:05 Intermission.

10:20 ENVR 31. Ferrate (VI) mediated degradation and detoxification of the potent cyanotoxin, cylindrospermopsin. C. Zhao, V.K. Sharma, D. Dionysiou, K.E. O'Shea

10:45 ENVR 32. Ferrate oxidation of bromide: Formation of bromate in deionized and natural waters. Y. Jiang, J. Goodwill, D. Reckhow, J. Tobiason

11:10 ENVR 33. Role of manganese oxide in the formation of disinfection byproducts. A. Bazilio, J.E. Tobiason

11:35 ENVR 34. Efficient production of ozone in an oxygen microplasma for water treatment. J. Lozano

Section E

Boston Park Plaza Hotel and Towers Tremont

Assessing Transformation Products by Non-Target and Suspected Target Screening: The New Frontier in Environmental Chemistry and Engineering

Financially supported by AEESP (Association of Environmental Engineering and Science Professors) S. A. Snyder, *Organizer*

J. Drews, T. Letzel, *Organizers, Presiding*

8:00 Introductory.

8:05 ENVR 35. Fate of antiviral compounds and their transformation products in the urban water cycle. C. Prasse, D.L. Sedlak, T.ernes

8:25 ENVR 36. HRMS approaches for evaluating transformations of pharmaceuticals in the aquatic environment. D. Barcelo, B. Zonja, S. Perez

8:45 ENVR 37. Identifying transformation products of organic micropollutants in conventional wastewater treatment by high-resolution mass spectrometry and differential non-targeted screening. G.J. Getzinger, L. Ferguson

9:05 ENVR 38. Transformation and products of thiol drugs with the presence of humic substance in water during enzymatic catalysis. P. Du, H. Zhao, H. Cao

9:25 ENVR 39. Accurate mass screening and data evaluation approaches for ozonation by-products in wastewater treatment plant effluents. C. Zwiener, S. Merel, S. Lege

9:45 ENVR 40. Target, suspected-target, and non-target LC-MS/MS screening: New strategies for transformation products and metabolites in water bodies. T. Letzel

10:05 Intermission.

10:20 ENVR 41. Linking trace organic chemical attenuation to the metabolic capability of the microbiome in complex environments: Insights from laboratory- and full-scale managed aquifer recharge systems. J. Regnery, D. Li, S. Roberts, C.P. Higgins, J.E. Drewes

10:40 ENVR 42. Characterization of products of 2,4-dinitroanisole (DNAN) microbial biotransformation using liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (LC-QToF-MS) and their inhibitory impact to methanogens. C.I. Olivares, L. Abrell, J. Chorover, R. Sierra-Alvarez, J. Field

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11:00 ENVR 43. Identification of transformation products in sulfate radical based groundwater remediation and toxicity implications. W. Li, D. Schlenk, H. Liu

11:20 ENVR 44. Formation of bioactive transformation products during glucocorticoid chlorination. N.C. Pflug, A. Kupsco, E.P. Kolodziej, D. Schlenk, J.B. Gloer, D.M. Cwiertny

11:40 ENVR 45. NORMAN Association: A network approach to scientific collaboration on emerging contaminants and their transformation products in Europe. J. Slobodnik

12:00 Concluding Remarks.

Section F

Boston Park Plaza Hotel and Towers
Cambridge Room

Hydrothermal Carbonization: Possibilities and Limits for Feedstocks, Processes and Applications

HTC Fundamentals and Sorption

Cosponsored by AGRO

Financially supported by AEEESP (Association of Environmental Engineering and Science Professors) S. Chang, J. A. Libra, *Organizers*

C. Coronella, K. Ro, *Organizers, Presiding*

8:00 ENVR 46. Sustainable carbon materials and chemicals from biomass via hydrothermal carbonization. M. Titirici, F. Pileidis, A. Marinovic

8:35 ENVR 47. Putting the “hydro” in hydrothermal — chemistry of hot water and its influence on process efficiency of hydrothermal carbonization. A. Funke, T. Schäfer, A. Kruse

9:00 ENVR 48. Mechanochemical modification of hydrothermal chars. M.T. Timko, A. Brown, B. McKeogh, J. Venegas, G. Tompsett, N.A. Deskins

9:25 ENVR 49. Hydrothermal carbonization (HTC) for producing a biocarbon with coal like properties from undervalued lignocellulosic biomass. A. Dutta

9:50 Intermission.

10:15 ENVR 50. Characterization and adsorption ability of CO₂ activated hydrochars. J. Fang, B. Gao

10:40 ENVR 51. Hydrochar as sorbent for organic contaminant removal: connecting the effect of the char physicochemical properties with sorption capacity for pyrene and pharmaceuticals and personal care products (PPCPs). K. Sun, L. Han, K. Ro, J. Libra, H. Sun, B. Xing

11:05 ENVR 52. Developing livestock odor reduction system using biochar/hydrochar - characteristics. S. Cho, O. Hwang, D. Han, K. Ro

Section G

Boston Park Plaza Hotel and Towers
Stuart Room

Next Generation Nanomaterials: Advances and Perspectives for Biomedicine, Energy, and Environmental Protection

Biomedicine/Energy

Cosponsored by ENFL

J. Mi, J. Song, *Organizers, Presiding*

8:00 ENVR 236. Targeted polymeric nanoparticles: From discovery to clinical trials. O. Farokhzad

8:30 ENVR 237. Allosteric ligands and nanoparticle conjugates for photocontrol of unmodified neurons. D.R. Pepperberg

9:00 ENVR 238. Nanoscale metal oxide clusters for biomedicine and water splitting. J. Mi, J. Song

9:20 ENVR 239. Sustainable antimicrobial polymers and nano-assemblies for killing MRSA. C. Tang

9:40 Intermission.

9:55 ENVR 240. Thermostable RNA motif as boiling-resistant polymers in material science and nanotechnology. P. Guo

10:25 ENVR 241. Synthesis, assembling, and actuation of plasmonic-active rotary nanomotors for controlled biochemical release and detection with Raman spectroscopy. X. Xu, K. Kim, D. Fan

10:45 ENVR 242. Novel antibiotic/silver nanomaterial hybrid as a surface coating on medical devices. D.E. Gorka, M. Arifuzzaman, J.C. Timmerman, R. Widenhoefer, S. Abraham, J. Liu

11:05 ENVR 243. Mobility of iron oxide nanoparticles under representative reservoir conditions. B.A. Lyon, A. Kmetz II, M.D. Becker, E.L. Foster, E.E. Urena Benavides, M. Iqbal, Y. Fei, E. Moaseri, C.J. Ellison, K.P. Johnston, L.M. Abriola, K.D. Pennell

Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization and Storage

CO₂ Capture Using Advanced Materials

Sponsored by ENFL, Cosponsored by ENVR†

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Sponsored by PHYS, Cosponsored by ENVR

Pesticide Dose: Effects on the Environment and Target and Non-Target Organisms

Sponsored by AGRO, Cosponsored by ENVR

Biofuels for Powering the World: Discovery to Application

Catalytic Fast Pyrolysis

Sponsored by ENFL, Cosponsored by CATL and ENVR

SUNDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers
Statler Room

New Challenges in Water Quality, Treatment, Reuse and Sustainability: Chemistry and Application of Advanced Oxidation Processes for Removal of Contaminants of Concern and Transformation Products

Reactors

Cosponsored by CEI

R. de Fatima Peralta Muniz Moriera, D. D. Dionysiou, D. Minakata, K. E. O'Shea, *Organizers*

G. Li Puma, *Organizer, Presiding*

J. Sánchez Pérez, *Presiding*

1:30 ENVR 53. Effect of liquid depth and iron concentration on micropollutant removal by solar photo-Fenton in raceway pond reactors. J. Sánchez Pérez, J. Casas Lopez, J. Garcia Sánchez, G. Rivas Ibañez, P. Soriano

2:10 ENVR 54. Novel microfluidic approach for extremely rapid photochemical transformations of chemical and biological species. N.M. Reis, G. Li Puma

2:35 ENVR 55. Solar CPC reactor design using boundary layer of photon absorption and ray-tracing. H.L. Otálvaro-Marín, M.Á. Mueses, J.C. Crittenden, F. Machuca-Martinez

3:00 ENVR 56. Cyanide removal by photo-Fenton process, assisted with ferrioxalate, under the sunlight, using a parabolic cylindrical rotary reactor (PCRR). A. Barbosa Lopez, D. Gil, K. Pajaro

3:25 Intermission.

3:40 ENVR 57. Photovoltaic-driven UV-LED photo-Fenton: A new approach for micropollutant removal. J. Casas Lopez, G. Rivas Ibañez, I. de la Odra, M. Perez Garcia, J. Sánchez Pérez

4:05 ENVR 58. Kinetics and modeling of reacted oxidants in saltwater ozonation. Y. Jung, E. Hong, M. Kwon, Y. Jung, H. Kye, J. Kang

4:30 ENVR 59. Method for hydroxyl radical rapid production using a strong ionization discharge combined with effect of water jet cavitation. M. Bai, Z. Zhang, Y. Yu, H. Li, Y. Zhang

4:55 ENVR 60. Effect of the absorption process over the discoloration of dyes by solar heterogeneous photocatalysis. M. Almansa-Ortegon, M. Hernandez-Famirez, M. Mueses, J.A. Colina-Marquez, F. Machuca-Martinez

Section B

Boston Park Plaza Hotel and Towers
St. James Room

Designing Safer Chemicals

Cosponsored by CEI†

P. T. Anastas, *Organizer*

A. Voutchkova, J. B. Zimmerman, *Organizers, Presiding*

1:30 ENVR 61. Alerts about toxicity alerts. A. Tropsha, D. Fourches, R. Politi, Y. Low, E. Muratov

2:00 ENVR 62. Chemical design process at the crossroads of product efficacy and risk assessment. C. Yang, J.F. Rathman, C.H. Schwab, B. Bienfait

2:30 ENVR 63. Use of computational toxicology for evaluating potential endocrine bioactivity and exposure. K. Markey

2:50 ENVR 64. Assessing the accuracy of software predictions of mammalian and microbial metabolites. M. Card, C. Tebes-Stevens, E.J. Weber

3:10 ENVR 65. Quantitative structure-fragmentation relationships (qFRs): Development of a data-driven workflow for alternatives ingredient assessments for in silico molecular repurposing. M.R. Goldsmith, D.T. Chang, A. Deschenes

3:30 Intermission.

3:45 ENVR 66. Quantitative structure-activity relationships for predicting toxicity and biodegradability of biosynthetic and bio-inspired glycolipid surfactants. J. Pemberton, R. Polt, L. Szabo, R. Palos Pacheco, L. Kegel, C. Coss, A. Fathi, R. Gonzalez, R. Eismir

4:05 ENVR 67. Screening/prioritization of chemicals and QSAR “Benign by Design” approach: The cumulative PBT index model in QSARINS. P. Gramatica, E. Papa, S. Cassani, A. Sangion

4:25 ENVR 68. Analysis of xenobiotic properties leading to electrophilic or radical activation of Nrf2-keep1 pathway in ToxCast. F. Melnikov, J. Kosal, L. Sehn, A. Voutchkova, J.B. Zimmerman, P.T. Anastas

4:45 ENVR 69. Quantum chemistry blueprints for greener chelating agents. E.J. Beckman, M.N. Vo, J.A. Keith, K. Johnson

5:05 ENVR 70. Coupling the power of high throughput zebrafish screening and synthetic chemistry to design safer chemicals. R.L. Tanguay, M. Simonich, L. Truong

Section C

Boston Park Plaza Hotel and Towers
Berkeley/Clarendon Room

Nano-Enabled Environmental Technologies

Technologies for Treatment of Inorganic Water Contaminants

Financially supported by Boston University, Division of Materials Science & Engineering K. D. Hristovski, *Organizer*

K. Doudrik, J. L. Goldfarb, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 71. Goethite nanoparticles impregnated cross-linked macroporous polymer for arsenic removal: full-scale system modeling. K. Taleb, J.S. Markovski, K.D. Hristovski, V. Rajaković-Ogrjanović, A. Mariniković

2:00 ENVR 72. Engineering superparamagnetic metal oxide nanocrystals for chromium and arsenic sorption, and separation. C. Kim, S. Lee, W. Li, J. Fortner

2:25 ENVR 73. Evidence of facilitated surface diffusion of arsenate in nano-metal (hydr)oxide hybrid ion exchange media. S. Dale, K.D. Hristovski

2:50 Intermission.

3:05 ENVR 74. Using hybrid ion exchanger with nanoscale zirconium oxide particles (HIX-NanoZr) to mitigate fluoride crisis in Africa and Asia. A.K. Sengupta, J. Li, M. German

3:30 ENVR 75. Removal of fluoride using a nanostructured diatom-ZrO₂ composite synthesized from algal biomass. M. Thakkar, S. Mitra

3:55 ENVR 76. Nanocoated fiber optics for photocatalytic drinking water treatment. H. Stanci, J. Robinson, P.K. Westerhoff, K.D. Hristovski

4:20 Panel Discussion.

4:45 Concluding Remarks.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

Section D

Boston Park Plaza Hotel and Towers
Beacon Hill Room

Advances in Drinking Water Disinfection: Byproducts Occurrence, Formation, Treatment, Health Effects, Epidemiology and Regulation

E. Sahle-Demessie, G. Sorial, *Organizers, Presiding*

1:30 ENVR 77. Electrochemical drinking water disinfection — are all problems solved? **M.E. Bergmann**, W. Schmidt, A. Grunert, T. Grummt

1:55 ENVR 78. Comparative study in treating disinfection by products (DBPs) in biotrickling filters (BTFs) under different environmental conditions. **B. Mezgebe**, K. Palanisamy, G. Sorial, E. Sahle-Demessie

2:20 ENVR 79. Optimizing coagulation for treatment of high TOC surface water and minimizing disinfection byproduct formation potential. A. Waldron, A. Manikonda, C. Bellona

2:45 ENVR 80. Modeling THM removals from a horizontal in-line diffused aeration system in pressurized water distribution pipes. **M.R. Collins**

3:10 Intermission.

3:25 ENVR 81. Saving our bees: Removing neonicotinoids from waters using oxidizing radicals. **B. Daws**, J.J. Kiddle, S.P. Mezky

3:50 ENVR 82. Exploratory statistical analysis of drinking water treatments and water characteristics in Scotland: Best predictors of trihalomethanes (THMs) formation. **M.A. Valdivia-Garcia**, D. Werner, P. Weir

4:15 ENVR 83. Prioritizing environmental health and household demographic factors impacting biosand filter maintenance and diarrheal occurrences in Brazil. **L.E. Voth-Gaeddert**, D. Oerther

Section E

Boston Park Plaza Hotel and Towers
Tremont

Heterogeneous Catalysis for Environmental Applications

Photocatalysis for Energy and Environment

Cosponsored by CATL

A. Savara, *Organizer*

A. Orlov, S. Zhao, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 84. Effect of crystal defects on visible-light photoreactivity. **C. Huang**

2:00 ENVR 85. Directed assembly of cuprous oxide nanocluster catalyst for CO₂ reduction coupled to heterobinuclear light absorber in mesoporous silica. **W. Kim**, H.M. Frei

2:20 ENVR 86. Development of a continuous flow photoreactor for the destruction of water soluble ethers using TiO₂ and visible/near UV light. **R.D. Barreto**

2:40 ENVR 87. Exploring tunability of catalysts for light induced reactions: Subnanometer particles and their interactions with support, reactants, and light. **A. Orlov**, Q. Wu, S. Zhao, Y. Li

3:05 ENVR 88. Understanding the influence of catalyst structure on activity and stability in the oxygen evolution reaction (OER) using crystalline oxides as a platform. **G. Gardner**, J. Al-Sharab, Y.B. Go, M. Greenblatt, G.C. Dismukes

3:25 Intermission.

3:40 ENVR 89. Electrospun nanofibers of TiO₂-PEDOT for heterogeneous photodegradation of pharmaceutical pollutants. **J. Liu**, D.L. McCarthy, M.J. Cowen, K.H. Skorenko, S.M. Boyer, L. Tong, W.E. Bernier, W.E. Jones

4:00 ENVR 90. In-situ ATR-FTIR observation of selenate reduction by photocatalytic nano-metal oxides. **A.W. Lounsbury**, J.B. Zimmerman

4:20 ENVR 91. Supporting of TiO₂ with metallic nanoparticles to improve the decomposition of paracetamol by photocatalysis: The effect of ultrasound. **N.H. Ince**

4:40 ENVR 92. Efficient photocatalytic removal of aqueous NH₄⁺-NH₃ by palladium-modified nitrogen-doped titanium oxide nanoparticles under visible light illumination, even in weak alkaline solutions. **D. Sun**, W. Sun, W. Yang, **Q. Li**, J.K. Shang

5:00 ENVR 93. Novel microchannel photocatalytic reactor for environmental applications. **N. Padoin**, J. Angelo, A. Mendes, L. Andrade, R.F. Moreira, **C. Soares**

5:20 ENVR 94. Simultaneous photocatalytic elimination of gaseous NO and SO₂ in a BiOI/Al₂O₃ wet scrubber system. **C. He**, L. Hu, W. Pan, Y. Hou

Section F

Boston Park Plaza Hotel and Towers
Cambridge Room

Hydrothermal Carbonization: Possibilities and Limits for Feedstocks, Processes and Applications

Municipal and Agricultural Applications and Economics of HTC

Cosponsored by AGRO

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
C. Coronella, K. Ro, *Organizers*

S. Chang, J. A. Libra, *Organizers, Presiding*

1:30 ENVR 95. Hydrothermal carbonization (HTC) of sewage sludge: Challenges and synergies for future waste water treatment. **B. Wirth**, L. Herklotz, U. Lüder

1:55 ENVR 96. Hydrothermal carbonization and wet oxidation of sewage sludge. **B. Weiner**, G. Riedel, R. Koehler, J. Poerschmann, F. Kopinke

2:20 ENVR 97. Food waste as feedstock for hydrothermal carbonization and its products. **S. Bae**, S. Lee, S. Lee, Y. Hwang, S. Park

2:45 ENVR 98. Understanding the environmental impact of the hydrothermal carbonization of food wastes for energy generation using life cycle assessment. **N.D. Berge**, L. Li, J. Flora, K. Ro

3:10 Intermission.

3:35 ENVR 99. Leachate water quality from soils amended with swine manure based biochars. **K. Ro**, J.A. Libra, S. Bae

4:00 ENVR 100. Hydrothermal carbonization (HTC) of cow manure: Carbon and nitrogen distribution in HTC products. **M. Reza**, M. Lu, T. Song, K. Conrad, S. Hiibel, H. Lin, **C. Coronella**

4:25 ENVR 101. Economics of decentralized hydrothermal carbonization of biogas digestate: A case study from Germany. **K. Suwelack**, D. Wüst, A. Kruse

Section G

Boston Park Plaza Hotel and Towers
Stuart Room

Next Generation Nanomaterials: Advances and Perspectives for Biomedicine, Energy, and Environmental Protection

Energy/General

Cosponsored by ENFL

J. Mi, J. Song, *Organizers, Presiding*

1:30 ENVR 279. Giving new life to materials for energy, the environment, and medicine. **A.M. Belcher**

2:00 ENVR 280. Probing structure and dynamics of nanomaterials for energy applications. **S. Corr**

2:30 ENVR 281. Microbial interactions of carbon nanotube-titania-platinum nanohybrid electrocatalyst. **N.B. Saleh**, N. Aich, D. Das, M. Kirisits, T. Sabo-Attwood

2:50 ENVR 282. Plasmonic hot electron driven reactions: New insights gained from plasmon-enhanced spectroscopic studies. **H. Wang**

3:10 Intermission.

3:25 ENVR 283. Optimization strategies for nanostructured cobalt-based water oxidation catalysts. **G.R. Patzke**

3:55 ENVR 284. Environmentally benign supercapacitor based on "green"chemistry and easily disposable material. **B. Dyatkin**, V. Presser, M. Heon, M.R. Lukatskaya, M. Beidaghi, Y. Gogotsi

4:15 ENVR 285. Production of synthetic natural gas from catalytic syngas conversion using biomass waste. **K. Kawamoto**

4:35 ENVR 286. Nanocomposite of silver nanoparticle loaded on graphene: Synthesis and spectroscopic behaviors. **T. Saleh**, A.A. Al-Saadi

4:55 ENVR 287. EDTA functionalized superparamagnetic nanoparticles for heavy metal remediation. **Y. Huang**, A.A. Keller

Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization and Storage

Perspects on CO₂ Capture and Conversion

Sponsored by ENFL, Cosponsored by ENVR†

Latest Trends in Environmental Fate and Exposure Assessments: Filling in Knowledge and Data Gaps Across the Commodity Groups

Sponsored by AGRO, Cosponsored by ENVR

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Sponsored by PHYS, Cosponsored by ENVR

Pesticide Dose: Effects on the Environment and Target and Non-Target Organisms

Sponsored by AGRO, Cosponsored by ENVR

Urban Agriculture: Turf, Ornamentals, Household Products, and Water-Re-Use

Sponsored by AGRO, Cosponsored by ENVR

Biofuels for Powering the World: Discovery to Application

Sponsored by ENFL, Cosponsored by CATL and ENVR

Current Topics in Seed Treatment

Sponsored by AGRO, Cosponsored by ANYL and ENVR

MONDAY MORNING

Section A

Boston Park Plaza Hotel and Towers
Statler Room

New Challenges in Water Quality, Treatment, Reuse and Sustainability: Chemistry and Application of Advanced Oxidation Processes for Removal of Contaminants of Concern and Transformation Products

Disinfection/Natural Organic Matter

Cosponsored by CEI

R. de Fatima Peralta Muniz Moriera, D. D. Dionysiou, D. Minakata, K. E. O'Shea, *Organizers*

G. Li Puma, *Organizer, Presiding*

J. Marugan, *Presiding*

8:00 ENVR 102. Photocatalytic disinfection and removal of emerging pollutants from real effluents of biological wastewater treatment. **J. Marugan**, K. Philippe, R. Timmers, R. van Grieken

8:40 ENVR 103. Influence of variable amino acids on the photolysis and photochemical degradation of microcystins (cyanotoxins) in terms of reaction kinetics and mechanism. **X. He**, A.A. de la Cruz, **D. Dionysiou**

9:05 ENVR 104. Hybrid microfiltration-UV process for removal and photocatalytic inactivation of viruses. **B. Guo**, B. Starr, I. Xagorarakis, **V. Tarabara**

9:30 Intermission.

9:45 ENVR 105. Characteristics and fate of natural organic matter during UV oxidation processes. **Y. Ahn**, D. Lee, M. Kwon, H. Kye, I. Choi, S. Nam, J. Kang

10:10 ENVR 106. Advanced oxidation process effects on natural organic matter profiles in Nova Scotia drinking water. **S. MacIsaac**, G. Gagnon, L. Hu

Section B

Boston Park Plaza Hotel and Towers
Plaza Ballroom

ACS Award for Creative Advances in Environmental Science and Technology: Symposium in Honor of Dr. Paul B Shepson

A. M. Grannas, K. A. Pratt, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR 107. Influence of sea spray aerosols on cloud and climate. **K.A. Prather**

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- 8:35 ENVR 108.** Composition and chemistry of urban grime: a field and laboratory study. **D. Donaldson**, A. Baergen, S.A. Styler, H. Herrmann
- 9:00 ENVR 109.** Mercury chemical transformation and speciation in atmosphere. **P.A. Ariya**, A. Ghoshdastidar, M. Subir, D. Deeds, U. Kurien, A. Feinberg
- 9:25 ENVR 110.** Air-ice chemical interactions from the molecular to the global scale: Honoring Paul Shepson. **V.F. McNeill**
- 9:50** Intermission.
- 10:15 ENVR 111.** Modeling of air quality from materials used in passenger vehicle interiors. **G.D. Edwards**, S. Canaday, P. Stratton
- 10:40 ENVR 112.** Connecting secondary organic aerosol in the field with the laboratory: Microspectroscopic analysis of aerosol particles from the SOAS field campaign and comparisons with proxies. **A.P. Ault**, A. Bondy, R.L. Craig, J.D. Rindelaub, M. Nhlizyo, S.B. Bertman, K.A. Pratt, P.B. Shepson
- 11:05 ENVR 113.** Air chemistry in a central Amazonian forest during 2014. **J.D. Fuentes**
- 11:30 ENVR 114.** Nutrient carry-over in fermented beverages. **T. Starn**, M. Van Vliet, L. McGoldrick

Section C

Boston Park Plaza Hotel and Towers
Berkeley/Clarendon Room

Sensing of Environmentally Relevant Contaminants

Cosponsored by AGRO

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
B. P. Chaplin, D. Jassby, *Organizers, Presiding*

8:00

8:20 ENVR 115. Estimation of occupational risks from exposures to polycyclic aromatic hydrocarbons and trace metals in soils of automobile repair shop environs in Uyo, Nigeria. **N.O. Offiong**, F.M. Ibang, J. Edet, E. Inam

8:45 ENVR 116. Real time emissions monitoring of diesel engines aboard marine vessels. **B. Sarnacki**, R. Kimball, T. Wallace, T. Lokocz, G. Harakas

9:10 ENVR 117. Filter-based measurements of airborne particulate matter and metals in indoor environments using OPSIS SM200 system and ICP-MS. **J. Niu**, P.E. Rasmussen

9:35 ENVR 118. Advances in the visualization of urban air quality data and environmental monitoring using TIBCO Spotfire® and the Elm sensor network. **K.A. Kuhr**

10:00

10:10 ENVR 119. Electrochemical detection of ciprofloxacin with a boron-doped diamond electrode modified with nafion-coated multi-walled carbon nanotubes. **B.P. Chaplin**, P. Gayen

10:35 ENVR 120. Developing an electrochemical aptamer-based sensor to detect endocrine disrupting compounds in natural waters. **S. Akki**, S.K. Silverman, R.M. Crooks, C.J. Werth

11:00 ENVR 121. Voltammetric analysis of naturally occurring reductants in prairie pothole wetland sediment pore water. **B. McAdams**, Y. Chin, W. Arnold

11:25 ENVR 122. 2-Aminobenzothiazole imines as sensitive colorimetric anion sensors. **Y.M. Hiji**, H. Aleasa

Section D

Boston Park Plaza Hotel and Towers
Beacon Hill Room

Advanced Materials and Technologies for Desalination and Wastewater Reuse

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
J. Kim, *Organizer*

Q. Li, *Organizer, Presiding*

8:00 ENVR 123. Efficacy of hydrophilic, polyethylene glycol-grafted reverse osmosis membranes in the presence of mineral scalants and natural organic matter. **J. Ray**, W. Wong, Y. Jun

8:20 ENVR 124. Biofouling mitigation in forward osmosis by functionalization of thin-film composite polyamide membranes with graphene oxide nanosheets. **F. Perreault**, H. Jaramillo, M. Xie, M. Elimelech

8:40 ENVR 125. UVC-radioluminescent materials for membrane biofouling control using X-rays. **T. Johnson**, E.L. Cates, F. Li

9:00 ENVR 126. Block copolymer functionalized thin-film composite membranes for antifouling and antimicrobial properties using atom-transfer radical polymerization. **J. Lee**, G. Ye, F. Perreault, M. Elimelech

9:20 ENVR 127.

9:40 ENVR 128. Organic fouling of molecular layer-by-layer polyamide with different surface functionalities: A direct comparison of QCM and bench-scale membrane fouling. **M.E. Tousley**, D. Shaffer, C.O. Osuji, J. Lee, M. Elimelech

10:00

10:15 ENVR 129. Novel photothermal nanocomposite membrane using electrospun fibers for direct solar membrane distillation. **J. Wu**, K.R. Zodrow, Q. Li

10:35 ENVR 130. In-situ and self-healing of water filtration membranes for wastewater reuse applications. **B. Getchew**, S. Kim, J. Kim

10:55 ENVR 131. Mixed charge mosaic membranes prepared by layer-by-layer assembly for ion selective separations. **S. Rajesh**, M. Summe, **W.A. Phillip**

11:15 ENVR 132. Effective organic draw solutions for engineered osmosis processes. **M. Islam**, M. Lemieux, M. Rahaman

11:35 ENVR 133. Carbon nanotube enhanced membrane distillation: A new generation membranes for sea or brackish water desalination. **S. Ragunath**, S. Roy, S. Mitra

Section E

Boston Park Plaza Hotel and Towers
Tremont Room

Heterogeneous Catalysis for Environmental Applications

Heterogeneous Catalysis for Energy and Environment

Cosponsored by CATL

S. Zhao, *Organizer*

A. Orlov, A. Savara, *Organizers, Presiding*

8:00

8:05 ENVR 134. Hydrogen evolution on nickel phosphide electrocatalysts: A comparative study of efficiency and corrosion tolerance. **A.B. Laursen**, B. Liu, K.R. Patraju, M.J. Whitaker, M. Retuerto, T. Sakar, N. Yao, K.V. Ramanujachary, M.K. Greenblatt, G.C. Dismukes

8:30 ENVR 135. First principles investigation of the hydrogen evolution reaction on nickel phosphides Ni₂P and Ni₃P₂. **R. Wexler**, J.M. Martinez, **A.M. Rappe**

8:50 ENVR 136. Heterogeneous catalysis for sustainable energy: Atomically dispersed gold clusters for hydrogen production. **N. Yi**, M. Stephanopoulos

9:10 ENVR 137. Aromatic-hydroxyl interaction of a lignin model-compound on SBA-15, present at pyrolysis temperatures. **A. Savara**, M. Kandziolka, M. Kidder, L.W. Gill, Z. Wu

9:35

9:50 ENVR 138. Study of the mechanism for the formation of formic and levulinic acids from HMF. **E. Weitz**, A. Das, T. Drake, P.C. Stair

10:10 ENVR 139. Understanding and enhancing the selectivity of reductive lignin disassembly over doped porous metal oxides. **C.M. Bert**, J.A. Barrett, M.A. Chui, G. Bottari, H. Maneesuan, K. Barta, S.L. Scott, P.C. Ford

10:30 ENVR 140. Exploring the nature of active sites in Cu-exchanged SSZ-13 under realistic conditions. **F. Goettl**, A. Love, P. Sautet, I. Hermans

10:50 ENVR 141. Study of NH₃-SCR over Cu-zeolites: From straight channel zeolites to cage-type zeolites with D6R unit. **R. Xu**, B. Chen, Y. He, R. Zhang

11:10 ENVR 142. Drawing bio-inspiration to design environmental catalysts. **J. Liu**, C.J. Werth, **T.J. Strathmann**

Section F

Boston Park Plaza Hotel and Towers
Cambridge Room

Green Chemistry and the Environment

Cosponsored by YCC

S. O. Obare, *Organizer*

A. M. Balu, R. Luque, *Organizers, Presiding*

8:00

8:05 ENVR 143. Organic reactions in water: A green avenue to add-value chemicals. **C. Len**

8:45 ENVR 144. Ionic liquids as solvents for metal extraction: Engineering consideration. **C. Janssen**, M.N. Kobrak, M. Aguilar Martinez

9:05 ENVR 145. Using the waste materials to generate nanoparticles and electrospun the nanofibers. **Z. Katircioglu**, S. Dursun, M. Yavuz

9:25 ENVR 146. Controlling phosphorus as a preservation strategy for products with high organic load. **Y. Azimi**, I.P. Thompson

9:45

10:00 ENVR 147. Nitrilotriacetic acid functionalized *Adansonia digitata* bio-adsorbent: A potential means of waste water treatment in developing nations. **A. Adewuyi**

10:20 ENVR 148. Removal of acid red 114 and basic blue 3 from aqueous solutions by activated carbon obtained from waste tire. **G. Camargo**, P. Jimenez, J. Granados, J.C. Moreno

10:40 ENVR 149. Immobilization of *Moringa* protein extracts on solid adsorbents for use in water disinfection. **J. Barajas**, S.A. Pagsuyoin

11:00 ENVR 150. Lead removal from aqueous solution using pine wood biochar modified with chitosan. **N.W. Bombuwala Dewage**, T.E. Misna

ACS Scholars: Rising Stars in Academe

Sponsored by PRES, Cosponsored by AGRO, CARB, CMAA, COLL, ENFL, ENVR, PROF, SCHB and YCC

Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization and Storage

CO₂ Conversion, Utilization and Storage

Sponsored by ENFL, Cosponsored by ENVR

Global Research Needs: Identifying and Prioritizing Efforts to Sustain Environmental Quality

Sponsored by AGRO, Cosponsored by ENVR and TOXI

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits

Sponsored by CHED, Cosponsored by BMGT, CEI, ENVR, I&EC, MEDI, PROF, SCHB and YCC

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Sponsored by PHYS, Cosponsored by ENVR

Environmental Fate, Transport and Modeling of Agricultural Chemicals

Sponsored by AGRO, Cosponsored by ENVR

Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications

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Biofuels for Powering the World: Discovery to Application

Hydrotreating, Upgrading and Gasification

Sponsored by ENFL, Cosponsored by CATL and ENVR

MONDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers
Statler Room

New Challenges in Water Quality, Treatment, Reuse and Sustainability: Chemistry and Application of Advanced Oxidation Processes for Removal of Contaminants of Concern and Transformation Products

Electrochemical/Inorganics

Cosponsored by CEI

R. de Fatima Peralta Muniz Moriera, D. D. Dionysiou, D. Minakata, K. E. O'Shea, *Organizers*

G. Li Puma, *Organizer, Presiding*

X. Quan, *Presiding*

1:30 ENVR 151. Removal of ionizable organic contaminants from water by electro-assistant adsorption in a carbon-fiber filter. **X. Quan**, X. Li, S. Wang, M. Liu, S. Chen

2:10 ENVR 152. Degradation of phenol by the Electro-Peroxo process. **D. Pino-Sandoval**, R. Núñez-Salas, **J. Rodríguez-Acosta**, N. Marriaga-Cabrales

2:35 ENVR 153. Photoelectrocatalytic oxidation of phenol by using TiO₂/ITO anode. **J. Villota-Zuleta**, **J. Rodríguez-Acosta**, J. Benavides-Guerrero, N. Marriaga-Cabrales

3:00

3:15 ENVR 154. Bromate formation from bromide oxidation by the UV/peroxymonosulfate process. **D. Zhang**, L. Ling, J. Fang, C. Shang

3:40 ENVR 155. Removal of nitric oxide by combined aqueous persulfate and ferrous-edta systems: Effects of persulfate and edta concentrations, temperature, and pH. **Y.G. Adewuyi**

4:05 ENVR 156. Treatment of landfill leachate by Fenton-based process in batch reactor with ferric sludge reuse. **N. Dulova, E. Kattel, M. Trapido**

4:30 ENVR 157. Treatment of fecal sludge in a prototype supercritical water oxidation reactor. **M.A. Deshusses, W. Jacoby**

4:55 ENVR 158. Data based modeling of the photo-Fenton process for soft-sensing applications. **F. Audino**

Section B

Boston Park Plaza Hotel and Towers
Plaza Ballroom

ACS Award for Creative Advances in Environmental Science and Technology: Symposium in Honor of Dr. Paul B Shepson

A. M. Grannas, K. A. Pratt, *Organizers, Presiding*

1:30 ENVR 159. Measurements of atmospheric halogens using chemical ionization mass spectrometry. **G. Huey**

1:55 ENVR 160. Probing the connections between aerosol particles, clouds, and climate in the high Arctic summer. **J.P. Abbatt, H. Bozem, J. Burkart, A. Herber, P. Hoor, F. Koellner, R. Leaitch, J. Schneider, M. Willis**

2:20 ENVR 161. Evidence for snow photochemistry and surface emissions from a polluted, midlatitude snowpack in the Uinta Basin, Utah. **C. Thompson, J. Hueber, D. Helmig, J. de Gouw, A. Koss, J. Roberts, P. Veres**

2:45 ENVR 162. Natural organic matter in cryosphere-atmosphere interactions: Chemistry and characterization. **A.M. Grannas, A. Fedde, V. Catanzano**

3:10 Intermission.

3:35 ENVR 163. Influence of Arctic leads on sea spray production and snow chemistry. **K.A. Pratt, N. May**

4:00 ENVR 164. ODE to Paul Shepson. **J.W. Bottenheim, S. Netcheva, R. Staebler, A. Steffen**

4:25 ENVR 165. Award Address (ACS Award for Creative Advances in Environmental Science and Technology). Heterogeneous photochemical processes in a changing Arctic. **P.B. Shepson**

Section C

Boston Park Plaza Hotel and Towers
Berkeley/Claarendon Room

Sensing of Environmentally Relevant Contaminants

Cosponsored by AGRO

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
B. P. Chaplin, D. Jassby, Organizers, Presiding

1:30 Introductory Remarks.

1:40 ENVR 166. Direct and rapid detection of adenovirus in environmental waste waters by SWCNTs modified biosensor system. **N. Yildirim, J. Lee, H. Cho, S. Somu, A. Busnaina, A. Gu**

2:05 ENVR 167. Groundwater monitoring system for microbial activity. **S.R. Burge, K.D. Hristovski, R.G. Burge**

2:30 ENVR 168. Comparison between various observing systems for monitoring harmful algal blooms and preliminary concept of innovative sensing network for in situ monitoring of biological toxins. **H. Zamankhan Malayeri, S. Cho, J. Park, S. Jung, H. Choi**

2:55 ENVR 169. Portable detection of Ochratoxin A based on a structure-switching aptamer using a personal glucose meter (PGM). **C. Gu, H. Shi**

3:20 Intermission.

3:40 ENVR 170. Study on integrated phytoremediation measures for enhancing energy crops' performance in treating heavy metal-polluted soil. **T. Yeh**

4:05 ENVR 171. Comparing the partition and sorption behavior to agricultural soils of bisphenol A (BPA) and BPA alternatives: BPS and BPAF. **Y. Choi, L.S. Lee**

4:30 ENVR 172. Withdrawn.

4:55 ENVR 173. Direct-reading exposure assessment through wireless chemical sensor and position tracking. **K. Brown, K.R. Mead, P.B. Shaw, R.J. Kovein, R. Voorhees, A.R. Brandes**

Section D

Boston Park Plaza Hotel and Towers
Beacon Hill Room

Advanced Materials and Technologies for Desalination and Wastewater Reuse

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
Q. Li, Organizer

J. Kim, Organizer, Presiding

1:30 ENVR 174. Binder-free carbon nanotube electrode for electrochemical removal of chromium. **C. Na, H. Wang**

1:50 ENVR 175. Selective electrochemical sorption of anions through heterogeneous redox processes for water remediation and waste control. **X. Su, T. Hatton**

2:10 ENVR 176. Continuous-flow device for photocatalytic degradation and full mineralization of priority pollutants in water. **G. Rytwo, T. Klein, G. Daskal**

2:30 ENVR 177. Coupling capacitive deionization with microbial fuel cells for water purification. **C. Hou, C. Tsai, C. Ma**

2:50 ENVR 178. Exploiting the benefits of ionic liquids for the re-use of industrial and mining wastewater. **C. Janssen, M.N. Kobrak, M. Aguilar Martinez**

3:10 ENVR 179. Recyclable epichlorohydrin free magnetic chitosan hydrogel film in removal of Cr(VI) from water. **M. Kassaei, M. Mirabedini**

3:30 Intermission.

3:45 ENVR 180. Removal of hexavalent chromium from electroplating wastewater using ammoniated wheat straw. **X. Yao, S. Deng, S. Hong, Z. Du**

4:05 ENVR 181. Use of steel slag coated with sodium hydroxide for treatment of highly concentrated wastewater. **T. Park, V. Ampunan, E. Chung**

4:25 ENVR 182. Enhanced bromate removal using polypyrrole-grafted activated carbon. **S. Hong, X. Yao, S. Deng**

4:45 ENVR 183. Predictive modeling of bi-solute adsorption by polymeric resin based on adsorbed solution theories (ASTs). **H.J. Zhang, S. Wang**

5:05 ENVR 184. Adsorption performance of hydroxyapatite powder in the removal of dyes in wastewater. **A.A. Okoya**

Section E

Boston Park Plaza Hotel and Towers
Tremont Room

Heterogeneous Catalysis for Environmental Applications

Heterogeneous Catalysis for Water and Air Treatment

Cosponsored by CATL

A. Savara, Organizer

A. Orlov, S. Zhao, Organizers, Presiding

1:30 Introductory Remarks.

1:35 ENVR 185. Development of a fast measurement system for gaseous total reduced nitrogen species. **Y. Liu, J. Roberts**

1:55 ENVR 186. SO₂ tolerant CO oxidation catalysts and the effect of TiO₂ and ZrO₂ supports on catalytic activity. **K. Taira, K. Nakao, K. Suzuki**

2:15 ENVR 187. Experimental and computational study of CO oxidation promoted by Nb in manganese oxide octahedral molecular sieve. **H.C. Genuino, D. Valencia, S.L. Suib**

2:35 ENVR 188. Crystal structure- and morphology-dependent of MnO₂ for catalytic decomposition of ozone. **J. Jia, P. Zhang**

2:55 Intermission.

3:10 ENVR 189. Tunable soft templated mesoporous manganese oxide as an efficient heterogeneous catalyst for solvent free aerobic oxidation of hydrocarbons. **S. Biswas, S.L. Suib**

3:30 ENVR 190. Bimetallic palladium-indium catalyst technology for nitrate treatment in waste ion exchange (IX) brine to enable brine reuse. **A. Bergquist, J. Choe, T.J. Strathmann, C.J. Werth**

3:50 ENVR 191. Shape- and size-dependent activity of Pd/Cu₂O nanoparticles for sustainable light-activated hydrodehalogenation of polychlorinated biphenyls (PCBs). **E. Zahran, W.A. Ranson, M.R. Knecht, L.G. Bachas**

Section F

Boston Park Plaza Hotel and Towers
Cambridge Room

Green Chemistry and the Environment

Cosponsored by YCC

A. M. Balu, Organizer

R. Luque, S. O. Obare, Organizers, Presiding

1:30 Introductory Remarks.

1:35 ENVR 192. On the use of the United States Environmental Protection Agency's toxics release inventory to assess implementation and impact of green chemistry practices by the pharmaceutical manufacturing sector. **S. DeVito**

2:35 ENVR 193. Sustainable chemistry: Hybrid photocatalysts for solar energy conversion. **T. Jin, B. Stewart, S. Pantovich, G. Li**

2:55 ENVR 194. Designing polymer materials for degradation: The use of molecular simulations for green chemistry applications. **M.A. Pasquini**

3:15 Intermission.

3:30 ENVR 195. Using the principles of green chemistry in biomass valorization. **F.M. Kerton, C. Bottaro, K. Hawboldt, Y. Liu, G. Margoutidis, J. Murphy, V.H. Parsons**

3:50 ENVR 196. Catalysis using earth abundant transition metals. **C.M. Kozak**

4:10 ENVR 197. Cellulose valorisation by catalytic hydrolytic hydrogenation towards sugar alcohols. **P.A. Lazaridis, A. Panteli, S.A. Karakoulia, S.M. Coman, V. Parvulescu, K. Triantafyllidis**

4:30 ENVR 198. Life cycle assessment of lignin-derived chemicals from catalytic depolymerization of candlenut shells. **M. Montazeri, E.S. Beach, M. Eckelman**

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What's in Your Chemical Toolbox?

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Endangered Species Risk Assessment for Pesticides: Advances in Methods and Process

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Undergraduate Research Posters

Environmental Chemistry

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MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

D. D. Dionysiou, Organizer

8:00 - 10:00

158. See previous listings.

ENVR 199. Developing novel perovskite-based nano-composite materials for photocatalytic energy applications. **Q. Wu, J. Cen, Y. Zhao, E.L. Connors, D. Su, S. Zhao, M.G. White, A. Orlov**

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ENVR **200.** Selective detection of aliphatic alcohols via proximity-induced fluorescence modulation. D.J. DiScenza, M. Levine

373, 391, 412-413, 416-417, 420-421, 426-427, 432, 434, 443-445, 448, 451, 453-455, 458, 463, 468-469, 472, 475, 478-480, 482, 485-489, 491-492, 513, 517, 526-527, 531, 537, 540, 542, 552, 556-557, 559-561. See subsequent listings.

TUESDAY MORNING

Section A

Boston Park Plaza Hotel and Towers
Statler Room

New Challenges in Water Quality, Treatment, Reuse and Sustainability: Chemistry and Application of Advanced Oxidation Processes for Removal of Contaminants of Concern and Transformation Products

Pharmaceuticals and Contaminants of Emerging Concern

Cosponsored by CEI

R. de Fatima Peralta Muniz Moriera, D. D. Dionysiou, D. Minakata, K. E. O'Shea, *Organizers*

G. Li Puma, *Organizer, Presiding*

D. Avisar, *Presiding*

8:00 ENVR 201. Withdrawn.

8:40 ENVR 202. On the removal of ketoprofen drug in persulfate aqueous systems: Thermal vs. chemical activation processes. A. Ghauch, N. Awad, S. Naim

9:05 ENVR 203. Time-dependent by-product formation from ibuprofen degradation by the UV/chlorine process. Y. Xiang, J. Fang, J. Sun, C. Shang

9:30 ENVR 204. Chlorine atom reactions with antibiotics in wastewater: Kinetics and mechanisms. C.A. Rice, S.P. Mezyk

9:55 Intermission.

10:10 ENVR 205. Sulfate-radical based remediation of pharmaceutical-contaminated waters: Evaluation of chemical association constants. T. Reutershan, S.P. Mezyk

10:35 ENVR 206. Oxidation of amino acids by peroxymonosulfate. M. Ruiz, A. Chesney, C. Booth, C. Lietz, L. Li, J.A. Pedersen

11:00 ENVR 207. Photocatalytic degradation of perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS). P. Zhang

11:25 ENVR 208. Plasma-based water treatment: An effective method to degrade perfluorooctanoic acid and other emerging contaminants. S. Mededovic, F. Dai, G. Stratton, C. Bellona, T.M. Holsen, E. Dickenson

Section B

Boston Park Plaza Hotel and Towers
Plaza Ballroom

Microorganism-Membrane Interactions: Towards Understanding Pathogen Removal and Membrane Biofouling

Cosponsored by AGRO

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)

S. Chang, C. Coronella, J. A. Libra, K. Ro, *Organizers*

T. H. Nguyen, V. Tarabara, *Presiding*

8:00 ENVR 209. Probing virus capture during virus filtration with confocal microscopy: Effects of membrane morphology and solution conditions. A.L. Zydney, S.K. Dishari, M. Micklin, K. Sung, A. Venkiteshwaran, J. Earley

8:30 ENVR 210. Selective cell interactions and antibacterial behavior of functional fibrous membranes. S. Xu, B.S. Hsiao, C.C. Han, B.T. Chu

8:50 ENVR 211. Random sequential adsorption of human adenovirus on membrane surface. R. Lu, Q. Li, T.H. Nguyen

9:10 ENVR 212. Human adenovirus removal by hollow fiber membranes: Effect of membrane fouling by suspended and dissolved matter. Z. Yin, V. Tarabara, I. Xagorarakis

9:30 ENVR 213. Withdrawn.

9:50 Intermission.

10:00 ENVR 214. Initiation and succession of biofouling communities on hydrophobic and hydrophilic membrane surfaces in a submerged membrane bioreactor. G. Matar, G. Gonzalez-Gil, S. Bagchi, S. Nunes, J. Vrouwenvelder, P. Saikaly

10:20 ENVR 215. Pyrosequencing of 16S rRNA gene reveals large differences in the sessile bacterial community in five full-scale membrane bioreactors. G. Matar, S. Bagchi, K. Zhang, D. Oerther, P. Saikaly

10:40 ENVR 216. Microbial dynamics and membrane biofouling in suspended and attached-growth anaerobic membrane bioreactors treating low-strength wastewater. M. Harb, Y. Xiong, G. Amy, P. Hong

11:00 ENVR 217. Interactions between GAC sizes, particle sizes and biofouling in anaerobic fluidized membrane bioreactor. J. Kim, M. Aslam, D. Kwon, R. Ahmad, J. Bae, P. McCarty

11:20 ENVR 218. Quantification of extracellular polymeric substance (EPS) surrogate adsorption on polyamide water filtration membranes. A. Vozar, B.J. Marinas, J. Moore, A. Yang

11:40 ENVR 219. Using luminescence to determine the impact of assimilable organic carbon on biological fouling of reverse osmosis membranes in seawater desalination. L.A. Weinrich

Section C

Boston Park Plaza Hotel and Towers
Berkeley/Clarendon Room

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Electron and Energy Transfer: From Molecular to Device Engineering for Minimizing Environmental Impacts

Cosponsored by CEI, ENFL, ORGN and PHYS

K. Rajeshwar, V. I. Vullev, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 220. DNA-based molecular wires and devices for photoinduced charge separation. F.D. Lewis

8:45 ENVR 221. Charge and exciton transport: Can conjugated chains be "molecular wires". J.R. Miller, A.R. Cook, M. Bird, T. Mani, X. Xi, G. Rumbles, O. Reid, R. Holroyd

9:25 ENVR 222. Light energy conversion aspects of organic metal halide perovskites. P.V. Kamat, Y. Chen, J. Manser, J. Christians

10:05 Intermission.

10:20 ENVR 223. Inorganic spin chemistry in sustainable chemistry processes. M.D. Forbes

11:00 ENVR 224. Developing new electron transfer proteins using a de novo protein design approach. V.L. Pecoraro, A. Tebo, J.S. Plegaria

11:40 ENVR 225. Stark spectroscopy at the dye-sensitized TiO₂ interface. C. Ward, R. O'Donnell, G.J. Meyer

Section D

Boston Park Plaza Hotel and Towers
Beacon Hill Room

Reclamation, Remediation, Restoration: Novel Approaches to Environmental Challenges

Cosponsored by AGRO

L. S. Lee, M. Mashtare, L. Royer, *Organizers, Presiding*

8:00 Introductory Remarks.

8:20 ENVR 226. Radionuclide and heavy metal remediation via biological calcium carbonate precipitation. E. Lauchnor, L. Schultz, T.D. dos Santos, R. Gerlach

8:40 ENVR 227. Environmental fate of 14C-radiolabeled 2,4-dinitroanisole (DNAN) in anaerobic saturated soils. C.I. Olivares, L. Abrell, R. Sierra-Alvarez, J. Chorover, J. Field

9:00 ENVR 228. Reductive transformation of explosives in soil with zero-valent iron-bearing biochar. S. Oh, Y. Seo

9:20 ENVR 229. Effect of nanosized zero-valent iron on the spectroscopic characteristics of a terrestrial humic acid. C. Kim, J. Ahn, Y. Chin, I. Hwang

9:40 ENVR 230. Metal removal mechanisms using passive treatments in mining-impacted water. S.R. Al-Abed, P. Pinto, C.D. Holder, S.M. Lomnicki, J. McKernan

10:00 Intermission.

10:10 ENVR 231. Zerovalent metals and vitamin B12 potential for remediation of persistent perfluoroalkyl acids in groundwater. L.S. Lee, S. Park, J.E. Zenobio

10:35 ENVR 232. Spectroscopic investigation of interfacial interaction of organic compounds and manganese oxides. M. Shaikh, S. Taujale, H.J. Zhang, K. Artyushkova, J.M. Cerrato

10:55 ENVR 233. Withdrawn.

11:15 ENVR 234. Characterization of valuable materials of the acid waste from a hydrometallurgical process. M.E. Gutierrez Ruiz, K. Martin del Campo, S. Castillo Blum, V. Luna Pabello

11:35 ENVR 235. NMR evaluation of cyclodextrin-perfluorinated surfactant host-guest interactions. M.J. Weiss, K.E. O'Shea

11:55 Concluding Remarks.

Section F

Boston Park Plaza Hotel and Towers
Cambridge Room

Green Chemistry and the Environment

Cosponsored by YCC

R. Luque, *Organizer*

A. M. Balu, S. O. Obare, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 244. Investigation of sonochemistry for biomass conversion: That sounds like a good idea. G. Chatel, D. Rinsant, K. De Oliveira Vigier, F. Jérôme

8:30 ENVR 245. Carbon dioxide solvent applications for biodiesel production with a heterogeneous catalyst. L. Soh, C. Chen, J.B. Zimmerman

8:55 ENVR 246. Insights on the solubility of CO₂ in 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide from the microscopic point of view. L.T. Costa, D. Van Der Spoel, T. Lourenço

9:20 ENVR 247. Trends in environmental releases of toxic chemicals from the automotive sector. C. Keenan

9:45 Intermission.

9:55 ENVR 248. Does pollution prevention work? Evidence from twenty years of TRI reporting data. M. Ranson, B. Cox, C. Keenan, D. Teitelbaum

10:20 ENVR 249. Trapping of methylglyoxal (MGO), a dicarbonyl metabolite derived from glucose by flavonoids present in okra seed extract and its implications in the down-regulation of receptor for advanced glycation end products (RAGE), a key cellular target. B. Dayal

10:45 ENVR 250. Preparation and properties of a novel interpenetrating network hydrogel with chitosan and hyaluronic acid. Y. Zhang, X. Fan, Q. Wang, P. Wang, L. Cui, J. Yuan, J. Xu, Y. Yu

11:10 ENVR 251. Innovative benign by design methodologies for the synthesis of advanced nanomaterials. R. Luque

11:35 ENVR 252. Analysis of perfluorinated compounds (PFCs), select pesticides, and a biocide using quick sample extraction/preparation followed by UPLC/MS/MS analysis. L. Zintek, D. Wesolowski, B. Shrestha, C. Bhardwaj

Section G

Boston Park Plaza Hotel and Towers
Tremont Room

Environmental Applications and Implications of Graphene-Based Nanomaterials

I. Chowdhury, M. Hersam, *Organizers*

D. C. Bouchard, *Organizer, Presiding*

W. M. Henderson, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR 253. Simultaneous sensing and degradation of nitroaromatics with graphene oxide based multifunctional catalyst mat. P.V. Kamat, R. Alam

8:45 ENVR 254. Monitoring a nitrifying biofilm using a graphene biotransistor. M. Brown, L. Barker, L. Semprini, E.D. Minot

9:05 ENVR 255. Pd and Pd/Au nanocatalysts supported on exfoliated graphite for high throughput dehalogenation by nanocomposite membranes. C.A. Crock, V. Tarabara

9:25 Intermission.

9:40 ENVR 256. Graphene-based adsorbents for the removal of aqueous contaminants. B. Gao

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

10:00 ENVR 257. Enhanced hydrogen production by carbone-doped TiO₂ decorated with rGO under visible light irradiation. L. Kuang, W. Zhang

10:20 ENVR 258. TiO₂-graphene photocatalyst interfaces elucidated through density functional theory modeling. N.A. Deskins, B. Bukowski

10:40 Concluding Remarks.

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TUESDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers Statler Room

New Challenges in Water Quality, Treatment, Reuse and Sustainability: Chemistry and Application of Advanced Oxidation Processes for Removal of Contaminants of Concern and Transformation Products

Materials

Cosponsored by CEI

R. de Fatima Peralta Muniz Moriera, D. D. Dionysiou, D. Minakata, *Organizers*

G. Li Puma, K. E. O'Shea, *Organizers, Presiding*

1:30 ENVR 259. Roles of pH and carbonate radical on photochemical destruction of oxytetracycline. Y. Liu, X. He, X. Duan, Y. Fu, D.D. Dionysiou

1:55 ENVR 260. Insights into the formation of POPS (persistent organic pollutants) during application of AOPs to wastewater containing organo-chlorinated compounds. I. Ortiz, M. Vallejo, P. Fernández, M. San Román, Á. Irabien

2:20 ENVR 261. Phenomenal synergistic pathway for degradation of organic pollutants using reduced graphene oxide supported photocatalyst under diffused sunlight. S. Ganesh Babu, B. Neppolian

2:45 ENVR 262. Mineralization of phenol in presence of sulphate radicals using modified ZnAl layered double hydroxides. A. Mantilla, G. Romero, M. Suarez Quezada, V. Suarez, E. Navarro Ceron, F. Tzompantzi, L. Lartundo

3:10 Intermission.

3:25 ENVR 263. Radiocatalytic materials for pursuing fixed-bed heterogeneous advanced oxidation using X-rays. F. Li, T.A. Johnson, E.L. Cates

3:50 ENVR 264. Detection and remediation of pesticides contamination in water. S. Ahuja

4:15 ENVR 265. Mass balance of fipronil in a wastewater treatment train and engineered wetland. S. Supowit, A.M. Sadaria, E.J. Reyes, R.U. Halden

Section B

Boston Park Plaza Hotel and Towers Plaza Ballroom

The Debate: How Do We Respond to Climate Change

Cosponsored by CEI#

C. W. Avery, L. E. Pence, *Organizers, Presiding*

3:30 Introductory Remarks.

3:35 Opening Statements.

3:45 ENVR 266. The debate: How do we respond to climate change? C.W. Avery, L.E. Pence

5:05 Concluding Remarks.

Section C

Boston Park Plaza Hotel and Towers Berkeley/Clarendon Room

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Designs: From Molecules to Functional Materials

Cosponsored by CEI, ENFL, ORGN and PHYS

K. Rajeshwar, V. I. Vullev, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 267. Mimics of the Tyr₂-His redox relay of photosystem II in water splitting schemes. A.L. Moore, T.A. Moore, D. Gust, A. Teillant, M.J. Llansola-Portelés, J.J. Tomlin, M.E. Tejada-Ferrari

2:15 ENVR 268. Electrochemical conversions of carbon with enzymes from the reverse TCA cycle. S.J. Elliott, B. Li, P. Steindel

2:55 ENVR 269. Designing bioinspired molecular electrets for hole-transfer. J. Larsen, E.M. Espinoza, V.I. Vullev

3:15 Intermission.

3:30 ENVR 270. Protein-based hybrid catalysts for hydrogen production. G. Ghirlanda

4:10 ENVR 271. Introducing Cu(I)-photosensitizers in artificial photosynthetic supramolecular assemblies. L. Kohler, K.L. Mulfort, S. Soltan, L.M. Utschig-Johnson

4:50 ENVR 272. Multivalency through dendritic building blocks: Fabrication of functionalizable hydrogels. R. Sanyal

Section D

Boston Park Plaza Hotel and Towers Beacon Hill Room

C. Ellen Gonter Awards Symposium

T. Anderson, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 273. Stability of endocrine disrupting estrogens in dairy manure during pasteurization-anaerobic digestion process. K.M. Noguera-Oviedo, D.S. Agar

2:00 ENVR 274. Changes in physico-chemical and transport properties of a reverse osmosis membrane exposed to chloraminated seawater. L. Valentino, T. Renkens, T. Maugin, J. Croue, B.J. Marinas

2:25 ENVR 275. Polysulfone membranes modified with bioinspired polydopamine and silver nanoparticles formed in situ to mitigate biofouling. L. Tang, K. Livi, K. Chen

2:50 Intermission.

3:05 ENVR 276. Influence of dissolved organic matter on the rates and mechanisms of 2,2',4,4'-tetrabromodiphenyl ether (BDE-47) photolysis. M.L. Wei-Haas, Y. Chin

3:30 ENVR 277. Using in situ passive samplers to assess porewater concentrations in sediment beds influenced by groundwater flow. J. Apell, J.K. MacFarlane, P.M. Gschwend

3:55 ENVR 278. Aerobic bioremediation of PAH contaminated soil results in increased toxicity and no change in excess lifetime cancer risk. L. Chibwe, M. Geier, J. Nakamura, R.L. Tanguay, M. Aitken, S.L. Simonich

Section F

Boston Park Plaza Hotel and Towers Cambridge Room

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

Membranes, Absorption and H₂O₂ Production

Cosponsored by AGRO

F. A. Monterrubio, I. S. Sardonil, *Organizers*

V. K. Sharma, *Organizer, Presiding*

M. E. Bergmann, E. Roberts, *Presiding*

1:30 Introductory Remarks.

1:55 ENVR 288. Combining adsorption with electrochemical oxidation for the treatment of dissolved organic contaminants in water. H. Mohammad, S.N. Hussain, A.D. Martin, N.W. Brown, E. Roberts

2:15 ENVR 289. High-throughput fabrication of all carbon nanotube hollow fiber membranes with improved performance in permeability and selectivity for water treatment. G. Wei, X. Quan

2:35 ENVR 290. Development of reactive electrochemical membranes for water treatment applications. B.P. Chaplin, Y. Jing, L. Guo

2:55 ENVR 291. Characterization of electroactive membranes based on carbon nanotubes/Fe-nanoparticles and application in the degradation of emerging pollutants. J.E. Yanez Heras, C. Zwiener

3:15 Intermission.

3:30 ENVR 292. Electro-peroxone: a promising electrochemical advanced oxidation process for water and wastewater treatment. Y. Wang, H. Wang, W. Yao

3:50 ENVR 293. Enhancement of pharmaceutical degradation and inhibition of bromate formation by adapting ozonation to electro-peroxone process. H. Wang, Y. Li, J. Zhan, Y. Wang

4:10 ENVR 294. Mass transport characterization of oxygen reduction reaction to produce hydrogen peroxide using boron doped diamond, graphite felt and reticulated vitreous carbon cathodes in a filter press cell, using two types of supporting electrolyte. G. Coria, T. Perez, I. Sirés, J.L. Nava

4:30 ENVR 295. Modular advanced oxidation process enabled by cathodic hydrogen peroxide production. J. Barazesh, D.L. Sedlak

4:50 ENVR 296. Degradation of metribuzin by electrochemical advanced oxidation processes using a boron-doped diamond anode. F. Gozzi, S.C. de Oliveira, A. Machulek Junior, E. Brillas, I. Sirés

5:10 ENVR 297. Mineralization of trans-ferulic acid by anodic oxidation, electro-Fenton and photoelectro-Fenton. N.E. Flores, I. Sirés, P.L. Cabot, F. Centellas, R. Rodríguez, J. Garrido, E. Brillas

Section G

Boston Park Plaza Hotel and Towers Stuart Room

Environmental Applications and Implications of Graphene-Based Nanomaterials

I. Chowdhury, M. Hersam, *Organizers*

D. C. Bouchard, *Organizer, Presiding*

W. M. Henderson, *Presiding*

1:30 Introductory Remarks.

1:35 ENVR 298. Sunlight-induced transformations of graphene-based nanomaterials in aquatic environments. R.G. Zepp, D.C. Bouchard, W. Hou, I. Chowdhury, H. Fairbrother, D.G. Goodwin, W. Henderson, C. Knights, C. Chen

2:15 ENVR 299. Withdrawn.

2:35 ENVR 300. Toxicological potential and environmental fate of molybdenum disulfide (MoS₂), a post-graphene 2D material. L.M. Guiney, N.D. Mansukhani, P. Kim, X. Wang, Z. Ji, C. Chang, M. Wang, Y. Liao, T. Song, B. Sun, R. Li, J.D. Lanphere, C.J. Luth, S.L. Walker, T. Xia, A. Nel, M. Hersam

2:55 ENVR 301. Low-level of Graphene inhibits the activity of ABC transporters and acts as chemosensitizer. S. Liu

3:15 Intermission.

3:30 ENVR 302. Heteroaggregation of graphene oxide with nanometer- and micrometer-sized hematite colloids: Rates and conformation. K. Chen, Y. Feng

3:50 ENVR 303. Assessing the exposure and toxicological implications of environmental transformations of graphene oxide using in vitro methods. W.M. Henderson, I. Chowdhury, X. Chang, W. Hou, R.G. Zepp, D.C. Bouchard, S.J. Martin

4:10 ENVR 304. Efficient removal of indoor pollutants by using graphene-layered double hydroxide composites in room temperature. F. Liu, P. Zhang

4:30 ENVR 305. Ecotoxicity of carbon nanotubes to algae, *Dunaliella tertiolecta*. M. Thakkar, S. Mitra, L. Wei

4:50 Concluding Remarks.

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WEDNESDAY MORNING**Section A**Boston Park Plaza Hotel and Towers
Tremont Room**Anaerobic Sewage Treatment: Dissolved Methane and Nitrogen Control**

G. Wells, Organizer

P. Joonhong, H. Lee, Organizers, Presiding

8:00 Introductory Remarks.**8:05 ENVR 306.** Direct interspecies electron transfer by syntrophic interaction between exoelectrogens and methanogens via granular activated carbon. J. Lee, H. Park**8:20 ENVR 307.** Toward mainstream nitrification-anammox bioprocesses for reactive nitrogen management in effluent from anaerobic dilute wastewater treatment. G. Wells**8:35 ENVR 308.** Use of dissolved methane gas for denitrification- process kinetics and microbiology. R. Goel, A. Bhattacharjee**8:50 ENVR 309.** Removing nitrogen from effluents of anaerobic wastewater treatment processes: Understanding control and operation through biofilm modeling. J. Delgado Vela, K.J. Martin, A. McFarland, N. Beaton, L.B. Stadler, S. Skerlos, L. Raskin, C.B. Bott, N. Love**9:05 ENVR 310.** Modeling soluble methane in an anaerobic baffled reactor. D. Sills, D. Cowell**9:20** Intermission.**9:35 ENVR 311.** Complimentary or competitive — exploring dynamics between denitrifiers and anode-respiring bacteria in bioelectrochemical biofilms. V. Srinivasan, C. Butler**9:50 ENVR 312.** Enrichment of an anammox MBBR to treat mainstream wastewaters. Z. Li, K. Chandran**10:05 ENVR 313.** Anaerobic methane oxidation coupled to nitrate reduction using membrane biofilm reactors. H. Lee, W. Alrashed**10:20 ENVR 314.** Nitrous oxide (N₂O) recovery from ammonia oxidizing culture (AMO) in membrane aerated biofilm reactor with high NH₃ strength wastewater. T.V. Doan, J. Lee, S.K. Shukla, M. Lee, J. Park**10:35 ENVR 315.** Comparison of dissolved methane removal processes: Removal efficiency, energy consumption and application of recovered methane. J. Bae**10:55 ENVR 316.** Performance of anaerobic electrochemical membrane bioreactor using graphene-coated nickel hollow fiber membrane as cathode electrode. C. Werner, K.P. Katuri, H. Anandarao, W. Chen, Z. Lai, B. Logan, G. Amy, P. Saikaly**11:10 ENVR 317.** Methane-driven microbial fuel cell for dissolved methane management in anaerobic effluents. S. Chen, A. Smith**Section B**Boston Park Plaza Hotel and Towers
Stuart Room**Status and Trends of Biological and Persistent Organic Chemicals in the Great Lakes**

D. D. Dionysiou, J. J. Pagano, Organizers, Presiding

8:00 ENVR 318. The Great Debate: Investigating the roles of nitrogen and phosphorus in driving the growth and toxicity of cyanobacterial harmful algal blooms in western Lake Erie. T. Davis, T. Johengen, M. Harke, G. Bullerjahn, S. Watson**8:30 ENVR 319.** Products of oxidation of microcystin-LR by ferrate(VI) as a function of reactant molar ratios and pH. L. Chen, Y. Rezenom, D.H. Russell, D. Dionysiou, K.E. O'Shea, B. Marsalek, R. Zboril, V.K. Sharma**8:50 ENVR 320.** Removal of cyanotoxins (microcystins and cylindrospermopsin) using UV-based processes. X. He, A.A. de la Cruz, D.D. Dionysiou**9:10 ENVR 321.** Sorption of human and veterinary antimicrobials in soils and sediments. S.A. Pagsuyoin, J. Yap**9:30 ENVR 322.** Sediments as sinks of antimicrobials in rivers. S.A. Pagsuyoin**9:50** Intermission.**10:20 ENVR 323.** Microplastics in surface water in and entering nearshore areas of the lower Great Lakes. G. Zimmer, M. Stones, J. Thibeau, W. Page, A. Sims, B. Thornburn, P.A. Helm**10:40 ENVR 324.** Trends and toxic equivalence of PCDD/F and DL-PCBs in lake trout from the Great Lakes: 2004-2013. J.J. Pagano, A. Garner, B.S. Grimmins, M. Milligan, X. Xia, P.K. Hopke, T.M. Holsen**11:00 ENVR 325.** Spatial distribution and diffusive air-water exchange of dissolved flame retardants and synthetic musks in the lower Great Lakes. C.A. McDonough, R. Lohmann**11:20 ENVR 326.** Long term spatial and temporal trends of PBDEs and their replacements in the Great Lakes atmosphere. L. Liu, A. Salamova, M. Venier, R.A. Hites**11:40 ENVR 327.** Spatial distribution, air-water exchange and source apportionment of polychlorinated biphenyls in the lower Great Lakes Basin. M. Khairiy, D.C. Muir, C. Teixeira, R. Lohmann**Section C**Boston Park Plaza Hotel and Towers
Berkeley/Clarendon Room**Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials****Energy Storage, Solar Fuels, and Biofuels: Satisfying the Energy Needs While Decreasing the Carbon Footprint**

Cosponsored by CEI, ENFL, ORGN and PHYS

K. Rajeshwar, V. I. Vullev, Organizers, Presiding

8:00 Introductory Remarks.**8:05 ENVR 328.** Bioinspired approaches for energy storage: Molecular excited states that drive bond formation. G.J. Meyer**8:45 ENVR 329.** Bioinspired structural motifs for multi-functional behavior in the design of molecular catalysts for CO₂/H₂ interconversion with formic acid. J.T. Muckerman, M.Z. Ertem, Y. Himeda, E. Fujita**9:25 ENVR 330.** Electrosynthesis of hybrid organic/inorganic photocathodes for solar fuel generation. D. Hursan, K. Rajeshwar, C. Janaky**9:55** Intermission.**10:10 ENVR 331.** Homogeneous solar hydrogen photocatalysis. F.N. Castellano**10:50 ENVR 332.** Running on sun: Bioinspired approaches to achieving solar fuels. G.F. Moore, D. Khushnutdinova, A. Beiler, S. Jacob, E. Skibo, A. Echeverri**11:30 ENVR 333.** Microbial conversion of methane to methanol in a packed bed reactor by *Methylosinus trichosporium* OB3b immobilized in alginate beads. P. Molzahn, A. Taylor, L. Semprini**Section D**Boston Park Plaza Hotel and Towers
Beacon Hill Room**Resource Recovery and Contaminant Elimination in Waste Streams of Increasing Concern****Nutrient Recovery: Source Separated Urine**Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
T. H. Boyer, C. Huang, Organizers, Presiding**8:00** Introductory Remarks.**8:10 ENVR 334.** Removal of pharmaceuticals in source separated urine using biochar for nutrient recovery. A. Solanki, T.H. Boyer**8:35 ENVR 335.** Contaminant removal from source separated urine will enhance opportunities for nutrient recovery. K. Landry, P. Sun, C. Huang, T.H. Boyer**9:00 ENVR 336.** Unconventional treatment for unconventional waste: Removal of pharmaceuticals and metabolites by AOPs in source-separated human urine. P. Sun, R. Zhang, C. Huang**9:25** Intermission.**9:40 ENVR 337.** Implications of implementation scale on the environmental sustainability of wastewater treatment with resource recovery. Q. Zhang, P. Cornejo, J. Mihelcic**10:15 ENVR 338.** Adsorption applications for total nutrient recovery from urine. T.H. Boyer**10:40 ENVR 339.** Evaluating ion exchange and electrochemical nitrogen recovery from source-separated urine. W. Tarpeh, K. Nelson**11:05 ENVR 340.** Coupling chemical and biological processes for nutrient recovery and removal for better source separated urine management. R. Goel, P. Huang**Section E**Boston Park Plaza Hotel and Towers
Statler Room**Environmental Transformation of Nanoparticles: Processes, Mechanisms, and Ecological Impacts****Physicochemical Transformations**

M. Cledon, B. Lau, W. Yan, Organizers

K. D. Hristovski, P. Larese-Casanova, Organizers, Presiding

8:00 Introductory Remarks.**8:05 ENVR 341.** Case studies in the environmental transformations of nonequilibrium nanomaterials. R. Hurt**8:35 ENVR 342.** Surface interaction of gold and fullerene nanoparticles with pyrogenic carbonaceous materials. S.M. Uchimiya, J.J. Pignatello, J.C. White**9:05 ENVR 343.** Heteroaggregation between cerium oxide nanoparticles and nanoparticles of pyrolyzed biomass. P. Yi, J.J. Pignatello**9:25 ENVR 344.** Release and transformations of silver nanoparticles in polymeric nanocomposites exposed to environmental scenarios. T.A. Dankovich, G. Lowry**9:45 ENVR 345.** Measure the deposition of titanium dioxide nanoparticles on model rough surfaces using generalized ellipsometry technique. N. Kananizadeh, D. Peev, C. Rice, T. Hofmann, M. Schubert, S. Bartelt-Hunt, Y. Li**10:05** Intermission.**10:20 ENVR 346.** Role of nanoparticles in the fate and transport of hydrophobic pollutants. E. Sahle-Demessie, A. Zhao, Y. Shan**10:40 ENVR 347.** Evaluation and improvement of sample preparation protocols for the single particle ICP-MS measurement of silver nanoparticles. J. Liu, K.E. Murphy, V.A. Hackley, M.R. Winchester**11:00 ENVR 348.** Co-transport of gold nanospheres with single-walled carbon nanotubes in saturated porous media. A. Afroz, D. Das, C.J. Murphy, P.J. Vikesland, N.B. Saleh**11:20 ENVR 349.** Influence of natural organic matter on the interaction of functionalized diamond nanoparticles with supported lipid bilayer. A.C. Mensch, M. Torelli, J.A. Pedersen, R.J.J. Hamers**11:40 ENVR 350.** Withdrawn.**Technical program information known at press time.****The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015**

Section F

Boston Park Plaza Hotel and Towers
Cambridge Room

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

Electrocoagulation and Electro-Fenton Processes

Cosponsored by AGRO

F. A. Monterrubio, I. S. Sardonil, V. K. Sharma, *Organizers*

E. Brillas, J. Luis Nava Montes de Oca, *Presiding*

8:00 ENVR 351. Advances in electrocoagulation: Self-powered systems and use of low-cost aluminium. D.M. Valero Valero, E. Expósito, V. García-García, A. Aldaz Riera, V. Montiel Leguey

8:20 ENVR 352. Electrocoagulation of tannery wastewater: Optimization and comparison between pulse and direct current. A. Suarez, A.F. Lopez Vasquez, A.R. Albis, N. Agudelo

8:40 ENVR 353. Treatment of food color additives in different water matrices by single and combined electrochemical processes. A. Thiam, E. Brillas, R. Rodriguez, J. Garrido, F. Centellas, P.L. Cabot, I. Sirés

9:00 ENVR 354. Optimization of the electro-Fenton process for removal of pharmaceuticals from water: Minimization of energy consumption, treatment time, and improvement of biodegradability. O. Ganzenko, N. Oturan, D. Huguenot, E. van Hullebusch, G. Esposito, M. Oturan

9:20 Intermission.

9:35 ENVR 355. Combined electro-Fenton pre-treatment and a biological process for the mineralization of the pharmaceuticals Furosemide and Ranitidine. H. Olvera Vargas, N. Oturan, D. Buisson, M.A. Oturan

9:55 ENVR 356. Rapid and complete removal of nitrophenols by heterostructured gold-magnetite nanocatalysts. R. Doong, F. Lin

10:15 ENVR 357. Transformation products of oxidation of microcystin-LR by ferrate(V) and ferrate(IV): similarities and differences with ferrate(VI). L. Chen, Y. Rezenom, D.H. Russell, D. Dionysiou, K.E. O'Shea, B. Marsalek, R. Zboril, V.K. Sharma

10:35 ENVR 358. Recent development in enhanced electro-Fenton process efficiency: Electrode materials and coupling possibilities with other methods. M.A. Oturan

Subsurface Geochemistry for Energy & the Environment

Mineral Reactions in Geologic Carbon Sequestration

Sponsored by GEOC, Cosponsored by ENVR

Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage, and Monitoring Data

Sponsored by AGRO, Cosponsored by ENVR

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Sponsored by PHYS, Cosponsored by ENVR

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by CINF, Cosponsored by AGRO, COMP, ENVR and MEDI

Environmental Fate, Management, and Mitigation of Nitrogen in Agricultural Systems

Sponsored by AGRO, Cosponsored by ENVR

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds

Sponsored by AGRO, Cosponsored by ANYL and ENVR

Pesticides and Hydrophobic Compounds in Sediment

Sponsored by AGRO, Cosponsored by ENVR

WEDNESDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers
Trenton

Detection and Fate of Health-Related Microorganisms in Water

Cosponsored by AGRO

K. Bibby, K. Wigginton, *Organizers, Presiding*

1:00 ENVR 359. Novel microbial source tracking microarray for pathogen detection and fecal source identification in environmental systems. J. Weidhaas, X. Li, V. Harwood

1:20 ENVR 360. Development of CrAssphage as an Improved indicator of human fecal pollution in the environment. E. Stachler, K. Bibby

1:40 ENVR 361. Diversity of potentially pathogenic bacteria in municipal wastewater treatment plants. Q. Chen

2:00 ENVR 362. Methods for the detection of infective enveloped viruses in municipal wastewater. Y. Ye, M. Ellenberg, K. Wigginton

2:20 ENVR 363. Effect of chlorinated phenol in point-of-use drinking water filters on antibiotic resistance and opportunistic pathogens. C. Wu, N. Love, T.M. Olson

2:40 ENVR 364. Public health and potable reuse: Challenges in pathogen control and detection. B. Pecsion, S. Trussell, A.N. Pisarenko, R. Trussell

3:00 ENVR 365. Removal of bacterial contaminants and antibiotic resistance genes by conventional wastewater treatment processes in Saudi Arabia: Is the treated wastewater safe to reuse for agricultural irrigation compared to the groundwater? P. Hong, N. Al-Jassim, M. Ansari, M. Harb

3:20 ENVR 366. Predicting the fate of waterborne viruses in surface water using photochemistry tools. M.J. Mattle, D.V. Vione, T. Kohn

3:40 ENVR 367. Fate and persistence of NDM-9 *Escherichia coli* in aerobic and anaerobic sludge under different micro-selective conditions. D. Mantilla, P. Hong

4:00 ENVR 368. Fate of pathogens and indicator organisms in direct and indirect wastewater irrigation systems in the Cochabamba valley of Bolivia. M.E. Verbyla, M. Iriarte, A. Mercado, J. Mihelcic

Section B

Boston Park Plaza Hotel and Towers
Stuart Room

Using Passive Sampling Techniques to Detect Organic Contaminants

Cosponsored by AGRO and ORGN

Financially supported by AEESP (Association of

Environmental Engineering and Science Professors)

C. A. McDonough, *Organizer*

R. Lohmann, *Organizer, Presiding*

1:30 ENVR 369. Calibration of a novel passive sampler for the measurement of 34 polar organic contaminants in aquatic systems. J. Chailis, M. Hanson, C.S. Wong

1:50 ENVR 370. Phytoforensics and novel passive samplers to assess vapor intrusion risk. J.L. Wilson, M. Limmer, J.G. Burken

2:10 ENVR 371. Passive sampling in the water column using "fast" performance reference compounds. D.P. Prendergast, P.M. Gschwend

2:30 ENVR 372. Polyethylene uptake of gaseous hydrophobic organic contaminants (HOCs). C.A. McDonough, R. Lohmann

2:50 ENVR 373. Estimating sampling rate of polyethylene passive samplers using samplers of different thickness. C. Sun, R. Lohmann

3:10 ENVR 374. Calculating the diffusive flux of DDTs and PCBs across the sediment-water interface at the Palos Verdes Shelf Superfund site using polyethylene and polyoxymethylene passive samplers. L. Fernandez, G.M. Flavetta, R.M. Burgess

3:30 ENVR 375. Atmospheric polybrominated diphenyl ethers from an e-waste dismantling area: seasonal variation and sample pattern comparison. X. Jiao, H. Cao

3:50 ENVR 376. Spatial and temporal variations of PCBs and OH-PCBs in the Metropolitan Chicago area using passive air sampling. N.J. Herkert, A. Martinez, K.C. Hornbuckle

4:10 ENVR 377. HCBz and PAHs trend in the atmosphere and surface seawater along a cruise pathway from the East China Sea to the Arctic Ocean. M. Cai, W. Zhao, D.A. Adelman, R. Lohmann

4:30 ENVR 378. Application of GCxGC and passive dosing for characterizing mixture toxicity of hydrophobic organic chemicals (HOCs). A. Tcaciuc, R. Nelson, L. Rotkowitz, C. Reddy, P.M. Gschwend

4:50 ENVR 379. Passive sampling and target/non-target analyses as tools for tracking chemicals of concern in the Great Lakes. P.A. Helm, M. Robson, E. Reiner, M. Pena, P. Yang, D. Morse, K. MacPherson, I.D. Brindle

Section C

Boston Park Plaza Hotel and Towers
Berkeley/Clarendon Room

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Artificial Photosynthesis: Challenges and Strategies to Meet Energy Needs in an Environmentally Benign Manner

Cosponsored by CEI, ENFL, ORGN and PHYS

K. Rajeshwar, V. I. Vullev, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 380. Artificial photosynthesis — Helping nature regain control of the global carbon cycle. T.A. Moore, A.L. Moore, D. Gust

2:15 ENVR 381. High valence homogeneous and amorphous metal oxide clusters as biomimetic catalysts: Identifying ligand-dependent changes in domain structure. D.M. Tiede, G. Kwon, D. Fazi, J.D. Emery, A.B. Martinson, J. Thomsen, S.W. Sheehan, G.W. Brudvig, R.H. Crabtree

2:55 ENVR 382. Stabilization of oxygen sensitive hydrogenases towards oxidative damage by redox hydrogels. O. Rüdiger, A.A. Oughli, F. Conzuelo, M. Winkler, T. Happe, W.W. Lubitz, W. Schuhmann, N. Plumere

3:25 Intermission.

3:40 ENVR 383. Photocatalysis inspired by FAD/NAD cofactors: Merging dye-sensitized solar cells with catalysis. K. Glusac

4:20 ENVR 384. Solar fuel biohybrids: Aqueous light-driven hydrogen production by photosensitizer-protein-molecular catalyst systems. S. Soltan, J. Niklas, P.D. Dahlberg, D.M. Tiede, O. Poluektov, K.L. Mulfort, L.M. Utschig-Johnson

4:40 ENVR 508. Synthesis and characterization of p-type semiconductor inorganic nanocrystals for photoelectrochemical fuel generation. A. Kormanyos, A.L. Thomas, K. Rajeshwar, C. Janaky

5:00 ENVR 385. In-situ structure function characterization of the cobalt oxide water oxidation catalyst films. G. Kwon, H. Kim, J.D. Emery, D. Fazi, A.B. Martinson, P.C. Stair, D.M. Tiede

Section D

Boston Park Plaza Hotel and Towers
Beacon Hill Room

Resource Recovery and Contaminant Elimination in Waste Streams of Increasing Concern

Metal Recovery: From Lithium to Gold

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
T. H. Boyer, C. Huang, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 386. Assessment of U.S.-based coal fly ashes as an alternative resource for rare earth elements. H. Hsu-Kim, R. Taggart, J.C. Hower, G.S. Dwyer

2:10 ENVR 387. Lithium recovery from low temperature geothermal brines through membrane distillation and manganese oxide sorption. J. Renew, J. Rajterowski, J. Wos

2:35 ENVR 388. Tunable anion exchange to treat Marcellus flowback wastewater and recover barium using impaired acid mine drainage (AMD). A.K. Sengupta, J. Li, M. German

3:00 Intermission.

3:15 ENVR 389. Precious metal and rare earth element recovery from waste streams: Technical developments and life cycle considerations of recovering and recycling gold from nanomaterial waste streams. P. Pati, P.J. Vikesland, S. McGinnis

3:40 ENVR 390. Silver removal and recovery from waste streams: role of co-contaminants and regenerants and purity of silver recovered. T. Nawaz, S. Sengupta

4:05 ENVR 391. Bioinspired adaptively reconfigurable material systems: A new paradigm for autonomous metal ion separation. H. Nan, Z. Zhao, J. Liu, X. He

4:30 ENVR 392. Removal of PFOS and its alternative from electroplating wastewater using granular reactivated carbon. Z. Du, S. Deng, D. Liu, X. Lu, X. Yao, W. Bin, Y. Huang, Y. Wang, G. Yu

4:55 Concluding Remarks.

Section E

Boston Park Plaza Hotel and Towers
Statler Room

Environmental Transformation of Nanoparticles: Processes, Mechanisms, and Ecological Impacts Biotransformations and Bioavailability

K. D. Hristovski, P. Larese-Casanova, B. Lau,
Organizers

M. Cledon, W. Yan, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 393. Heteroaggregation of nanoparticles with bio-colloids and geocolloids. A.A. Keller, H. Wang, A.S. Adeleye, Y. Huang

2:05 ENVR 394. Can carbon-based nanomaterials modulate the toxic activity of organic pollutants in the environment? D. Barcelo, J. Sanchis, M. Farre

2:35 ENVR 395. Toxicity of rare earth element oxide nanoparticles on *E. coli*. V. Craver, N. Anaya, F. Solomon

2:55 ENVR 396. Uptake, distribution, and physiological impacts of metal oxide nanoparticles in mature crop plants: Evidence for nanophototoxicity? J. Conway, S. Mazer, A.A. Keller

3:15 ENVR 397. Lithium nickel manganese cobalt oxide (NMC) nanomaterials: Interactions with biological systems. M.N. Hang, I. Gunsolus, J. Bozich, H.A. Wayland, E. Melby, A.C. Mensch, K. Hurley, J.A. Pedersen, R. Klaper, C.L. Haynes, R.J. Hamers

3:35 Intermission.

3:50 ENVR 398. Interaction of engineered materials with microbial biofilms and its potential applications. H. Jing, D. Clark, S. Palmer, V. Sumner, E. Sahle-Demessie, M.J. Kupferle, G. Sorial

4:05 ENVR 399. Microbial aging of fullerene C₆₀ nanoparticle aggregates in water. S. Chae, D.E. Hunt, C.K. Gunsch, M.R. Wiesner

4:25 ENVR 400. Tracking trace amounts (ppb) of silica nanoparticles in complex fluids and sewage water plants using DNA tracers. R.N. Grass, D. Paunescu, R. Kaegi, W.J. Stark

4:45 ENVR 401. Influence of phytoplankton on fate, transformations, and effects of iron nanoparticles. A.S. Adeleye, A.A. Keller

5:05 ENVR 402. Evaluation of silver nanoparticle – impregnated textiles across their life cycle. R.B. Reed, M. Marco, T. Zaikova, A. Barber, J.E. Hutchison, J.F. Ranville, R.L. Tanguay, P.K. Westerhoff, K.D. Hristovski

5:25 ENVR 403. Preparation and characterization of strawberry fruit extraction loaded nano biodegradable chitosan particles. R. Pulicharla, C. Marques, S. Brar, T. Rouissi, M. Cledon, S. Sarma

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

Section F

Boston Park Plaza Hotel and Towers
Cambridge Room

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

(Bio)electro-Oxidation

Cosponsored by AGRO

F. A. Monterrubio, I. S. Sardonil, V. K. Sharma,
Organizers

M. Rodrigo, I. S. Sardonil, *Presiding*

1:30 Introductory Remarks.

1:55 ENVR 404. Electrochemical engineering for safer advanced oxidation processes (AOPs). M.E. Bergmann

2:15 ENVR 405. Electrochemical disinfection of urban treated wastewater: An alternative to conventional disinfection processes. S. Cotillas, A. Raschitor, J. Pérez, M. Martín de Vidales, J. Llanos, C. Sáez, M. Rodrigo, P. Cañizares

2:35 ENVR 406. Pharmaceutical wastewater treatment associated with energy recovery in microbial fuel cell. Z.Z. Ismail, A.A. Habeeb

2:55 Intermission.

3:10 ENVR 407. Preparation of a dimensional stable anode for the production of heterogeneous hydroxyl radicals used to oxidize persistent organic compounds. Z.G. Aguilar-Rico, J.L. Nava, M.M. Salazar

3:30 ENVR 408. Effect of different parameters on the electro-oxidation treatment of Congo red. H. Jalife, R. Feria, A. Alatorre, S. Gutierrez, J. Peralta-Hernandez

3:50 ENVR 409. Treatment of soil washing solutions by electro-oxidation with BDD anode: Selective removal of target pollutants and biodegradability enhancement. C. Trellu, Y. Péchaud, N. Oturan, D. Huguenot, E. van Hullebusch, G. Esposito, M. Oturan

4:10 ENVR 410. Electrolytic and electro-irradiated processes with diamond anodes for the removal of persistent pollutants. M. Martín de Vidales, A. Raschitor, J. Pérez, S. Cotillas, J. Llanos, C. Sáez, M. Rodrigo, P. Cañizares

4:30 ENVR 411. Synergistic coupling between electrochemical and ultrasound treatments for organic pollutant degradation as a function of the electrode material (IrO₂ and BDD) and the ultrasonic frequency (20 and 800 kHz). R.A. Torres-Palma, G. Fernando, C. Pétrier, G. Peñuela, E. Herrera-Calderón, C. Pulgarin

Subsurface Geochemistry for Energy & the Environment

Mineral Reactions in Subsurface Energy and Waste Operations

Sponsored by GEOC, Cosponsored by ENVR

Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage, and Monitoring Data

Sponsored by AGRO, Cosponsored by ENVR

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Sponsored by PHYS, Cosponsored by ENVR

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by CINF, Cosponsored by AGRO, COMP, ENVR and MEDI

Degradation of Halogenated Compounds in the Environment

Sponsored by AGRO, Cosponsored by ENVR

Recent Advances in the Analysis of Environmental Contaminants in Foods and Feeds

Sponsored by AGRO, Cosponsored by ANYL and ENVR

Formulation Technologies for Improved Crop Protection

Sponsored by AGRO, Cosponsored by ENVR and ORGN

WEDNESDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Advanced Materials and Technologies for Desalination and Wastewater Reuse

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
J. Kim, Q. Li, *Organizers*

6:00 - 8:00

ENVR 412. Investigation of fluoride removal from brackish groundwater by single-pass capacitive deionization. W. Tang, P. Kovalsky, D. Waite

ENVR 413. Characterization of fouling potential through the use of fluorescence techniques. L. Strahs, J. VanBriesen, K.L. Jones

ENVR 414. Aqueous synthesis of polyvinyl alcohol-alginate-montmorillonite nanocomposite particles for applications in wastewater purification. M. Bee, E. Kalivas, J.C. Schwabacher, M.R. Hartings, D. Fox

ENVR 415. Adsorption of metal ions by magnetic carbon tubes. C. Chang, B. Wang

Section A

Boston Convention & Exhibition Center
Hall C

Advances in Chemistry for Carbon Capture, Utilization and Sequestration

Cosponsored by ENFL

P. Fennell, N. Florin, *Organizers*

M. Zhao, *Organizer, Presiding*

6:00 - 8:00

ENVR 416. Synthesis of a porphyrin polymer with benzimidazole linkages for CO₂ capture. V. Neti

ENVR 417. CPO-27-Ni incorporated in nickel foam for efficient CO₂ capture. Z. Liu, W. Han, K.L. Yeung

ENVR 418. Study of sorption kinetics of CO₂, CO, CH₄, and N₂ on an organic molecular porous material (cucurbit[6]uril). J. Lee, B. Min, H. Kim, Y. Park, D. Chun, J. Moon

ENVR 419. CO₂ and H₂S mixed gas absorption in mixed aqueous solutions of sulfolane and MDEA. B. Min, J. Lee, Y. Park, J. Moon

Section A

Boston Convention & Exhibition Center
Hall C

Advances in Drinking Water Disinfection: Byproducts Occurrence, Formation, Treatment, Health Effects, Epidemiology and Regulation

E. Sahle-Demessie, G. Sorial, *Organizers*

6:00 - 8:00

ENVR 420. Adsorption of selected antibiotics and endocrine disrupting compounds from aqueous solution by carbon nanomaterials. X. Li, S. Chen, X. Quan

ENVR 421. On THM formation in direct electrochemical drinking water disinfection. M.E. Bergmann, J. Hartmann, T. Iourtchouk

ENVR 422. Revealing the mechanism and kinetics of UV-254 nm/H₂O₂-based degradation of active sunscreen ingredient PBSA. W. Abdelraheem, X. He, D.D. Dionysiou

Section A

Boston Convention & Exhibition Center
Hall C

Anaerobic Sewage Treatment: Dissolved Methane and Nitrogen Control

P. Joonhong, H. Lee, G. Wells, *Organizers*

6:00 - 8:00

ENVR 423. Anaerobic digestion of renewable materials for biogas production: Experimental stage to the field. O.O. Adetule

ENVR 424. Improved stability of methane-producing anaerobic biological reactors through novel use of ion-exchange fibers. Y. Tian, D. Brown, A. SenGupta

ENVR 425. Tale of two cities (Boston and Detroit). S. Simoliunas, I. Welch, C. Darrah, S. McDonald, C. Dougherty

Section A

Boston Convention & Exhibition Center
Hall C

Assessing Transformation Products by Non-Target and Suspected Target Screening: The New Frontier in Environmental Chemistry and Engineering

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
S. A. Snyder, J. Drews, T. Letzel, *Organizer*

6:00 - 8:00

ENVR 426. Withdrawn.

ENVR 427. Suspected-target screening strategy to investigate degradation by ozonation or photolysis of urban micropollutants in wastewaters. P. Bados, B. Mathon, J. Choubert, J. Chovelon, M. Coquery, C. Miede, T. Brzokewicz

ENVR 428. Widening the analytical perspective – polarity extended separations for the detection of trace organic compounds in environmental samples. S. Bieber, J. Drews, T. Letzel

ENVR 429. Biofiltration: An advanced treatment process for removal of EDCs and PPCPs. S. Zhang, S. Gitungo, L.B. Axe, J.E. Dyksen, R.F. Raczko

ENVR 430. Characterization and determination of oxygen types present in weathered Deepwater Horizon oil by Fourier transform ion cyclotron resonance mass spectrometry. S.M. Rowland, R.P. Rodgers

ENVR 431. Product formation and energy efficiency during algae-mediated transformation of estrogens and other emerging chemicals. Y. Zhang, K. Grimes, L.M. Colosi

ENVR 432. Fate of six neonicotinoids during full-scale wastewater treatment and passage through an engineered wetland. A. Sadaria, S. Supowit, R.U. Halden

Section A

Boston Convention & Exhibition Center
Hall C

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Cosponsored by CEI, ENFL, ORGN and PHYS

K. Rajeshwar, V. I. Vullev, *Organizers*

6:00 - 8:00

ENVR **433.** Glucose entrapped in titania under mild environmental conditions. Z. Yu, P. Huang, X. Wang

ENVR **434.** Analysis of *Cryptococcus* and *Rhodotorula* fungi in the extraction of lipids for biodiesel production. S. McGee, A.J. Reese, L.A. Welch

Section A

Boston Convention & Exhibition Center
Hall C

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

Cosponsored by AGRO

F.A. Monterrubio, I. S. Sardonil, V. K. Sharma, *Organizers*

6:00 - 8:00

ENVR **435.** Influence of nitrates, chlorides, and humic substances on electrochemical reduction of trichloroethylene. L. Rajic, N. Fallahpour, R. Nazari, A. Alshawabkeh

ENVR **436.** 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, S. Yuan, A. Alshawabkeh

ENVR **437.** Electrochemical degradation of chlorobenzene in simulated groundwater using Pd-catalytic electro-Fenton's reaction. R. Nazari, A. Ciblak, I. Mousa, A. Alshawabkeh

ENVR **438.** Degradation of chlorophenols in the Fe/TPP/air system: The role of reactive oxygen species on the degradation kinetics and mechanism. W. Li, L. Zhang

ENVR **439.** Electrochemical oxidation of carbaryl on platinum and boron-doped diamond anodes using electro-Fenton process. N. Oturan, M. Sönmez Celebi, M.A. Oturan

ENVR **440.** Degradation and mineralization of the phenylurea herbicide fluometuron in aqueous media by electro-Fenton process. N. Oturan, P.A. Diaw, M.D. Gaye Seye, J. Aaron, M.A. Oturan

ENVR **441.** Fe@Fe₂O₃ promoted E-Fenton mineralization of atrazine under a low current of 30 mA. D. Xing, L. Zhang

ENVR **442.** Electrochemical treatment of p-phenylenediamine by self electro-generative Fenton process. S. Yen, W. Hsieh

ENVR **443.** Remediation of bovine slurry wastewater using a combination of anaerobic biological digestion and solar photoelectro-Fenton processes. J. Vidal, R. Salazar, C. Huiñir

ENVR **444.** Degradation and mineralization of Malathion by Solar Photo electro-Fenton in a 200 mL electrochemical reactor and in a10L flow plant. G. Palacios, D. Chavez, A. Hernandez-Ramirez, L. Hinojosa-Reyes, J. Guzman, E. Ruiz

ENVR **445.** Degradation of antihypertensive drug hydrochlorothiazide in water by electro-oxidation with BDD: Application of method to pharmaceuticals tablets. R. Salazar, N. Contreras

ENVR **446.** Electrochemical degradation of the antihypertensive losartan in neutral aqueous medium by electro-oxidation with BDD electrode. C.A. Salazar, N. Contreras, H.D. Mansilla, J. Yanez, R. Salazar

ENVR **447.** Withdrawn.

ENVR **448.** Electrochemical treatment of petrochemical industry effluent using Ti/IrO₂-Ta₂O₅ and BDD. S. Souza Leal Castro, D. Ribeiro da Silva, C. Martínez-Huitle

ENVR **449.** New oxygen-diffusion electrodes for hydrogen peroxide electrogeneration: Application in wastewater decontamination and disinfection. F.A. Monterrubio, G. Alvarez, E. Brillas, H. Grande, O. Miguel, I. Sirés

ENVR **450.** Electrocatalysis enhanced activated carbon catalyzing peroxydisulfate for the degradation of Acid Orange 7 in simulated water at ambient temperature. J. Li, L. Yang, M. Chen, H. Zhang

ENVR **451.** Treatment of industrial wastewater by electrochemical techniques: Systems powered by photovoltaic energy. D.M. Valero Valero, V. García-García, E. Exposito, A. Aldaz Fiera, V. Montiel Leguey

ENVR **452.** Electrochemical and photoelectrochemical degradation of tetracyclines and quinolones on Ti/TiO₂ electrode. P. Moreira, P. Molina, C. Berrios

Section A

Boston Convention & Exhibition Center
Hall C

Environmental Applications and Implications of Graphene-Based Nanomaterials

I. Chowdury, M. Hersam, D. C. Bouchard, *Organizers*

6:00 - 8:00

ENVR **453.** Electrochemical carbon nanotube filters for removal of perfluoroalkyl acids in the presence of natural organic matter. Y. Zhi, A. Bakr, M. Rahaman, J. Liu

ENVR **454.** Graphene as passive sampler material for Polycyclic Aromatic Hydrocarbons (PAHs): Effect of chemical properties and sample characteristics on partitioning and equilibration times. R. Sevanti-Dilipan, M. Green, A. Jackson

Section A

Boston Convention & Exhibition Center
Hall C

Environmental Transformation of Nanoparticles: Processes, Mechanisms, and Ecological Impacts

D. C. Bouchard, I. Chowdury, M. Hersam, *Organizers*

6:00 - 8:00

ENVR **455.** Use of single particle ICP-MS and asymmetric flow field flow fractionation to investigate silver nanoparticle corrosion in environment waters. J. Liu, J.M. Pettibone, M.R. Winchester, V.A. Hackley

ENVR **456.** Effects of ultra-violet light on silver nanoparticle mobility and dissolution. A. Mittelman, J. Fortner, K.D. Pennell

ENVR **457.** Shape-controlled synthesis of CuO/ZnO composites and their photocatalytic performance. L. Tan, J. Li, M. Yang, H. Gao

ENVR **458.** C₆₀ transformation(s) in water: Elucidating and connecting critical oxidation/reduction pathways and products. J. Wu

ENVR **459.** Quantum dot dissolution kinetics monitored with SEC-ICP-MS. P. Paydary, P. Larese-Casanova

ENVR **460.** Monitoring the environmental effects of CeO₂ and ZnO nanoparticle through the life cycle of corn (*Zea mays*) and cucumber (*Cucumis sativus*) plants. L. Zhao, Y. Sun, J.L. Gardea-Torresdey, J.R. Peraltavidea, J. Hernandez-Viezas, J. Hong, S. Majumdar, A. Servin, M. Duarte-Gardea

ENVR **461.** Effects of nano- and microscale microplastics on the transformation and *Daphnia* bioaccumulation of phenanthrene in fresh water. Y. Ma, R. Ji

Section A

Boston Convention & Exhibition Center
Hall C

General Posters

D. D. Dionysiou, *Organizer*

6:00 - 8:00

ENVR **462.** Chlorine-free disinfection of water contaminated with *E. coli* by combination of electrolysis and photochemical treatment: Role of electrode material. N. Barashkov, T. Sakhno, I. Irgibayeva

ENVR **463.** Study of the redox and optical properties of NOM with different origin and pre-treatments. S. Orsetti, E. Subdiaga, D.L. Macalady, S.B. Haderlein

ENVR **464.** Engineering superparamagnetic iron oxide nanocrystals for environmental applications. W. Li, S. Lee, J. Wu, Y. Jiang, C. Kim, C.H. Hinton, J.D. Fortner

ENVR **465.** Mineralization of oxalic acid via advanced oxidation technologies. Y. Kim, H. Kwon, J. Kim, S. Choi

ENVR **466.** Effect of pH on the activation of persulfate by zero-valent iron. Y. Kim, Y. Luo, S. Woo, M. Kim, W. Lim

ENVR **467.** Degradation of tetracycline in synthesized wastewater using immobilized TiO₂ on rotating corrugated aluminum drum. R. Bautista, W. Anderson, S. Pagsuyoin

ENVR **468.** Dissolved organic matter mediated photolysis of 17 α -ethynylestradiol. M.M. Freiburger, S.N. Eustis

ENVR **469.** Changes in redox properties of humic acid upon sorption to alumina. S. Orsetti, E. Subdiaga, S.B. Haderlein

ENVR **470.** Environmental fate of iron: study of the effect of the chelating and reductive properties of humic acids. J.R. Borgatta, J.G. Navea

ENVR **471.** Selective removal of As in heavy metal mixture solution using synthetic Fe-hydroxide. J. Kim, Y. Kim, J. Geum, J. Hwang

ENVR **472.** Characterization of α -Fe₂O₃ nanoparticles for removal of chemical warfare agent simulants. J.R. Soliz, W.O. Gordon, A. Balboa, J. Mahle, A.J. Hauser, K.M. Bussmann, M.S. Osofsky, C.J. Karwacki

ENVR **473.** Isotherm and kinetic studies on the adsorption of humic acid fractions onto clay minerals. M. Khalaf, M. Elsayed, J. Rice

ENVR **474.** Lead extraction from wastewater streams using diethylphosphatoethyl functionalized mesoporous silica. C. Gunathilake, M. Jaroniec, S. Huang, M. Kadanapitiye

ENVR **475.** New porous MgO-ZnO sorbent to capture CO₂ at 473 K. J. Zhu, Y. Li, Y. Wang

ENVR **476.** Interaction of tetracycline antibiotics with nanocarbonics. H. Juffer, E.E. Mojica

ENVR **477.** Derivatization of chlorinated phenols (CPs) for their detection and analysis by Nuclear Magnetic Resonance Spectroscopy. S. Hok, R.N. Leif, C.A. Valdez

ENVR **478.** Characterizing phenolic compounds by LC/MS in New Hampshire sugar maple sap. E. Brady, W.C. Shortle, M. Carlson, B. Rock, S. Tomellini

ENVR **479.** Distribution of di(2-ethylhexyl) phthalate (DEHP) in sediments of the Kaohsiung Ocean Disposal Site, Taiwan. C. Chen, C. Chen, Y. Ju, C. Hung, C. Dong

ENVR **480.** Effectiveness of *Eucalyptus Globulus* extract as an insect repellent. S. Bommakanti

ENVR **481.** Non-destructive screening of collagen content in archaeological bone samples using hand-held Raman spectroscopy. B.J. Vesper, M.D. Colvard, G.A. Cordell, W.J. Pestle

ENVR **482.** Degradation of polychlorinated biphenyls using magnesium/carbon with Ethanol/Ethyl Lactate solvent system and its potential applications for contaminated soil. F.M. Zullo, A. Almutairi, D.E. Richardson, C. Clausen, C. Yestrebtsky

ENVR **483.** Using an artificial oil platform to study the dissolution rates of different PAHs from micron sized droplets. K.A. Sandoval

ENVR **484.** Solid phase extraction of naproxen in environmental samples using molecularly imprinted polymer sorbents. R. Wise, E.E. Mojica

ENVR **485.** Analysis of continuous-flow column and batch bottle microcosm perchloroethylene biodegradation treatability studies. E.M. Driver, J. Roberts, P. Dollar, M. Charles, P. Hurst, R.U. Halden

ENVR **486.** Elemental distribution in influent, biosolids, and effluent of five wastewater treatment plants in Savannah, Georgia, USA. K. Sajwan, K. Ballou, T. Newsome, T. Morris, K. Meadows, B.G. Loganathan

ENVR **487.** Photo-enhanced biodegradation of a test substance using artificial sunlight with a ready biodegradation test design. S.P. McLaughlin, T. Timmons, A. Griffith, K. Malekani

ENVR **488.** *Triumfetta semitriloba mucilage* a promising natural flocculant for water treatment. L.G. Romero, A. Araya, J. Valverde, J. Jiménez, P. Rojas, A. Acuña

ENVR **489.** Phytotoxicity of copper nanowires in environmentally relevant species. D.E. Gorka, K.A. Marsh, P. Flowers, B.J. Wiley, J. Liu

ENVR **490.** Effects of environmental contaminants on the weathering of stone cultural properties in South Korea. J. Jung, M. Jung, B. Shon, K. Yoo, Y. Phee, H. Lim

ENVR **491.** Evaluating the operation of an enhanced acquisition system for conducting vapor pressure measurements on volatile organic compounds (VOCs). S. Abernathy

ENVR **492.** New technique for ppt levels of mercury in air and water. J.N. Driscoll, J.L. MacLachlan

ENVR **493.** Emissions changes of nitrous oxide from soil of native shrub forest in Brazil shifted to soybean plantation. C. Wilches, T. Tavares, S. Oliva, D. Vasconcellos, C. Carvalho

ENVR **494.** Illicit drugs in the air of three Northern European cities. A. Cecinato, C. Balducci, M. Perilli, R. Krejci, C. Johansson, D.C. Green, P. Pantelidis

- ENVR **495.** Illicit drugs in the indoor air. **A. Cecinato, C. Balducci, M. Perilli, P. Romagnoli**
- ENVR **496.** Comparison of various chemical scrubbing agents used in the simultaneous removal of SO₂ and NO_x in simulated flue gas systems. **Y.G. Adewuyi**
- ENVR **497.** Particle size distributions of trace elements in a community near industrial and traffic sources. **I. Han, Y. Guo, M. Afshar**
- ENVR **498.** Withdrawn.
- ENVR **499.** Withdrawn.
- ENVR **500.** Zinc-glutamate metal organic framework catalyst for the cycloaddition of CO₂ with epoxides. **A. Cherian K, K. Hwang, D. Park**
- ENVR **501.** Development of DMC synthesis process using adsorptive copper-based catalysts. **J. Moon, N. Yoo, J. Woo, Y. Park, H. Kim, D. Chun, G. Jin**
- ENVR **502.** Synthesis of metal-organic porous catalysts and their catalytic properties for the synthesis of propylene carbonate through CO₂ fixation to propylene oxide. **Y. Park, H. Kim, J. Moon, D. Chun**
- ENVR **503.** Mn-Fe/TiO₂ catalysts synthesized by deposition precipitation — promising for SCR of NO with NH₃ at low temperatures. **L. Schill, S. Putluru, R. Fehrmann, A.D. Jensen**
- ENVR **504.** Promoted V₂O₅/TiO₂ catalysts for selective catalytic reduction of NO with NH₃. **P. Siva Sankar Reddy, L. Schill, A.D. Jensen, R. Fehrmann**
- ENVR **505.** Selective gas absorption by ionic liquids. **R. Fehrmann, A. Riisager, S. Mossin, P.L. Thomassen, H. Kolding, A. Kunov-Kruse**
- ENVR **506.** Conversion of flue gas NO_x to nitric acid using ionic liquids — an optimized NO_x abatement strategy. **P. Thomassen, S. Mossin, A. Riisager, R. Fehrmann**
- ENVR **507.** Determining electronic waste flows. **J.A. Glaser**
- ENVR **509.** Water quality change along urbanization processes according to pesticides and PPCPs distribution within different population area in Suzhou, China. **S. Qin, H. Jeong**
- ENVR **510.** Polybenzoxazine-based carbon aerogel for carbon dioxide capture. **N. Jungsawat, U. Suriyaphradilok**
- ENVR **511.** Algal toxin photodegradation in coastal and marine environments. **K.M. Parker, W. Mitch**
- ENVR **512.** Different approaches of surface treatment on activated carbon for CO₂ captured enhancement. **N. Thongwicht, U. Suriyaphradilok**
- ENVR **513.** Ecotoxicological risk assessment of pesticidal persistent organic pollutants in the surface riverine water from eastern and north-eastern part of India. **P. Chakraborty, S. Khuman, S. Selvaraj, B. Loganathan**
- ENVR **514.** Carbohydrate aldehydes as homobifunctional cross-linker analogues for biopolymer stabilization and immobilized enzyme systems. **D.E. Wong, J.M. Goddard**
- ENVR **515.** Single particle ICP-MS (SP-ICP-MS) for the detection of metal-based nanoparticles in environmental matrices. **L. Pitts, C. Stephan, A. Hineman**
- ENVR **516.** Wastewater treatment using an integrated fixed-film activated sludge-sequencing batch biofilm reactor (IFAS-SBR): Impact of carbon nitrogen ratio on microbial population dynamics. **Y. Shao, Y. Shi, A. Mohammed, Y. Liu**

Section A

Boston Convention & Exhibition Center
Hall C

Green Chemistry and the Environment

Cosponsored by YCC

A. M. Balu, R. Luque, S. O. Obare, *Organizers*

6:00 - 8:00

- ENVR **517.** Selective oxofunctionalization of aliphatic compounds by semiconductor-based heterogeneous photocatalysis. **D. Contreras, A. Henriquez, F. Benitez, L. Cornejo, H.D. Mansilla, J. Freer**
- ENVR **518.** Crystallographic studies of fully dehydrated and partially Zn²⁺-exchanged zeolites Y (FAU, Si/Al = 1.56) depending on Zn²⁺ concentration of aqueous solution during exchange. **D. Moon, H. Kim, H. Lee, S. Choi, J. Kim, Y. Kim, W. Lim**
- ENVR **519.** Crystallographic determination of Mn²⁺-ion exchange sites in zeolite Y (FAU, Si/Al = 1.56). **D. Moon, S. Seo, J. Seo, H. Lee, H. Kim, C. Lee, W. Lim**
- ENVR **520.** Single-crystal structures of Cs⁺-exchanged Zeolite Y: dependence on Cs⁺ concentration of aqueous solution during exchange. **H. Kim, H. Lee, D. Moon, D. Chung, E. Lee, K. Kim, K. Lee, W. Lim**
- ENVR **521.** Investigation of the thermal behavior of magnesium ammonium phosphate hexahydrate. **M.V. Ramlogan, A. Rouff**
- ENVR **522.** Assessing quality of herbal medicines contaminated by heavy metals. **F. Hassaine-Sadi**
- ENVR **523.** Sustainable dyeing technique using environmental friendly solvents to eliminate waste streams from coloration of cotton. **B. Wang, L. Chen, X. Ruan, J. Chen, Y. Yang**
- ENVR **524.** Sustainable and hydrolysis-free dyeing process for polyalactic acid using nonaqueous medium. **S. Xu, J. Chen, B. Wang, Y. Yang**
- ENVR **525.** Non-toxic, renewable, and cost-effective crosslinking system based on citric acid and xylitol as a replacement of the formaldehyde-releasing N-methylol crosslinkers. **J. Liu, B. Wang, J. Chen, X. Xu, Y. Yang**

Section A

Boston Convention & Exhibition Center
Hall C

Heterogeneous Catalysis for Environmental Applications

Cosponsored by CATL

S. Zhao, A. Orlov, A. Savara, *Organizer*

6:00 - 8:00

- ENVR **526.** Withdrawn.
- ENVR **527.** Application of Fe₃O₄ activated persulfate oxidation for the degradation PAHs in sediments. **C. Hung, C. Chen, C. Chen, Y. Jhuang, C. Dong**
- ENVR **528.** Heterogeneous catalytic conversion of biomass-derived vicinal di-ols to epoxides. **T. Kim, J. Baek, C. Song, Y. Yun, D. Yun, W. Kim, J. Han, J. Yi**
- ENVR **529.** Infrared heating synthesis of carbon nitride nanorods with enhanced photocatalytic activities. **H. Li, M. Chen**

Section A

Boston Convention & Exhibition Center
Hall C

Hydrothermal Carbonization: Possibilities and Limits for Feedstocks, Processes and Applications

Cosponsored by AGRO

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)
S. Chang, J. A. Libra, C. Coronella, K. Ro, *Organizers*

6:00 - 8:00

- ENVR **530.** Withdrawn.
- ENVR **531.** Optimization of activated carbons for supercapacitors from hydrothermally carbonized sugars. **K. Lee, W. Hao, E. Björkman, F. Bjorefors, A.M. Andersson, N. Hedin**
- ENVR **532.** Herbicide sorption capacities of chars made from animal manures and food waste. **S. Lee, K. Ro, S. Bae**

Section A

Boston Convention & Exhibition Center
Hall C

Nano-Enabled Environmental Technologies

Financially supported by Boston University, Division of Materials Science & Engineering
J. L. Goldfarb, K. Doudrik, K. D. Hristovski, *Organizer*

6:00 - 8:00

- ENVR **533.** Aerogel catalysts for direct remediation of NH₃ malodor in air. **H. Chen, W. Han, Z. Liu, K.L. Yeung**
- ENVR **534.** Nanometal oxides as potential remediating materials in removing heavy metals in water samples. **M. Qiu, E.E. Mojica**

Section A

Boston Convention & Exhibition Center
Hall C

New Challenges in Water Quality, Treatment, Reuse and Sustainability: Chemistry and Application of Advanced Oxidation Processes for Removal of Contaminants of Concern and Transformation Products

Cosponsored by CEI

R. de Fatima Peralta Muniz Moriera, G. Li Puma, D. Minakata, K. E. O'Shea, D. D. Dionysiou, *Organizers*

6:00 - 8:00

- ENVR **535.** Decomposition of perfluorooctanoic acid by palladium doped nanoscale zerovalent iron conjugated with persulfate and peroxy-monosulfate. **W.A. Lawal, H. Choi**
- ENVR **536.** Regional distribution of styrene oligomer generated from polystyrene surrounding Japan. **B. Kwon, K. Koizumi, A. Okabe, H. Sato, S. Chung, D.M. Karl, M. Nishimura, Y. Kodera, K. Saïdo**
- ENVR **537.** Photolytic and photocatalytic decomposition of pharmaceuticals in water: Introduction of UV-LEDs and impact of wavelengths. **M. Eskandarian, M. Fazli, M. Rasoulfard, H. Choi**
- ENVR **538.** Comparative study on the catalytic degradation of paracetamol by Pd-TiO₂ and TiO₂ induced advanced oxidation processes. **A. Ziyilan Yavas**
- ENVR **539.** Fenton reaction driven by catechols. **D. Contreras, A. Henriquez, V. Melin, P. Salgado, H.D. Mansilla, L. Cornejo**
- ENVR **540.** Oxidation of three selected emerging contaminants by persulfate ion coupled with UV irradiation. **J. Benitez, F. Real, J. Acero, F. Casas**
- ENVR **541.** Evaluation of sensitizing effect of methyl red in the photocatalytic degradation of diclofenac under natural sunlight. **J. Diaz-Angulo, M. Mueses, F. Machuca-Martinez**
- ENVR **542.** TiO₂-graphene composites for the degradation of pollutants in aqueous and gaseous medium. **J. Suave, J. Angelo, L. Andrade, R.F. Moreira, A. Mendes**
- ENVR **543.** Photocatalytic oxidation of gentisic acid on ZnO using UVA and solar light. **H.D. Mansilla, K. Antil-Martini, D. Contreras, J. Yanez, L. Cornejo**
- ENVR **544.** Experimental evaluation, modeling, and simulation of a new pilot-scale photocatalytic solar reactor for wastewater treatment. **M.Á. Mueses, K.S. Ochoa-Gutiérrez, F. Machuca-Martinez, G. Li Puma**
- ENVR **545.** Degradation of commercial drugs with a solar flat plate reactor by means of supported TiO₂ - based photocatalysis. **J.A. Colina-Marquez, F. Machuca-Martinez, M.Á. Mueses**
- ENVR **546.** Advanced oxidation processes for sulfur molecules removal with Fe-Mo/C catalysts. **A. Barbosa Lopez, W. Licona, A. Alvarez**
- ENVR **547.** Evaluation of the catalytic effect of the ozone/graphene process: Comparison of GO, nGO, and oGO. **H. Oh, Y. Yoon, Y. Ahn, M. Kwon, W. Park, W. Yang, J. Kang**
- ENVR **548.** Reaction kinetics, decomposition pathways, and reactor modeling of anthraquinone dye reactive Blue 19 oxidation using ozone and UV radiation. **M. Lovato, M. Fiasconaro, C. Martin**
- ENVR **549.** Photocatalytic performance of WO₃/TiO₂-N on the degradation of diclofenac solution under visible light radiation. **A. Hernandez-Ramirez, A. Cordero-Garcia, M. Rodriguez-Ramirez, E. Ruiz-Ruiz, M. Villanueva-Rodriguez, L. Hinojosa-Reyes, J. Guzman-Mar**
- ENVR **550.** Enhanced degradation rate of emerging contaminants using luminescent materials promoted visible light active photocatalyst. **O. Sacco, D. Sannino, V. Vaiano, P. Ciambelli**
- ENVR **551.** Solar photocatalytic treatment of commercial dicloxacillin using a pilot-scale CPC reactor. **A. Arce-Sarria, H.L. Otálvaro-Marín, F. Machuca-Martinez, M.Á. Mueses, J.A. Colina-Marquez, A. Hernandez-Ramirez**
- ENVR **552.** Organotitanias: New approaches based in hybrid titanias for photocatalytic and solar cell applications. **M. Rico, A.E. Sepulveda, C. Ezquerro, E. Lalinde, E. Serrano, J.R. Berenguer, J. Garcia Martinez**
- ENVR **553.** Comparative study for the removal and destruction of pentachlorophenol using activated magnesium treatment systems. **A. Garbou, P.M. Cole, C. Clausen, C. Yestrebksy**
- ENVR **554.** Biosorption of phenolic compounds from aqueous solutions using marine macroalgae. **A. Hernandez-Vega, S. Marrero, C. Declet, L. Diaz, A. Navarro**
- ENVR **555.** Occurrence of glyphosate in agricultural farm drainage waters. **B.G. Loganathan, P. Yerneni, K. Sajwan**

Section A

Boston Convention & Exhibition Center

Hall C

Reclamation, Remediation, Restoration: Novel Approaches to Environmental Challenges

Cosponsored by AGRO

L. S. Lee, M. Mashtare, L. Royer, *Organizers*

6:00 - 8:00

ENVR 556. Sulfamethazine adsorption isotherms and kinetics with hypercrosslinked polymer MN250 at varying ionic strengths. **M.E. Grimm**

ENVR 557. Application of superoxide chemistry to ocean acidification. **M. Johnson**

Section A

Boston Convention & Exhibition Center

Hall C

Resource Recovery and Contaminant Elimination in Waste Streams of Increasing Concern

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)

T. H. Boyer, C. Huang, *Organizers*

6:00 - 8:00

ENVR 558. Removal of Cr(VI) using lignin and sericin beads. **K. Lee, H. Kwak, H. Yun**

ENVR 559. Strategic and rare earth elements in produced waters. **J. Rajterowski, J. Renew**

ENVR 560. Screening the effects of ligand chemistry and geometry on rare earth element partitioning from saline solutions to functionalized adsorbents. **C. Noack, K. Perkins, N. Washburn, D.A. Dzombak, A. Karamalidis**

Section A

Boston Convention & Exhibition Center

Hall C

Sensing of Environmentally Relevant Contaminants

Cosponsored by AGRO

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)

B. P. Chaplin, D. Jassby, *Organizers*

6:00 - 8:00

ENVR 561. Ratiometric Cu(II) sensor: Design and synthesis of a Zn(II)-chelator to minimize interference with Cu(II) sensing. **M. Abdalrahman**

Section A

Boston Convention & Exhibition Center

Hall C

Using Passive Sampling Techniques to Detect Organic Contaminants

Cosponsored by AGRO and ORGN

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)

C. A. McDonough, R. Lohmann, *Organizer*

6:00 - 8:00

ENVR 562. Evaluating the effectiveness of passive sampling as a surrogate for organism bioaccumulation. **A. Joyce, R.M. Burgess**

ENVR 563. Polyethylene: An alternative passive sampler for monitoring fluorotelomer alcohol. **E. Dixon-Anderson, R. Lohmann**

ENVR 564. Non-granular graphitic carbon passive samplers. **P. Benedetti, E. Guerriero, C. Crescenzi**

ENVR 565. Spatial distribution and source identification of dissolved PCBs, OCPs, and PAHs in the surface water of the Narragansett Bay Watershed using passive polyethylene samplers. **W. Zhao, M. Cai, D. Adelman, R. Lohmann**

THURSDAY MORNING

Section B

Boston Park Plaza Hotel and Towers

Tremont Room

Advances in Chemistry for Carbon Capture, Utilization and Sequestration

Cosponsored by ENFL

P. Fennell, N. Florin, M. Zhao, *Organizers*

8:00 ENVR 566. Thermodynamic properties of carbon dioxide clathrate hydrates toward CCUS application. **R. Belosludov, O. Subbotin, R. Zhdanov, V. Belosludov, Y. Kawazoe**

8:20 ENVR 567. Withdrawn.

8:40 ENVR 568. Analysis of nitrosamines in amine-based CO₂ capture. **M. Combs, J. Thompson, K. Liu**

9:00 ENVR 569. New approach to carbon dioxide utilization: The carbon molten air battery. **J.F. Stuart, J. Lau, J. Ren, F. Li, M. Lefler, S.L. Licht**

9:20 ENVR 570. Effective CO₂ capture by covalent organic polymers through amine binding and N₂ rejection. **J. Byun, H.A. Patel, D. Thirion, E. Ozdemir, S. Subramanian, C.T. Yavuz**

9:40 Intermission.

9:55 ENVR 571. CO₂ capture using metal oxyhydroxide-biochar nanocomposites. **A. Creamer, B. Gao**

10:15 ENVR 572. CO₂ solubility performance of deep eutectic solvents. **M. Atilhan, S. Aparicio-Martinez, R. Ullah**

10:35 ENVR 573. Minimizing nitrosamine formation in amine-based post-combustion CO₂ capture systems by amine selection. **N. Dai**

10:55 ENVR 574. Reactivity of CO₂ in molten alkali carbonates: A DFT study. **D. Corradini, F. Coudert, R. Vuilleumier**

11:15 ENVR 575. Ag@TiO₂/Graphene catalyst for CO₂ electroreduction. **L. Dawei, H. Xu, L. Zhang, H. Wang**

Section C

Boston Park Plaza Hotel and Towers

Berkeley/Clarendon Room

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Designs: From Molecules to Functional Materials

Cosponsored by CEI, ENFL, ORGN and PHYS

K. Rajeshwar, V. I. Vullev, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 576. Challenges to the use of anthocyanins as natural coloring agents and anti-oxidants. **F.H. Quina, C. Pacheco da Silva, B. Held, V. Oliveira Silva**

8:45 ENVR 577. Nitrotyrene derivatives for bioinspired charge-transfer system. **E.M. Espinoza, B. Xia, J.M. Larsen, V.I. Vullev**

9:05 ENVR 578. Erythrocyte-derived nanoparticles for actively targeted near infrared imaging of cancer biomarkers. **J. Mac, V. Nunez, B. Bahmani, Y. Guerrero, V.I. Vullev, B. Anvari**

9:25 ENVR 579. Transglutaminase-modified regenerated protein materials and their potential application in tissue engineering. **L. Cui, J. Gong, X. Fan, P. Wang, Q. Wang**

9:45 Intermission.

10:00 ENVR 580. Bioinspired superhydrophobic surfaces: From molecule to materials. **F. Guittard**

10:40 ENVR 581. Sticky coatings: Design and synthesis of functionalizable polymeric interfaces. **A. Sanyal**

11:20 ENVR 582. Nature-inspired synthesis of hybrid nanomaterials and nanoparticles based on a smart use of natural hyperbranched polyelectrolytes – humic substances. **I.V. Perminova, A.B. Volikov, S. Ponomarenko, A.Y. Polyakov, E.A. Shirshin, V.A. Lebedev, E.A. Goodilin, K. Hatfield**

11:40 ENVR 583. Characterization of metabolic changes in *Escherichia coli* under nitrate limitation. **E. Match, D. Butryn, M. Ghafari, D.S. Aga, G.E. Atilla-Gokcumen, B.Z. Haznedaroglu**

Section D

Boston Park Plaza Hotel and Towers

Beacon Hill Room

Resource Recovery and Contaminant Elimination in Waste Streams of Increasing Concern

Nutrient Recovery: Wastewater and Organic Byproducts

Financially supported by AEESP (Association of Environmental Engineering and Science Professors)

T. H. Boyer, C. Huang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 584. Efficient phosphate remediation using existing wastewater treatment plant technology. **D. Riccardi, C. Van Cleave, A.S. Hood, L.M. Pegram, D. Michael**

8:30 ENVR 585. Development of anion exchange resins using various waste lignocellulosic materials and environment friendly methods for the removal of phosphate from water. **M. Wazne**

8:55 ENVR 586. Withdrawn.

9:20 Intermission.

9:35 ENVR 587. Interaction of trace elements with struvite during phosphorus recovery from contaminated water. **A. Rouff**

10:10 ENVR 588. Phosphorus speciation in wastewater biosolids for efficient phosphorus recovery. **C.F. Gutierrez, L.E. Katz, K. Kinney**

10:35 ENVR 589. Recovering phosphorus from poultry litter: Impact of organic matter on recovery. **U. Shashvatt, K.P. Mangalgi, L.M. Blaney**

11:00 Panel Discussion.

Section E

Boston Park Plaza Hotel and Towers

Stuart Room

Environmental Transformation of Nanoparticles: Processes, Mechanisms, and Ecological Impacts

Physicochemical Transformations

M. Cledon, K. D. Hristovski, P. Laresse-Casanova, *Organizers*

B. Lau, W. Yan, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 590. Photo-induced transformations of polymeric coatings on gold nanoparticles. **S.M. Louie, E.A. McGivney, K.B. Gregory, V.A. Hackley**

8:30 ENVR 591. Influence of solution chemistry and protein corona on the interactions of silver nanoparticles with model biological membranes: Implications for nanotoxicity. **Q. Wang, M. Lim, K. Chen**

8:50 ENVR 592. Aggregation of chemical mechanical planarization nanoparticles and their interactions with model cell membranes. **X. Liu, K. Chen**

9:10 ENVR 593. Exchange of surfactant by natural organic matter on the surfaces of multiwalled carbon nanotubes. **X. Chang, D.C. Bouchard**

9:30 ENVR 594. Catalytic activity of interfacial iron on mineral nanoparticles: Effects of aqueous iron precursors and mineral substrates. **Y. Li, W. Yan**

9:50 Intermission.

10:05 ENVR 595. Aggregation kinetics of carbon nanotube and metal or metal oxide nanohybrids in aquatic environment. **D. Das, I.V. Sabaraya, N. Aich, N.B. Saleh**

10:25 ENVR 596. Nano-bio interaction: Influence of carbon nanotubes on virus like particle (VLP) transport through saturated porous media. **D. Das, A. Afroz, J. Lednický, T. Sabo-Attwood, N.B. Saleh**

10:45 ENVR 597. Methods for determining the weighted factors controlling silver nanoparticle size, state, and mass distribution in corrosive environmental waters using in situ measurements. **J.M. Pettibone, J. Liu**

11:05 ENVR 598. Detection and quantification of engineered metal nanoparticles in municipal wastewaters and biosolids. **M.M. Azodi, F. Piccapietra, N. Tufenkji, S. Ghoshal**

11:25 ENVR 599. Particles and VOC emissions properties from recent gasoline DI and DPF diesel vehicles. **H. Yamada, S. Inomata, H. Tanimoto**

11:45 ENVR 600. Formation, aggregation, and deposition of NOM-iron colloids formed at anoxic-oxic interfaces. **P. Liao, S. Yuan, D. Giammar, C. Pan**

Section F

Boston Park Plaza Hotel and Towers

Cambridge Room

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

Photo-Assisted Processes

Cosponsored by AGRO

F. A. Monterrubbio, I. S. Sardonil, V. K. Sharma, *Organizers*

M. A. Oturan, H. Zhang, *Presiding*

8:00 ENVR 601. Withdrawn.

8:20 ENVR 602. Simultaneously photoelectrochemical oxidation of azo dye and generation of hydrogen via C-N co-doped TiO₂ nanotube arrays. **Y. Peng, H. Chen, Q. Sun, Y. Chiu**

8:40 ENVR 603. Copper recovery combined with electricity production in a photoelectrochemical device. **C. He, L. Hu, W. Pan, Y. Hou**

9:00 ENVR 604. Salicylic acid degradation and mineralization by coupling advanced oxidation processes: Photo electro Fenton, anodic oxidation and heterogeneous photocatalysis. **B. Garza**, A. El-Ghenymy, E. Brillas, A. Hernandez-Ramirez, **E. Ruiz**

9:20 Intermission.

9:35 ENVR 605. Treatment of biologically treated landfill leachate by solar photoelectro-Fenton system using a recirculation reactor. **Z. Ye**, J. Geng, M. Chen, L. Wu, Y. Qian, L. Yang, **H. Zhang**

9:55 ENVR 606. Solar photoelectro-Fenton degradation of the antibiotic metronidazole using a flow plant with Pt/air-diffusion cell and a CPC photo-reactor. **T. Perez**, S. Garcia-Segura, A. El-Ghenymy, J.L. Nava, E. Brillas

10:15 ENVR 607. Solar photoelectro-Fenton treatment of organic pollutants in waters. **E. Brillas**

11:00 Concluding Remarks.

Biomonitoring for Pesticide Exposures

Sponsored by AGRO, Cosponsored by ENVR

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Sponsored by PHYS, Cosponsored by ENVR

Degradation of Halogenated Compounds in the Environment

Sponsored by AGRO, Cosponsored by ENVR

Spray Application Technology

Sponsored by AGRO, Cosponsored by ENVR

THURSDAY AFTERNOON

Data to Decisions: Software Solutions for Modern Analytical Workflows

Sponsored by AGRO, Cosponsored by ANYL and ENVR

Degradation of Halogenated Compounds in the Environment

Sponsored by AGRO, Cosponsored by ENVR

Spray Application Technology

Sponsored by AGRO, Cosponsored by ENVR

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FLUO

Division of Fluorine Chemistry

V. Petrov, Program Chair

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 208

Radiochemistry

Cosponsored by MEDI

N. Vasdev, Organizer

A. B. Packard, G. D. Tamagnan, Organizers, Presiding

S. V. Selivanova, Presiding

8:00 Introductory Remarks.

8:10 FLUO 1. Translational PET neuroimaging and drug development. **C. Haldin**

8:40 FLUO 2. General method for radiolabeling nonactivated arenes with [¹⁸F]fluoride and its transition to clinical use. **S. Liang**, B.H. Rotstein, N. Stephenson, L. Wang, N. Vasdev

9:00 FLUO 3. Comparison of several ¹⁹F-rhodamines for myocardial perfusion imaging. **V. Akurathi**, S. Zhang, T.S. Treves, A.B. Packard

9:20 FLUO 4. Synthesis of 3-fluoro and 3-iodo-8-hydroxyquinolines as potential PET and SPECT imaging agents for Alzheimer's disease (AD). **R.N. Hanson**

9:40 FLUO 5. New strategies for detecting pain and cancer. **F.T. Chin**

10:00 Intermission.

10:20 FLUO 6. Positron emission tomography: Enabling efficient drug development via in vivo quantification of target engagement. **E. Hostetler**

10:50 FLUO 7. Radiofluorinated aporphines: Selective D₂ agonist radioligands for brain imaging. **A.W. Sromek**, S. Zhang, V. Akurathi, Y. Chen, A.B. Packard, J.L. Neumeyer

11:10 FLUO 8. [C-11]Carbon disulfide: A versatile synthon for C-11 radiolabeling. **T. Haywood**, S. Kealey, C. Plisson, L. Allott, G. Smith, **P. Miller**

11:30 FLUO 9. Important parameters governing diaryliodonium salt radiofluorination reactions. **S.G. DiMaggio**

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 102B

Radiochemistry

Cosponsored by MEDI

G. D. Tamagnan, N. Vasdev, Organizers

A. B. Packard, Organizer, Presiding

S. V. Selivanova, Presiding

1:00 FLUO 10. Development of a fibrin-targeted radiopharmaceutical: Effect of chelate type, linker, and radiometal on in vivo efficacy. **P. Caravan**

1:20 FLUO 11. Radiometal labeling biomolecules for detection and therapy of disease. **J. Dearing**

1:40 FLUO 12. Effect of charge and nitrogen donors on the stability and labeling of fac-[^{99m}Tc(CO)₃]²⁺ + 1 complexes. **T.R. Hayes**, W.S. Slocumb, P.A. Lyon, C.L. Barnes, P.D. Benny

2:00 FLUO 13. Rhenium-cyclized somatostatin peptide analog: Synthesis and receptor affinity comparison. **Y. Li**, F. Gallazzi, M. Kuchuk, M.R. Lewis, S.S. Jurisson, **H.M. Hennkens**

2:20 FLUO 14. Site-specifically modified ⁸⁹Zr-labeled antibodies for PET and multimodal PET/optical imaging. **B.M. Zeglis**

2:40 Intermission.

3:00 FLUO 15. Click chemistry functionalization of heat induced radio-labeled (HIR) Feraheme nanoparticles. **L. Josephson**, H. Yuan

3:20 FLUO 16. 1,2,3-Triazole stabilized "click" radiopeptidomimetics for improved tumor targeting. **T.L. Mindt**, I.E. Valverde, C.A. Fischer, S. Vomstein, A. Bauman

3:40 FLUO 17. From therapeutics to theranostics: Synthesis and biological evaluation of porphyrin radiotracers. **F. Bryden**, G. Entract, H. Savoie, E.V. Rosca, R.W. Boyle

4:00 FLUO 18. Bioorthogonal ⁶⁸Ga-labeling approach to pretargeted in vivo imaging. **L. Carroll**, E. Aboagye

4:20 Concluding Remarks.

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 50

Radiochemistry

Cosponsored by MEDI

A. B. Packard, Organizer

G. D. Tamagnan, N. Vasdev, Organizers, Presiding

8:00 Introductory Remarks.

8:10 FLUO 19. Using the "matched pair" principle in radionuclide development for theranostics. **N. van der Meulen**

8:30 FLUO 20. Versatile method for producing multiple radiometals from a single cyclotron target. **E. Oehlke**, C. Hoehr, X. Hou, V. Hanemaayer, S. Zeisler, G. Dias, M.J. Adam, T.J. Ruth, A. Celler, K. Buckley, F. Benard, **P. Schaffer**

9:00 FLUO 21. Bringing radiotracing to titanium-based antineoplastics: Solid phase radiosynthesis, PET, and ex-vivo evaluation of antitumor agent [⁴⁵Ti] (salan)Ti(dipic). **G.W. Severin**, C.H. Nielsen, J. Fonslet, A.I. Jensen, A. Kjaer, **F. Zhuravlev**

9:20 FLUO 22. Cyclotron-produced ^{99m}Tc: From bench to bedside and beyond. **S.V. Selivanova**, E. Lavallée, H. Senta, L. Caouette, A. Zyuzin, B. Guerin, E. Turcotte, R. Lecomte

9:40 FLUO 23. Enhancement of low-energy electron emission in 2-D radioactive films. **A. Pronschinske**, **E.H. Sykes**

10:00 Intermission.

10:20 FLUO 24. Process chemistry for PET/SPECT imaging agents and the development of theranostic drugs. **J.F. Kronauge**

10:50 FLUO 25. Cyclotron production of radiometals in a solution target. **M.K. Pandey**, T.R. Degrado, J. Byrne, H. Jiang, H.P. Engelbrecht, A.B. Packard

11:10 FLUO 26. Collagen-targeted PET probes for pulmonary fibrosis imaging: Effect of the radioisotope on biodistribution. **P.A. desogere**, L. Vargas, T. Rietz, N. Rotile, F. Blasi, H. Day, M. Lanuti, P. Caravan

11:30 FLUO 27. Synthesis of fluorine-18 and gallium-68 positron emission tomography radiotracers in microfluidic reactors. **P. He**, H. Bignell, M. Tam, G. Clemente, B. Burke, N. Estahani, N. Pamme, N. Brown, **S.J. Archibald**

11:50 Concluding Remarks

GEOC

Division of Geochemistry

Y. Jun, Program Chair

SOCIAL EVENTS:

Social Hour and Reception,
5:30 PM: Tuesday

BUSINESS MEETINGS:

Business Meeting, 6:00 PM: Sunday

MONDAY MORNING

Section A

Seaport Hotel and World Trade Center
Beacon Hill 1

Structure & Reactivity of Mineral-Fluid Interfaces

S. N. Kerisit, S. Teich-McGoldrick, Organizers, Presiding

8:30 Introductory Remarks.

8:35 GEOC 1. Impact of ligands on co-precipitation and adsorption with aluminum hydroxide. **L.E. Katz**, K.A. Alfredo, M. Bartolo, I. Gee, J. Herboldt, D. Lawler

9:05 GEOC 2. Structural study of surface complexation of Pb(II) on a high-temperature annealed hematite(1-102) surface. **C. Qiu**, P.J. Eng, J. Stubbs, T.P. Trainor

9:25 GEOC 3. Modeling selenate and selenite adsorption by oxides, clay minerals, and soils using surface complexation models. **S.R. Goldberg**

9:55 GEOC 4. Adsorption to goethite-water interfaces: Molecular and surface complexation models. **L.J. Criscenti**, K. Leung, L.E. Katz

10:15 Intermission.

10:35 GEOC 5. Identifying reactivity factors in nanoparticle and mineral surface models through DFT calculations. **S.E. Mason**

11:05 GEOC 6. Linking adsorption enthalpy to surface reactivity at the mineral-water interface: New insights based on flow-adsorption microcalorimetry (FAMC). **A. Gale**, N. Kabengi

11:25 GEOC 7. Direct probes of mineral/water interfaces. **F. Geiger**

11:45 GEOC 8. Energetics of order-disorder in layered magnesium aluminum double hydroxides with interlayer carbonate. **R. Shivaramaiah**, A. Navrotsky

MONDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Beacon Hill 1

Structure & Reactivity of Mineral-Fluid Interfaces

S. N. Kerisit, S. Teich-McGoldrick, *Organizers, Presiding*

1:30 **GEOC 9.** Goethite nanoparticles in reactive systems. A.M. Stemig, J.H. Strehlau, J.A. Soltis, W. Arnold, R. Penn

2:00 **GEOC 10.** Iron Keggin-ion as a prenucleation cluster to ferrhydrite. M.D. Nyman, O. Sadeghi

2:20 **GEOC 11.** Orientational ordering of carbonate leads to superstructure in vaterite: Modeling and experiment. J. Wang

2:50 **GEOC 12.** Understanding the connection between composition, structure, and reactivity in amorphous precursors. D. Wang, A. Wallace, D. Krogstad, A. Fernandez-Martinez, S. Lin-Gibson

3:20 Intermission.

3:40 **GEOC 13.** Opposing effects of humidity on rhodochrosite surface oxidation. C. Na, Y. Tang, H. Wang, S.T. Martin

4:10 **GEOC 14.** Heteroepitaxial growth of (Cd_xCa_{1-x})CO₃ solid solution at the dolomite (104) surface: AFM and synchrotron X-ray studies. E. Callagon, P. Fenter, S. Lee, N. Sturchio, K.L. Nagy

4:40 **GEOC 15.** Molecular-scale controls on heteroepitaxy at mineral-water interfaces. S.N. Kerisit, S.L. Riechers, X. Man, E.S. Iltou, M.H. Engelhard, L. Kovarik, B. Arey, D.E. Perea, A.R. Felmy, K.M. Rosso

5:00 **GEOC 16.** Growth of barite and celestite as a function of the aqueous cation:anion ratio. J. Bracco, A.G. Stack, S.R. Higgins

GEOC 23. Association of strontium and chromate with quartz sand as a function of phase changes induced by variable water content. W.C. Weaver, T.C. Kibbey, C. Papelis

GEOC 24. Geochemical and mineralogical comparison of soil formation from mine tailings and undisturbed shale and their contribution to stream chemistry, Huff Run Watershed, Ohio. L. Zemanek, E. Herndon, D. Singer

GEOC 25. Effect of aqueous and solid-state calcium on uranium sorption behavior onto MnO-Fe₂O₄ composite. T. Park, J. Min, Y. Choi, M. Baik, S. Do

GEOC 26. Time-integrated, active sampling over 28-days in a contaminated coastal aquifer. I.B. Roll, E.M. Driver, R.U. Halden

GEOC 27. Diurnal fluctuations in groundwater concentrations of hexavalent chromium in a coastal aquifer. I.B. Roll, E.M. Driver, R.U. Halden

GEOC 28. Isotopic approach to characterizing biogeochemical transformations of selenium. A.E. Schellenger, L. Xia, A. Onnis-Hayden, D. Jaisi, P. Laresse-Casanova

GEOC 29. Are algae playing a role in mercury methylation through the production of thiols in aquatic biofilms? M. Leclerc, D. Planas, M. Amyot

GEOC 30. Climate change and the production of methylmercury in coastal sediments. N. Mazrui, E. Seelen, P.H. Balcom, V. Ortiz, B. Dimento, K. Gosnell, C.Y. Chen, B. Jackson, V. Taylor, K. Buckman, R.P. Mason

GEOC 31. Release of oxide oxygen during sorption of aqueous Fe(II) on goethite. P. Yue, P. Joshi, C. Gorski, P. Laresse-Casanova

GEOC 32. Electrochemical oxidation of organic molecules on mineral electrodes. O. Taran

TUESDAY MORNING

Section A

Seaport Hotel and World Trade Center
Beacon Hill 1

Structure & Reactivity of Mineral-Fluid Interfaces

S. N. Kerisit, S. Teich-McGoldrick, *Organizers, Presiding*

8:30 **GEOC 33.** Heterogeneous chemistry of biogenic exudates associated with nutrient acquisition. O. Duckworth

9:00 **GEOC 34.** Molecular-level interactions of organic ligands with iron oxide mineral/water interfaces studied using sum frequency generation (SFG). A.L. Miffitt

9:20 **GEOC 35.** Methane hydrate formation in the presence of clay mineral surfaces. S. Teich-McGoldrick, R.T. Cygan, M.E. Gordon

9:40 **GEOC 36.** Interactions and competitions at small molecule - mineral interfaces. D. Wu, X. Guo, H. Sun, A. Navrotsky

10:00 Intermission.

10:20 **GEOC 37.** U(VI) and Sr(II) sequestration in mesoporous materials: The importance of confined pore spaces. D. Singer, H. Guo, J.A. Davis

10:50 **GEOC 38.** Metal reactivity in abandoned uranium mine wastes. J.M. Cerrato, S. Avasarala, J. Blake, A. Ali, A. Breatley, K. Artyushkova, M. Spilde, J. Lezama-Pacheco

11:20 **GEOC 39.** Withdrawn.

11:40 **GEOC 40.** Spectroscopic evidence for Cr⁶⁺-Fe(II) electron transfer at clay mineral edge and basal sites. M. Bishop, H. Dong, M. Pentrak, J.W. Stucki

12:00 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Beacon Hill 1

Subsurface Geochemistry for Energy & the Environment

Operations and Resources

Cosponsored by ENVR

Y. Jun, C. A. Peters, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 **GEOC 41.** Effect of brine composition in carbon storage environment on arsenic release from arsenopyrite. A. Karamalidis, H. Parthasarathy, D.A. Dzombak

2:15 **GEOC 42.** Alteration of fracture geometries during flow of acidic fluids: Implications for subsurface energy technologies. B. Ellis, W. Fan, M. Tang, K.F. Hayes, W. Xiong, D. Giammar, P. Skemer

2:55 **GEOC 43.** What if? Evaluating geochemical changes to shallow groundwater under simulated carbon dioxide leakage conditions. A. Stichter, J. McCray, A. Wunsch

3:35 Intermission.

3:55 **GEOC 44.** Rare earth element geochemistry of kerogen samples from the Orange Basin. A. Akinlua

4:15 **GEOC 45.** Structural diversity of petroporphyrins and macromolecules isolated mesoproterozoic sedimentary successions and natural petroleum seeps by FT-ICR MS. A.M. McKenna, N. Gueneli, J.J. Brocks, C. Boreham, N. Ohkouchi, H. Chen, L. Krajewski, C. Reddy, D.L. Valentine, M. Kellerman

4:35 **GEOC 46.** Ab initio prediction of subsurface carbonate and hydrate formation. A.M. Chaka, A.R. Felmy

Transformation & Transport of Radionuclides in the Environment

Sponsored by NUCL, Cosponsored by GEOC

WEDNESDAY MORNING

Section A

Seaport Hotel and World Trade Center
Beacon Hill 1

Subsurface Geochemistry for Energy & the Environment

Mineral Reactions in Geologic Carbon Sequestration

Cosponsored by ENVR†

Y. Jun, *Organizer*

C. A. Peters, *Organizer, Presiding*

J. P. Fitts, *Presiding*

8:30 **GEOC 47.** In situ NMR reveals conversion of ¹³CO₂ to metal carbonates and pH monitoring for geosequestration studies. J.K. Moore, J. Surface, P. Skemer, M.S. Conradi, D. Giammar, S.E. Hayes

9:10 **GEOC 48.** Molecular-scale behavior at organo-mineral interfaces under supercritical CO₂ conditions. G.M. Bowers, B. Ferguson, H. Argersinger, N. Loganathan, R.J. Kirkpatrick, D.W. Hoyt, S.D. Burton

9:30 **GEOC 49.** Effect of salinity on CO₂ sequestration through iron bearing minerals. J.C. Dalessandro, K.D. Lammers, M.A. Schoonen, D.R. Strongin

9:50 **GEOC 50.** Probing particle-based crystal growth via dynamic force spectroscopy. X. Zhang, J. Liu, K.M. Rosso, J.J. De Yoreo, M.H. Engelhard, T.C. Droubay, M. Bowden

10:10 Intermission.

10:30 **GEOC 51.** Effects of sulfate and phosphate on seCO₂ saturated brine-biotite interactions: Wettability changes under geologic CO₂ sequestration (GCS) conditions. L. Zhang, Y. Jun

10:50 **GEOC 52.** Capillary pressure - saturation relations for supercritical CO₂ and brine in limestone/dolomite sands: Implications for geologic carbon sequestration in carbonate reservoirs. S. Wang, T. Tokunaga, J. Wan

11:10 **GEOC 53.** Geochemical alterations of carbonate fractures. H. Deng, J.P. Fitts, C.A. Peters

11:30 **GEOC 54.** Investigation on porosity and permeability evolution of Mount Simon sandstone under geological carbon storage conditions: A numerical simulation approach. L. Zhang, Y. Soong, R. Dilmore, C. Lopano

WEDNESDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Beacon Hill 1

Subsurface Geochemistry for Energy & the Environment

Mineral Reactions in Subsurface Energy and Waste Operations

Cosponsored by ENVR†

Y. Jun, *Organizer*

C. A. Peters, *Organizer, Presiding*

H. Deng, *Presiding*

1:30 **GEOC 55.** Evaluating the effects of shale-fluid reactions on produced water chemistry and shale formation permeability. A. Hakala, C. Lopano, A. Paukert, V. Marconi, C. Joseph, P. Scheuermann, S.W. Hedges, G. Guthrie

2:10 **GEOC 56.** Contaminant mobilization from shale during hydrofracturing and gas production. J.P. Fitts, K. Spokas, H. Hunter, C.A. Peters

2:50 **GEOC 57.** New insights into factors controlling bacterial adhesion to oil-water interfaces. S. Ghoshal, A. Akbari, S. Sultana

3:30 Intermission.

3:50 **GEOC 58.** Pyrite-hydraulic fracturing fluid interaction: Hydrolysis and catalysis of dazomet. N. Consolazio, G. Lowry, A. Karamalidis

4:10 **GEOC 59.** Carbonation of wollastonite in a shale matrix. Z. Tao, J.P. Fitts, A. Clarens

4:30 **GEOC 60.** Characterization of concentrated shale gas produced water treated with different water treatment technologies. E. Jang, E. Chung

4:50 **GEOC 61.** Two modes of iodine release of iodine-apatite in aqueous solution: Diffusion and dissolution. Z. Zhang, J. Wang

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

Y. Jun, *Organizer*

8:00 - 10:00

GEOC 17. Fecal sterols and the 15th-century demise of Norse Vikings. T.J. Barrasso, G. de Wet, I. Castañeda, R.S. Bradley

GEOC 18. Debris plastics are sources of chemical contaminations in coast and open sea. K. Saïdo, B. Kwon, S. Chung, A. Okabe, K. Koizumi, K. Kogure, N. Ogawa, D.M. Karl

GEOC 19. Comparing the solubility products of layered Me(II)-Al(III)-hydroxides based on sorption studies with Ni(II), Zn(II), Co(II), Fe(II), and Mn(II). L. Bhattacharya, E. Elzinga

GEOC 20. Role of pH and ionic strength in the structure and morphology of smectite-natural organic matter composite materials. H. Argersinger, B. Ferguson, R.J. Kirkpatrick, B. Arey, G.M. Bowers

GEOC 21. Impacts of sulfuric acid on chemical speciation of arsenic(V) and copper(II) bound to layer-structured minerals. S.P. Hyun, H. Moon, K. Kwon

GEOC 22. Evaluation of the leaching potential of components of brines applied for ice control. J. Wilson, C. Barrett, G. Gunawan, K. Pulido, D. Monge

THURSDAY MORNING

Section A

Seaport Hotel and World Trade Center
Beacon Hill 1

General Geochemistry Session

Y. Jun, *Organizer, Presiding*

8:10 GEOC 62. Europium in phosphogypsum: Solubility, location, and thermodynamic stability. **R. Shivaramaiah**, W. Lee, A. Navrotsky, D. Yu, H. Wu, P. Kim, R. Riman

8:30 GEOC 63. Biological redox cycling of iron in nontronite and its potential application in nitrate removal. **L. Zhao**, H. Dong, R. Kukkadapu

8:50 GEOC 64. Reduction of hexavalent chromium and [Cobalt(III)-EDTA] by thermophilic methanogen *Methanothermobacter thermoautotrophicus*. **R. Singh**, H. Dong, D. Liu, L. Zhao, A. Marts, E. Farquhar, D. Tierney, C. Almquist, B. Briggs

9:20 GEOC 65. Kinetics of Fe^{II}-polyaminocarboxylate oxidation by molecular oxygen. **J. Wilson**, K.J. Farley, R.F. Carbonaro

9:40 Intermission.

10:00 GEOC 66. Variations of soil *n*-alkanes δ D and glycerol dialkyl glycerol tetraethers (GDGTs) distributions along an altitudinal transect from southwest China. **C. Wang**, M.T. Hren, G. Hoke, C. Garziona, J. Liu

10:20 GEOC 67. Model study of the feedbacks between lightning activity and atmospheric temperature and composition changes. **L. Kolomeets**

10:40 GEOC 68. Enhanced indirect photochemistry of dissolved free and combined histidine through association with chromophoric dissolved organic matter. **C. Chu**, R. Lundeen, C.K. Remucal, M. Sander, K.P. Mc Neill

11:00 GEOC 69. Variation of anion concentration in aerosol at Mt. Kinabalu, Sabah, Malaysia. **H. Katsura**

11:20 GEOC 70. Spatial assessment of soil contamination from informal E-waste recycling site in Agbogboshie, Ghana. **V. Kyere**

Section B

Seaport Hotel and World Trade Center
Beacon Hill 2/3

Biogeochemical Cycling of Nutrients & Contaminants in Physically Complex Environments

B. D. Kocar, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 71. Reactivity of biogenic manganese oxides associated with an environmental remediation system at a Superfund site. **O. Duckworth**, M.Y. Andrews, E. Mitchell, T. Gardner, L.A. Sombers, C. Santelli, M.L. Polizzotto

8:55 GEOC 72. Radium adsorption to iron bearing minerals in variable salinity waters. **M.A. Chen**, B.D. Kocar

9:15 GEOC 73. Aqueous sulfide decreases transport of ferrihydrite colloids in anoxic porous media due to production of elemental sulfur. **P. Liao**, S. Yuan

9:35 GEOC 74. Biogeochemical cycling of methylmercury in estuaries. **R.P. Mason**, P.H. Balcom, C.Y. Chen, V. Ortiz, A.T. Schartrup, E. Seelen, E.M. Sunderland

9:55 Intermission.

10:15 GEOC 75. Link between methylmercury and nutrient levels in thaw ponds of the Canadian North. **G. MacMillan**, C. Girard, I. Laurion, J. Chételat, **M. Amyot**

10:35 GEOC 76. Mercury methylation by syntrophs and methanogens in peatlands. **L. Zhang**, X. Liu, S. Sampath, W. Sidelinger, Y. Wang, D. Krabbenhoff, T. Barkay, J. Schaefer, M. Hines

10:55 GEOC 77. Phosphorus at the water-soil interface: Not just phosphate. **M.A. Pasek**

11:15 GEOC 78. Terrestrial carbon sequestration depends on Ca biogeochemistry and forest growth. **W.C. Shortle**, K.T. Smith

11:35 Concluding Remarks

HIST

Division of the History of Chemistry

S. Rasmussen, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Professional Legacy of Henry Hill (see *PROF, Sunday*)

Fifty Years of Innovation: The Legacy of the Westheimer Report (see *MPPG, Tuesday*)

Henry A. Hill Centennial Symposium: Innovation in Polymer Science (see *POLY, Tuesday*)

SOCIAL EVENTS:

Award Banquet, 7:00 PM: Tuesday

BUSINESS MEETINGS:

Business Meeting, 1:30 PM: Sunday

Exec Committee Meeting, 5:00 PM: Sunday

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 50

Edwin Land and Instant Photography: Massachusetts' First National Historic Chemical Landmark

Sponsored by PRES

M. P. Filosa, V. K. Walworth, *Organizers*

J. N. Driscoll, *Organizer, Presiding*

2:00 HIST 1. What does it take to start chemical manufacturing from scratch? **W.C. Hollinsed**

2:30 Panel Discussion.

Professional Legacy of Henry Hill

Sponsored by PROF, Cosponsored by CEPA, CMA, ETHC, HIST†, ORGN, PMSE, POLY†, PRES and SCHB†

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 50

Memories of Henry Hill: His Legacy in Science and in Professional Service

Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES†, PROF and SCHB

J. Hayes, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 HIST 2. Dr. Henry Hill, ACS President 1977: Firsts and leading lights. **J. Hayes**

9:05 HIST 3. Henry Hill's entrepreneurial beginnings. **A.S. Obermayer**

9:35 HIST 4. A Shared Responsibility: Diversity and inclusion at ACS. **J. Titus-Young**

10:05 Intermission.

10:25 HIST 5. Henry Hill: My forerunner as ACS President. **J.S. Francisco**

10:45 HIST 6. Henry Hill: An ACS pioneer. **A.E. Pavlath**

11:15 HIST 7. The legacy of Henry Hill as viewed by a member of the Northeastern ACS Local Section. **D.J. Phillips**

11:40 Panel Discussion.

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 50

HIST Tutorial & General Papers

S. C. Rasmussen, *Organizer, Presiding*

1:00 HIST 8. Science anniversaries 2015: A philatelic celebration. **D. Rabinovich**

1:30 HIST 9. Learning the principles of organic chemistry in context using the historical development of this science. **M.M. Green**

2:00 HIST 11. Autograph books of Tetsuo Nozoe: July 19, 1953 to October 16, 1994. **J. Seeman**

2:30 Intermission.

2:45 HIST 12. From the history of stereochemistry: Louis Pasteur's language for molecular chirality. **J. Gal**

3:15 HIST 13. Legacy of British biochemist Frederick Sanger. **J.S. Jeffers**

3:45 HIST 14. Karl Karlovich Klaus (1796-1864): Discoverer of ruthenium. **D.E. Lewis**

4:15 HIST 15. Early history of polyaniline: Discovery and origins. **S.C. Rasmussen**

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector

Sponsored by SCHB, Cosponsored by CMA, COLL, HIST, I&EC, POLY, PRES and PROF

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

S. C. Rasmussen, *Organizer*

8:00 - 10:00

9, 13-14. See previous listings.

HIST 16. 100 years of service to chemistry in Virginia. **A.M. Sullivan**, K.S. Smetana, L.M. Watkins, J.A. Asper, J.M. Crockett

HIST 17. Aspirin: Incorporating the history of chemistry in the community college classroom. **G. Perkins**

HIST 18. Edwin Land and instant photography: An ACS National Historic Chemical Landmark. **J.L. MacLachlan**, J.N. Driscoll

TUESDAY MORNING

Fifty Years of Innovation: The Legacy of the Westheimer Report

Sponsored by MPPG, Cosponsored by HIST†

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Sponsored by POLY, Cosponsored by HIST, PMSE†, PRES and PROF†

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 50

HIST Award Symposium Honoring Christoph Meinel

G. D. Patterson, *Organizer*

A. J. Roche, *Organizer, Presiding*

1:00 HIST 19. Quiet revolution revisited: Theory vs. practice in nineteenth-century German chemistry. **A.J. Roche**

1:30 HIST 20. Tale of three generations: Interactions between historical context and disciplinary development among German chemists, 1871-1945. **J.A. Johnson**

2:00 HIST 21. Mixed messages: Divergent motives and frontier science at the Hickrill Chemical Research Laboratory. **S.J. Weininger**

2:30 HIST 22. John Tyndall and chemical physics. **W. Brock**

3:00 Intermission.

3:15 HIST 23. History and philosophy as an emergency exit? The case of Maurice Delacoe (1862-1938). **B. van Tiggelen**

3:45 HIST 24. History of recent chemistry: New wine in old flasks? **C. Reinhardt**

4:15 HIST 25. How science historians helped create chemistry as a discipline. **C. Meinel**

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Sponsored by POLY, Cosponsored by HIST, PMSE†, PRES and PROF†

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Division of Industrial and Engineering Chemistry

P. Smith, Program Chair

OTHER SYMPOSIA OF INTEREST:

Analytical Chemistry in Nuclear Technology (see NUCL, Sunday, Monday)

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control (see PMSE, Sunday, Monday, Tuesday)

Industrial Innovations in Polymer Chemistry (see POLY, Monday)

New Advances in Nanostructured Polymeric Membranes for Filtration (see PMSE, Monday, Tuesday)

Ring Opening Polymerization (see POLY, Monday, Thursday)

Ionic Liquids in Polymer Design: from Energy to Health (see POLY, Tuesday, Wednesday, Thursday)

SOCIAL EVENTS:

Luncheon, 11:45 AM: Tuesday

SUNDAY MORNING

Section A

Renaissance Boston Waterfront
Pacific Blrm D

Industrial & Engineering Fellow: Symposium in Honor of Kenneth L. Nash

Solution Chemistry

S. B. Clark, T. C. Shehee, *Organizers*

L. R. Martin, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 1. My time with Professor Nash: Reflections of a junior scientist. J. Braley

8:30 I&EC 2. Game of second chances: A decade's worth of separations. P.R. Zalupski

8:55 I&EC 3. Repeatedly finding new frontiers in f-element solution chemistry. K.L. Nash

9:25 I&EC 4. Assay of selective radio-nuclides using highly specific radiochemical separations and gamma-ray spectrometry with Ge well detectors. M.R. Kriz, J. Cadieux

9:50 Intermission.

10:10 I&EC 5. Covalency in actinyl ions evaluated using oxygen K-edge X-ray absorption spectroscopy and density functional theory. S.G. Minasian, E.R. Batista, C. Booth, J.M. Keith, W.W. Lukens, S.A. Kozimor, R.L. Martin, D.K. Shuh

10:35 I&EC 6. Studies of the protonation and complexation with Ln(III) of N-(2-hydroxyethyl)ethylenediamine-N,N',N'-triacetic acid in aqueous solutions: Temperature effect and coordination analysis. Z. Zhang, X. Li, G.L. Helms, S.B. Clark, L.R. Martin, L. Rao

11:00 I&EC 7. Prospects for improved TALSPEAK holdback reagents based on derivatives of 2,2'-bipyridine-6,6'-dicarboxylic acid. N.E. Uhnak, K.L. Nash

11:25 I&EC 8. Alternative aqueous holdback complexants for trivalent An/Ln differentiation. C.R. Heathman, P.R. Zalupski

11:50 Concluding Remarks.

Section B

Renaissance Boston Waterfront
Pacific Blrm C

Symposium in Honor of the 2013 & 2014 ACS Fellows in the Division of Industrial & Engineering Chemistry

S. Alexandratos, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 I&EC 9. Investigation of CF telomers in response to changing regulations, from molecules to application. J.M. Smith

8:55 I&EC 10. Molecular recognition, bioseparations, screening, and diagnostics: A cereer in I. R.C. Willson

9:15 I&EC 11. Effect of promoter type and amount on Fischer-Tropsch synthesis using iron catalysts on carbon supports. D. Dadyburjor

9:35 I&EC 12. Adventures in molybdenum oxide chemistry. A.W. Ablett, C.K. Perkin, N.F. Materer, B. Kiran

9:55 Intermission.

10:10 I&EC 13. Spectroelectrochemical sensor for technetium applicable to Hanford and other DOE sites. S.A. Bryan

10:30 I&EC 14. On the road to a new large-scale sweet sorghum industry in rural America. G. Eggleston

10:50 I&EC 15. Broadening the graduate student experiences — research internships with national laboratories and industry. P.K. Dorhout

11:10 I&EC 16. Entrepreneurship, scientific outreach, and responsibility: It all works together. B.J. Streusand

11:30 I&EC 17. ACS, career, and diversity. N.B. Jackson

SUNDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Pacific Blrm D

Industrial & Engineering Fellow: Symposium in Honor of Kenneth L. Nash

Solvent Extraction

S. B. Clark, L. R. Martin, *Organizers*

T. C. Shehee, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 I&EC 18. Calorimetric determination of organic-phase extractant interactions in the ALSEP process. A.T. Johnson, T.S. Grimes, L.R. Martin

2:00 I&EC 19. Synthesis, characterization, and extraction performance of new diglycolamide ligands. B.G. Tokheim, S.S. Kelly, R.C. Ronald, K.L. Nash

2:25 I&EC 20. Complexation and extraction studies of high valency actinides by Schiff base-ligands. M. Nilsson, C. Hawkins, C. Bustillos, I. May, R. Copping

2:50 I&EC 21. Precipitation stripping in the solvent extraction and separation of the rare earths. P.M. Smith

3:15 Intermission.

3:35 I&EC 22. Design and operation of a solvent radiolysis and hydrolysis test loop. D.R. Peterman

4:00 I&EC 23. Spectrophotometric investigations of actinyl cation-cation complexes in mixed-solvent solutions. A.G. Burn, L.R. Martin, K.L. Nash

4:25 I&EC 24. Effect of solvent extraction processes on Am(VI) reduction kinetics. T.S. Grimes, B.J. Mincher

4:50 I&EC 25. Titanate sorbents for radiochemical separations. D.T. Hobbs, K.M. Taylor-Pashow, C.A. Nash

5:15 Concluding Remarks.

Section B

Renaissance Boston Waterfront
Pacific Blrm C

Industrial & Engineering Fellow: Symposium in Honor of Henry C. (Hank) Foley

M. Strano, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 I&EC 26. From nanoporous carbon membranes to carbon nanotubes and monolayer graphene barriers. M. Strano

1:25 I&EC 27. Smaller scale gas-to-liquid processes. J.J. Lerou

1:45 I&EC 28. In celebration of nice guys. M. Acharya

2:05 I&EC 29. Clean green energy from coal via biotechnology. P. Dhurjati

2:25 I&EC 30. Catalysis — an indispensable tool. S. Sengupta

2:45 Intermission.

3:00 I&EC 31. Carbon molecular sieve membranes: Enabling large scale energy efficient separations. W. Koros

3:20 I&EC 32. Supported catalysts, does surface roughness matter? A case study with in VO_x-SBA-15. M.A. Smith

3:40 I&EC 33. New approaches to developing high performance ultra-filtration membranes. A.L. Zydney

4:00 I&EC 34. Ionic liquids from phase behavior to applications. M.B. Shiflett

4:20 I&EC 35. Membrane fouling due to chemically-driven transport. D. Velegol

4:40 Concluding Remarks.

True Stories from Entrepreneurs: BRIC Edition

Sponsored by SCHB, Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

MONDAY MORNING

Section A

Renaissance Boston Waterfront
Pacific Blrm D

Industrial & Engineering Fellow: Symposium in Honor of Kenneth L. Nash

Novel Separations

L. R. Martin, T. C. Shehee, *Organizers*

S. B. Clark, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 36. New polymer-supported complexants for uranyl recovery from acidic solutions. S. Alexandratos, X. Zhu

8:30 I&EC 37. Development of a selective americium separation process using TPAEN as a water-soluble stripping agent. C. Marie, M. Duchesne, E. Russello, N. Boubals, P. Kaufholz, G. Modolo, M. Miguirditchian

9:20 I&EC 38. Solid-supported ionic liquids for metal ion separation and preconcentration: Progress and prospects. M.L. Dietz, M.A. Momen, C.A. Hawkins, S.L. Garvey

9:45 Intermission.

10:05 I&EC 39. Withdrawn.

10:30 I&EC 40. Recent results of development and demonstration of the sodium bismuthate process for the oxidation and separation of americium from the lanthanides in engineering-scale equipment. J. Law, B.J. Mincher, R. Tillotson, T. Garn, N. Schmitt

10:55 I&EC 41. Recovery of precious metals from spent nuclear waste. P.D. Benny, S.C. Bortoff, A.S. Powell, T.R. Hayes

11:20 I&EC 42. Plutonium oxide characterization and morphology for process intensification. T.C. Shehee, N. Bridges

11:45 Concluding Remarks.

True Stories from Entrepreneurs: BRIC Edition

Sponsored by SCHB, Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits

Sponsored by CHED, Cosponsored by BMGT, CEI, ENVR, I&EC, MEDI, PROF, SCHB and YCC

MONDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Pacific Blrm D

Industrial & Engineering Fellow: Symposium in Honor of Gary M. Seabolt

E. Frank, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 I&EC 43. Industrial applications of polymer self assembly and association. J. Klier

1:50 I&EC 44. Kinetic study of Pd-catalyzed hydrogenation of N-benzyl-4-fluoroaniline. A. Varma, H. Hwang

2:30 I&EC 45. Surface characterization of alpha alumina catalyst carriers. D. Gough, N. Wickramaratne, P. Nguyen

3:10 I&EC 46. 2015 American Chemical Society Industrial and Engineering Chemistry Division Applied Chemical Technology Fellow Award presentation. G.M. Seabolt

3:50 Concluding Remarks.

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector

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Incorporating Green Chemistry Innovations and Applications into the Classroom and Outreach

Sponsored by CHED, Cosponsored by CEI, I&EC and SOCED

Undergraduate Research Posters

Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored by I&EC and SOCED

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

P. M. Smith, *Organizer*

8:00 - 10:00

63-64, 69-72, 79, 82-83. See subsequent listings.

TUESDAY MORNING

Section A

Renaissance Boston Waterfront
Pacific Blrm D

Industrial and Engineering Chemistry Division Graduate Student Award Symposium

P. Savage, *Organizer*

M. A. Matthews, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 I&EC 47. Amidoxime-modified mesoporous silica for uranium adsorption under seawater conditions. C. Gunathilake, M. Jaronec, J. Gorka, S. Dai

8:55 I&EC 48. Multiphase reaction studies in stirred tank and trickle-bed reactors. S. Lee, A. Varma

9:15 I&EC 49. Synthesis of hierarchical Sn-MFI as Lewis acid catalysts for isomerization of cellulose sugars. H. Cho, P. Dornath, W. Fan

9:35 I&EC 50. Vapor phase ethanol carbonylation over supported Rh based catalysts. S. Yacob, S. Park, B.A. Kilos, D.G. Barton, J.M. Notestein

9:55 Intermission.

10:05 I&EC 51. Heterogeneous nucleation of active pharmaceutical ingredients on polymers: Applications in continuous pharmaceutical manufacturing. L. Tan, A.S. Myerson, B.L. Trout

10:25 I&EC 52. Development of a new multimodal membrane adsorber for biologics purification. J. Wang, S.M. Husson

10:45 I&EC 53. Mechanistic insights into the electrochemical reduction of CO₂ to CO on nanostructured Ag surfaces. J. Rosen, F. Jiao

11:05 Closing Remarks.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

TUESDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Pacific Blrm D

Green Chemistry Makes a Difference: Pharmaceutical Industry/Academic Collaborations

Cosponsored by ORGN

M. E. Kopach, *Organizer, Presiding*

1:00 I&EC 54. Continuous flow multistep synthesis. T.F. Jamison

1:40 I&EC 55. Grignard, reaction past, present and future: Development of greener more sustainable processes. M.E. Kopach, T. Braden, M.D. Johnson, M.E. Kobierski

2:20 I&EC 56. UM/Dow collaboration on the development of catalytic fluorination reactions. M.S. Sanford

3:00 Intermission.

3:20 I&EC 57. Green chemistry at Pfizer. P.J. Dunn

4:00 I&EC 58. Green chemistry at Genentech. S.G. Koenig

4:40 I&EC 59. Process development of avibactam. M. Golden

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

TUESDAY EVENING

Section A

Boston Convention and Exhibition Center
Hall C

General Posters

P. M. Smith, *Organizer*

6:00 - 8:00

I&EC 60. Withdrawn.

I&EC 61. Removal of synthetic dye acid red 186 from water by activated carbon. A.M. Turky

I&EC 62. Comparative analysis of dependence of etching conditions (solution concentration, temperature and time) of track-etched membranes on ion beam fluence. D. Orazbayeva, Y. Koshman

I&EC 63. Investigation on the physico-chemical properties of poplar lignin carbon precursors before and after melt rheology. Q. Sun, A.J. Ragauskas

I&EC 64. Synthesis and characterization of CMC/Tb-Eu nanocomplexes with photoluminescence. W. Liang, J. Ye, J. Xiong

I&EC 65. Effect of pH on particles size and fluorescence properties of CMC/Eu nanocomposites with microwave assist. B. Wang, J. Ye, J. Xiong

I&EC 66. Activity coefficients of RbF in urea-water and formamide-water mixtures. M. Hu

I&EC 67. Size dependence of optical properties of gold nanoparticle. H. Dong, J. Liu, J. Zhao, Y. Song

I&EC 68. Synthesis of fat-based quaternary ammonium salts (QUATs). H. Yosry, K. Rasheed, H. Rasheed

I&EC 69. Simulation of drilling pressure profile in directional drilling and user program development. W. Panichaporn, R. Prurapark, K. Siemanond

I&EC 70. Study on removal of nickel ions in the mint wastewater during coagulation enhanced by pre-oxidation and pH adjustment. W. Qun, W. Tan, X. He, Z. Yang, S. Chen, B. Chai

I&EC 71. Effective radiative cooling and optimized heat dissipation for high power electronic devices. T. Hsiao, T.N. Eyassu, C. Lin

I&EC 72. Bioinspired ultrathin polydopamine coating skin layer on PDMS for enhanced hydrocarbon gas recovery. M. Fang, J. Li

I&EC 73. CFD modeling for fluid flow and mass transfer in spacer-filled channels for pervaporation. T. Wang, J. Li

I&EC 74. Pervaporation performance of Octavinyl-POSS cross-linked PDMS membranes for ethanol/water separation. X. Zhan, S. Ma, Y. Xia

I&EC 75. Pervaporation performance of cyclodextrin filled PDMS membranes for ethanol recovery from aqueous solution. X. Zhan, S. Ma, Y. Xia

I&EC 76. New computer controlled platforms for discovery and self-optimization bespoke flow systems. L. Porwol, A. Henson, V. Sans, L. Cronin

I&EC 77. Modularity and automation of multistep reactions combining 3D printing technology with continuous flow processes. V. Dragone, P. Kitson, V. Sans, L. Cronin

I&EC 78. Performance of a pilot-scale pervaporation system for the separation of an ethanol-water mixture. J. Liu, J. Chen, M. Fang, T. Wang, Y. Xia, X. Li, J. Li

I&EC 79. High performance membranes for organic solvent nanofiltration via surface modification of P84@ substrate followed by cross-linking. X. Li, J. Li

I&EC 80. Non equilibrium solution-diffusion phenomenon for osmosis membranes. W. Cai, Y. Xia, Y. Wang, J. Li, S. Zhu

I&EC 81. Distillate flux enhancement in direct contact membrane distillation modules with inserting carbon-fiber spacers under countercurrent-flow operations. C. Ho, P. Lin

I&EC 82. Oxalate formation during hydrogen peroxide bleaching waste paper pulp. H. Li, Y. Liu, Q. Zhang, H. Zhan

I&EC 83. Performance evaluation of vanadium redox flow battery adopting mesoporous carbon catalyst. Y. Kwon, J. Lee, K. Yoo

I&EC 84. Hindered diffusion of monomers and nanoaggregates of sulfur-containing compounds in petroleum residue fractions through polycarbonate membranes. Z. Chen, Y. Wu, Z. Xu, S. Zhao, C. Xu

I&EC 85. Modeling and NMR spectroscopy tools for understanding coalescent efficiency and partitioning in polymer latexes for coatings applications. S. Arumugam, K. Beshah, J. Sparks, S. Arturo, B. Rowe, J.R. Ell

WEDNESDAY MORNING

Section A

Renaissance Boston Waterfront
Pacific Blrm H

General Papers

P. M. Smith, *Organizer*

J. A. Ritter, *Presiding*

8:30 I&EC 86. Characterization of HFO-1233zd (E) leaching potential using numerical simulation. M.K. Mroziak, S. Mukhi, D. Perkins, K. Wright, M. Cheplick, G. Hancock

8:50 I&EC 87. Analyzing refinery unit kinetic models by reaction network visualization. S. He, Z. Hou, C. Bennett, S.R. Horton, M.T. Klein, Q. Shi, S. Zhao

9:10 I&EC 88. Synthesis of pogostone from biobased triacetic acid lactone. U.K. Wanninayake, G.A. Kraus

9:30 I&EC 89. Potassium fertilizers from ultrapotassic syenites. D. Ciceri, C.L. Gadois, T. Skorina, A. Allanore

9:50 Intermission.

10:05 I&EC 90. Comparison of boron fixation on different resins. H.T. Nguyen

10:25 I&EC 91. Engineering of DNA for the long-term storage of digital information. R.N. Grass, R. Heckel

10:45 I&EC 92. Developing workflows for continuous crystallisation processes within the pharmaceutical industry. T. McGlone, A.J. Florence

11:05 I&EC 93. ContinNMR: Monitoring and controlling continuous synthesis reactors with Benchtop NMR. S. Riegel, T. Rehm, J. Barten

Big Chemistry from Small Businesses

Sponsored by SCHB, Cosponsored by COLL, I&EC, PRES and PROF

International Symposium on Mesoporous Zeolites

Sponsored by ENFL, Cosponsored by CATL, I&EC and INOR

WEDNESDAY AFTERNOON

Section A

Renaissance Boston Waterfront
Pacific Blrm H

General Papers

P. M. Smith, *Organizer*

J. A. Ritter, *Presiding*

1:00 I&EC 94. Temperature dependence of gas transport and sorption in carbon molecular sieve membranes derived from four 6FDA based polyimides: entropic selectivity evaluation. S. Fu, E. Sanders, S. Kulkarni, W. Koros

1:20 I&EC 95. Pervaporation membrane for the efficient recovery of ionic liquid from mixed lignocellulosic feedstock processing. J. Sun, J. Shi, T. Dutta, B.A. Simmons, S. Singh

1:40 I&EC 96. Enhanced transdermal delivery of anti-inflammatory drugs synthesized as ionic liquids. W. Medina-Ramos, M.R. Prausnitz

2:00 I&EC 97. Methane oxidation on supported iron-based oxygen carrier with chemical looping redox reaction. L. Qin, Z. Cheng, J. Fan, M. Guo, D. Xu, D. Kopechek, N. Deshpande, L. Fan

2:20 I&EC 98. Withdrawn.

2:40 Intermission.

2:55 I&EC 99. Withdrawn.

3:15 I&EC 100. Transition metal modified mesoporous silica materials with zero surface microporosity for the adsorption of contaminants of emerging concern from aqueous solutions.

K. Ortiz-Martinez, K. Guerrero-Medina, F. Roman, A.J. Hernandez-Maldonado

3:35 I&EC 101. Flexible $\text{Cu}_2(\text{pzdc})_2$ [L = dipyrityl-based ligands] porous coordination polymers: Hysteretic adsorption and diffusion kinetics of CO_2 and CH_4 .

H. Chen, K. Riascos-Rodríguez, M.E. Marciano-González, A.J. Hernandez-Maldonado

3:55 I&EC 102. Fractionation of thermally produced bio-oils using supercritical fluids. L.M. Petkovic, D.M. Ginosar

International Symposium on Mesoporous Zeolites

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THURSDAY MORNING

Section A

Renaissance Boston Waterfront
Pacific Blrm H

General Papers

P. M. Smith, *Organizer*

J. A. Ritter, *Presiding*

8:30 I&EC 103. Biodegradable slashing agents from soy protein for textile industry. Y. Zhao, H. Xu, Y. Zhao, L. Xu, Y. Yang

8:50 I&EC 104. Novel Brønsted-acidic ionic liquids as catalysts for synthesizing trioxane. Y. Hu, J. Qi

9:10 I&EC 105. Effect of hydrolysis on pyrolytic characteristics of sunflower stalk. X. He, A. Zhou, L. Yang, H. Wu, J. Wei

9:30 I&EC 106. Green synthesis of 4-O-aryloxy carbonates from aryl/alkyl-oxy propanediols and dimethyl carbonate over nanocrystalline alkali promoted alkaline earth metal oxides. G.D. Yadav, P.S. Surve

9:50 Intermission.

10:05 I&EC 107. Dual functionalized ionic liquids [APmim][Gly] as an effective aqueous absorbent for CO_2 capture. B. Lv, Z. Zhou, G. Jing

10:25 I&EC 108. Membrane fouling mechanism and control for harvesting microalgae. B. Su, E. Kanchanapit, W. Den, N. Grisdanurak

10:45 I&EC 109. Adsorption of phenolic and chlorophenolic compounds using multiwall carbon nanotubes embedded on SiO_2 . S. Tulaphol, E. Kanchanapit, W. Den, N. Grisdanurak

11:05 I&EC 110. Perfluoroalkylsulfonfyl groups contained catalyst, stable for Friedel-Craft alkylation reaction. Y. He, Q. Zhang, X. Zhan, F. Chen, D. Cheng

INOR

Division of Inorganic Chemistry

N. Radu and S. Koch, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

2015 ACS Catalysis Lectureship
(see CATL, Monday, Tuesday)

SABIC Young Catalysis Investigator
Award: Symposium In Honor of
Melanie Sanford (see CATL, Tuesday)

Cope Award Symposium
(see ORGN, Tuesday)

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 160B

Main Group Chemistry

T. W. Hudnall, *Organizer*

J. D. Protasiewicz, D. Vidovic, *Presiding*

9:00 INOR 1. Alternate pyrrole and isoindoline-based BF_2 fluorophores. C.J. Ziegler, L. Crandall, I. Tamgho

9:20 INOR 2. Polyoxaphospholes: Polymeric organophosphorus compounds with luminescent properties. J. Gaffen, J.D. Protasiewicz

9:40 INOR 3. Luminescent materials featuring multiply bonded phosphorus groups. J.D. Protasiewicz

10:00 INOR 4. Computational design and characterization of organometallic molecules with unprecedented beryllium-beryllium double bonds. X. Wang

10:20 Intermission.

10:30 INOR 5. Tribora-cyclopropenyl dianion — a boron-based homoaromatic Hückel π system. T. Kupfer, H. Braunschweig

10:50 INOR 6. Synthesis and reactivity of phosphonium dications. D. Vidovic

11:10 INOR 7. Stabilization of reactive main group species by coordination to carbonyl-decorated carbenes. T.W. Hudnall, A. Ledet, K.M. Melancon, A.J. Torres

11:30 INOR 8. Redox- and anion-controlled modulation of a Au-Sb bond. S. Sen, I. Ke, F.P. Gabbai

11:50 INOR 9. Exploring the electronic structure of aluminum hydrides: X-ray absorption spectroscopic investigations of aluminum coordination complexes. A.B. Altman, J. Arnold, S.G. Minasian, S. Pemmaraju, D. Prendergast, D.K. Shuh, T. Tylliszczak

Section B

Boston Convention & Exhibition Center
Room 159

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

D. Mendoza-Espinosa, E. T. Papish, *Presiding*

8:00 INOR 10. Exploring the reactivity of Pd pincer complexes immobilized in a Zr(IV) metal-organic framework matrix. S.A. Burgess, C.R. Wade

8:20 INOR 11. Stabilizing high oxidation state first row metal complexes with a robust fluoroalkoxy carbene. A.J. Arduengo, S.P. Kelley, W.J. Marshall, J.W. Runyon

8:40 INOR 12. Heteroatom-functionalized 1,2,3-triazoliums: Ionic liquids for the Baylis-Hillman reaction and ligand precursors for MIC transition metal complexes. D. Mendoza-Espinosa, G. Negron-Silva, R. Gonzalez-Olvera

9:00 INOR 13. Synthesis and application of N-trifluoromethylated N-heterocyclic carbene ligands and their complexes. P. Engl, A. Togni

9:20 INOR 14. Tetranuclear Pd catalysts based on metal phosphonate cages for olefin polymerization. Q. Liu, N.D. Contrella, A.S. Filatov, R.F. Jordan

9:40 INOR 15. Metal-ligand cooperative pathway for intermolecular oxa-Michael additions to unsaturated nitriles. S. Perdriau, D. Zijlstra, E. Heeres, H. de Vries, E. Otten

10:00 INOR 16. New bifunctional ligands for catalysis. E.T. Papish, C.R. Thompson, E.A. Douglas, D.L. Gerlach

10:20 INOR 17. Threefold symmetric zerovalent cobalt is a potent reductant of N_2 . B.J. Cook, M. Pink, S. Bidwell, R.L. Lord, K.G. Caulton

10:40 INOR 18. Iridium $\text{PC}(\text{sp}^2)\text{P}$ -type complexes which exhibit unique ancillary interactions. D.C. Babbini, V.M. Iluc

11:00 INOR 19. Metal-ligand cooperativity between a new series of aryl-substituted PNP pincer-type ligands and an Ir(III) metal center. S.P. Vilanova, V.M. Iluc

11:20 INOR 20. Mono- and dimetalation of a tridentate bisimidazole-phosphine ligand. S.E. Flowers, B.M. Cossairt

11:40 INOR 21. Diastereoselective and enantioselective synthesis of P-stereogenic *Syn*-phosphiranes. J. Muldoon, B. Varga, M. Deegan, T.W. Chapp, D.S. Glueck, C. Moore, A.L. Rheingold

12:00 INOR 22. Pyridyl-functionalized 3H-1,2,3,4-triazaphospholes: Synthesis, coordination chemistry, and application in homogeneous catalysis. J. Sklorz, C. Mueller

Section C

Boston Convention & Exhibition Center
Room 162B

Solid-State Inorganic Chemistry

C. G. Lugmair, *Organizer*

V. Poltavets, *Organizer, Presiding*

A. Choudhury, *Presiding*

8:30 Introductory Remarks.

8:35 INOR 23. TiS_2 and TiS_3 layered materials: Intercalation and/or substitution to enhance the thermoelectric properties. A. Maignan

9:15 INOR 24. Magnetic anisotropy in new misfit layer compounds. S.M. Clarke, D.E. Freedman

9:35 INOR 25. Novel soft chemistry techniques for metastable materials synthesis. V. Poltavets, J.D. Davis, S.K. Kraemer

9:55 INOR 26. Controlling hard/soft magnetic exchange in core/shell nanoparticles. D. Carnevale, M. Shatruk, G.F. Strouse

10:15 Intermission.

10:30 INOR 27. Series of magnetically frustrated quaternary chalcogenides with interpenetrating lattices. A. Choudhury, S. Mohapatra, K. Ghosh

10:50 INOR 28. Single crystal growth and X-ray observation of charge-density-wave order in Ruddlesden-Popper nickelate $\text{R}_m\text{Ni}_x\text{O}_{10}$ ($\text{R}=\text{La}$ and Pr). J. Zhang, Y. Chen, H. Zheng, Y. Ren, J. Mitchell

11:10 INOR 29. Formation of transition metal oxide with high-aspect-ratio geometry by high pressure CVD. Y. Liu, V. Gopalan, J.V. Badding

11:30 INOR 30. Origin of superhardness in metallic tungsten monoboride. M.T. Yeung, J. Lei, R. Mohammadi, C.L. Turner, Y. Wang, S.H. Tolbert, R.B. Kaner

Section D

Boston Convention & Exhibition Center
Room 160C

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

F. N. Castellano, *Presiding*

8:00 INOR 31. Design and synthesis of ruthenium-EDOT based coordination polymers for use in inorganic-organic hybrid dye sensitized solar cells. S.M. Boyer, K.H. Skorenko, A. Nandur, F.H. Schreffler, M.I. Ehrlich, B.E. White, W.E. Bernier, W.E. Jones

8:20 INOR 32. Enhancements to electrocatalytic reduction of CO_2 by cobalt phthalocyanine upon immobilization in polyvinylpyridine membrane. W.W. Kramer, I.M. Ferrer, C.C. McCrory

8:40 INOR 33. Electrocatalytic reduction of carbon dioxide to carbon monoxide by manganese carbonyl complexes containing phenanthroline-type ligands: Catalytic turnover even in the absence of Brønsted acids. B. Dhakal, D.A. Kurtz, R.J. Hulme, G.A. Felton

9:00 INOR 34. Stoichiometric production and delivery of chlorine to substrates. A. Stastny, A.E. Norton, J.A. Krause, W.B. Connick

9:20 INOR 35. Hydrogenation of CO_2 and dehydrogenation of formic acid using iridium catalysts based on proton-responsive azole ligands. Y. Himeda, N. Onishi, S. Xu, Y. Suna, Y. Manaka, J.T. Muckerman, E. Fujita

9:40 INOR 36. Photochemical upconversion beyond the molecule. F.N. Castellano

10:00 Intermission.

10:10 INOR 37. Electrocatalytic reduction of CO_2 with manganese catalyst supported by pendant Brønsted-Lowry acid ligands. K. Ngo, R.P. Narayanan, B. Mahanti, B.R. Reed, S. Groysman, J.J. Rochford

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10:30 INOR 38. Rapid water oxidation electrocatalysis by a ruthenium complex with a facially coordinating polypyridyl ligand. **A. Walden**, A.J. Miller

10:50 INOR 39. Withdrawn.

11:10 INOR 40. Degradation of lignin model compounds through selective C-C bond cleavage using earth abundant vanadium catalysts driven by visible light. **S. Gazi**, W.K. Ng, R. Ganguly, H. Hirao, **H. Soo**

11:30 INOR 41. Chromophore-catalyst assemblies based on porphyrin and Ru(II) polypyridyl catalysts for light driven water oxidation. **A. Nayak**, R.R. Knaut, L. Alibabaei, J.L. Dempsey, T.J. Meyer

11:50 INOR 42. Volatile heterometallic precursors for the low-temperature synthesis of lithium ion battery cathode material. **Z. Wei**, H. Han, A.S. Filatov, E. Dikarev

Section E

Boston Convention & Exhibition Center
Room 161

Bioinorganic Chemistry: DNA, RNA and Inorganic Drugs

S. A. Koch, *Organizer*

J. Liu, *Presiding*

8:00 INOR 43. Ru(II) polypyridyl complexes as potent photosensitizers in photodynamic therapy. **C. Mari**, V. Pierroz, R. Rubbiani, M. Patra, S. Ferrari, **G. Gasser**

8:20 INOR 44. Small peptides-Re(CO)₃ conjugates synthesis using new lysine linkage approach. **K. Chanawanno**, V. Kondeti, S.M. Paruchuri, J.A. Caporoso, T. Leeper, R.S. Herrick, C.J. Ziegler

8:40 INOR 45. Lanthanide ion dependent DNazymes: In vitro selection and metal binding studies. **J. Liu**, P. Huang

9:00 INOR 46. Facile synthesis and biological evaluation of metalloce-nyl derivatives. **J. Hess**, M. Patra, A. Leonidova, V. Pierroz, S. Ferrari, G. Gasser

9:20 INOR 47. Practical and reliable method for long-term room temperature storage of RNA within silica. **M. Puddu**, W.J. Stark, R.N. Grass

9:40 INOR 48. Rationally designed glucose-platinum(II) conjugates for actively targeting cancer cells. **M. Patra**, T.C. Johnstone, K. Suntharalingam, S.J. Lippard

10:00 Intermission.

10:10 INOR 49. Biological consequences arising from the unique binding profile of phenanthriplatin. **I.A. Riddell**, G. Park, K. Agama, Y. Pommier, S.J. Lippard

10:30 INOR 50. On the cytotoxic activity of Pd(II), Pt(II) and Ru(II) complexes of N, N-disubstituted-N-acyl thioureas. **A. Batista**, A. Graminha, A.M. Plutin, A. Alvarez, R. Ramos, R. Mocelo, E. Castellano

10:50 INOR 51. Upconverting lipid vesicles for the red light activation of anticancer metalodrugs. **S. Bonnet**

11:10 INOR 52. Verstable and remarkably stable Mn-based MR imaging probe: Application to targeted thrombus imaging. **E. Gale**, I. Atanasova, F. Blasi, P. Caravan

11:30 INOR 53. In silico guided design and synthesis of new high relaxivity Gd(DOTA) derivatives. **E. Boros**, H. Kim, B. Tidor, P. Caravan, A. Horning

11:50 INOR 54. DNazyme sensors for cellular metal ion sensing. **K. Hwang**, Y. Lu

Section F

Boston Convention & Exhibition Center
Room 162A

Chemistry of Materials: Materials for Energy and Catalytic Applications

C. G. Lugmair, *Organizer*

A. Hall, *Presiding*

8:00 INOR 55. Graphite-conjugated pyrazines as molecularly-tunable electrocatalysts. **T. Fukushima**, Y. Surendranath

8:20 INOR 56. Electrocatalytic CO₂ reduction at ordered nanoporous metallic thin films. **A. Hall**, Y. Yoon, Y. Surendranath

8:40 INOR 57. Grain boundary rich metals: Synthesis and impact on electrocatalysis. **Y. Yoon**, A.S. Hall

9:00 INOR 58. Strain modulated electrocatalysis. **E. Benson**, D. Svedruzic, S. Ferrere, B.A. Gregg

9:20 INOR 59. Rhodium-based complexes and conducting metallopolymers for electrocatalytic CO₂ reduction. **Y. Liang**, L.A. Lytwak, **B.J. Holliday**

9:40 INOR 60. Imparting architecture control over colloidal nanocrystal frameworks for energy storage devices. **T.E. Williams**, A.W. Wills, B. Helms

10:00 Intermission.

10:10 INOR 61. Experimental and theoretical investigation of LiFeO₂ – tunnel: Fe²⁺/Fe³⁺ cathode for Li-ion batteries. **V. Poltavets**, J.D. Davis, S.R. Bruno, C. Blakely

10:30 INOR 62. Comparison of different TiO₂ phase structures and morphologies on dye-sensitized solar cell. **C. Tsui**, K.L. Yeung

10:50 INOR 63. Synthesis of mesoporous metal oxides via aerosol-assisted self-assembly pyrolysis for energy storage. **M. Sheehan**, M. Rudden, C. Tsung

11:10 INOR 64. Band edge control of crystalline silicon by chemical functionalization of the surface. **N.T. Plymale**, A.A. Ramachandran, A.N. Lim, B.S. Brunshwig, N.S. Lewis

11:30 INOR 65. Amplification of light energy conversion within the dielectric-band in a dye-sensitized solar cell coupled to an inverse opal compared with an inverse glass. **R. Fayad**, L.I. Halaloui

11:50 INOR 66. New iron-based polyanion compounds as cathode materials for rechargeable alkali-ion batteries. **H. Yaghoobnejad Asl**, A. Choudhury

Section G

Boston Convention & Exhibition Center
Room 160A

Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*

A. R. Fout, D. Rabinovich, *Presiding*

8:30 INOR 67. Isolation and characterization of intermediates involved in the silylation of dinitrogen using a dicobalt catalyst. **R. Siedschlag**, V. Bernales, K.D. Vogiatzis, L. Gagliardi, C. Lu

8:50 INOR 68. Synthesis and reactivity of new N-heterocyclic thione (NHT) and related ligands. **D. Rabinovich**

9:10 INOR 69. Linear oligopyrroles as redox-active ligands: Metal coordination and redox behavior. **E. Tomat**

9:30 INOR 70. Redox-state effects on small molecule bin multimetallic iron complexes. **G. de Ruiter**, N.B. Thompson, T. Agapie

9:50 INOR 71. Robust trinuclear complexes towards reactivity with challenging small molecule substrates. **J. Teesdale**, T. Betley

10:10 INOR 72. Investigating the role of a tripodal H-bond donor and acceptor ligand scaffold in small molecule activation. **C. Ford**, E.M. Matson, Y. Park, A. Fout

10:30 INOR 73. Bioinspired α -hydroxy acid containing tripodal amine chelates and photoactivity of their metal complexes. **J.E. Vernia**, M.J. Baldwin

10:50 INOR 74. Synthesis and characterization of trinuclear complexes featuring early transition metals. **A.K. Bartholomew**, T. Betley

11:10 INOR 75. Group transfer catalysis utilizing a pyrazolate-bridged Co₂ system. **B.J. Cook**, C. Chen, R.L. Lord, K.G. Caulton

11:30 INOR 76. New class of high-relaxivity Mn^{II}-based contrast agents as platforms for targeted intracellular magnetic resonance molecular imaging. **A. Barandov**, B. Bartelle, A. Jasanoff

11:50 INOR 77. Synthesis and coordination chemistry of chelating guanidinyll borate ligands. **N.A. Piro**, W.S. Kassel

12:10 INOR 78. Anion binding by cobalt complexes of an H-bond donor triguanidine ligand. **R.C. Scarrow**, J.A. Schneider, S.C. Schwartz, S. Park, T.M. Nguyen

Section I

Boston Convention & Exhibition Center
Room 158

Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*

A. De Bettencourt Dias, C. Thomas, *Presiding*

8:30 INOR 79. Linking [Fe^{III}] triangles with derivatised salicylaldoximes. **D.T. De Silva**, G.N. Jameson, E.K. Brechin, P.G. Plieger

8:50 INOR 80. Investigating the interaction and redox activity of novel polynuclear iron complexes with carbohydrates: Synthesis, structure, electrochemical, and spectroscopic investigation of their interactions with monosaccharides. **C.D. Stewart**, H. Arman, G.T. Musie

9:10 INOR 81. Towards selective Fe(II) optical sensors. **T.Y. Tittiris**, S.M. McLeod, J.R. Morrow

9:30 INOR 82. Isolation and characterization of a μ^3 -tricobalt nitride in four different oxidation states. **B. Lin**, T. Betley

9:50 INOR 84. Synthesis and reactivity of trinuclear Zn-Fe clusters. **C. Juda**, T. Betley

10:10 INOR 85. Synthesis and reactivity of a sterically demanding benzimidazole thione. **L. Hernandez**, D. Rabinovich

10:30 INOR 86. Synthesis and characterization of N-heterocyclic phosphonium/phosphide nickel complexes: Mono- and multimetallic. **D.A. Evers-McGregor**, M. Bezpalko, B.M. Foxman, C. Thomas

10:50 INOR 87. Coordination chemistry of mid-to-late first-row transition-metal complexes with tris(2-pyridyl)phosphine (PPy₃) and its oxide (OPPy₃). **K. Suppa**, C. Fairfield, D. Pericic, N.A. Piro, **W.S. Kassel**

11:10 INOR 88. Class I mixed-valent dirhenium complexes. **Y. Yan**, J.T. Mague, J.P. Donahue, **S. Sproules**

11:30 INOR 89. Dicarboxylate-connected and bisphosphine substituted dimolybdenum(II) coordination compounds. **D. Hoehne**, A. Pothig, E. Herdtweck, M. Cokoja, S. Haslinger, X. Cai, M. Koeberl, F.E. Kuehn, W. Herrmann

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Tutorial

Sponsored by PMSE, Cosponsored by INOR-F

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 160B

Inorganic Young Investigator Awards

J. M. Boncella, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR 90. Synthetic micro/nanomachines and their applications: Toward "Fantastic Voyage". **W. Gao**, J. Wang

2:05 INOR 91. Structure design of silicon anodes for high energy lithium-ion batteries. **N. Liu**, Y. Cui

2:35 INOR 92. Electronically doped colloidal semiconductor nanocrystals. **A.M. Schimpf**, D.R. Gamelin

3:05 Intermission.

3:15 INOR 93. Gas separations in metal-organic frameworks with open metal sites. **E.D. Bloch**, J.R. Long

3:45 INOR 94. Organometallic palladium complexes as chemoselective bioconjugation reagents. **E.V. Vinogradova**, C. Zhang, A.M. Spokoyrn, B.L. Pentelute, S.L. Buchwald

4:15 INOR 95. Exploring the trap state landscape of colloidal CdSe nanocrystals with cadmium halide ligands. **M.J. Greaney**, R.L. Brutchey

4:45 INOR 96. Models of the oxygen-evolving complex of photosystem II. **J. Kanady**, T. Agapie

5:15 INOR 97. Efforts toward the next generation of platinum drugs: Monofunctional complexes and nanodelivery. **T.C. Johnstone**, S.J. Lippard

Section B

Boston Convention & Exhibition Center
Room 159

Synthetic Chemistry Approaches to Magnetic Materials

D. E. Freedman, M. A. Green, E. E. Rodriguez, *Organizers*

D. Harris, *Organizer, Presiding*

1:30 INOR 98. Emergent chemical kinetics in a magnetic system. **S. Bramwell**

2:00 INOR 99. Withdrawn.

2:20 INOR 100. Synthetic chemical approaches to designing and understanding qubits. **J. Zadrozny**, M. Graham, M. Fataftah, S. Coste, D.E. Freedman

2:40 INOR 101. Electronic structure contributions to magnetic exchange interactions in photoexcited states. **M.L. Kirk**, D. Shultz

3:10 Intermission.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

- 3:20 INOR 102.** Controlled under pressure: Understanding magnetic anisotropy in heavy atom organic radicals. S. Hill, K. Thirunavukkuarasu, S. Winter, C.C. Beedle, R.T. Oakley
- 3:50 INOR 103.** Tunable superparamagnetism in n -type TM^{2+} - and Ln^{3+} -doped nanoparticles. J.D. Rinehart
- 4:10 INOR 104.** Effect of optical switching on the spin states of electronically bistable magnetic materials: Photoresponsive metal clusters. N. Frank
- 4:30 INOR 105.** Magnetic and multiferroic metal-organic frameworks. A. Cheetham

Section C

Boston Convention & Exhibition Center
Room 162B

Inorganic Catalysts

S. A. Koch, *Organizer*

K. A. Grice, *Presiding*

- 1:30 INOR 106.** Group 13 metal-containing catalysts and the development of more sustainable hydrocarbon oxidation reactions. C.R. Goldsmith, F. Bronston, C. Koellner, N.A. Piro, W.S. Kassel, C.R. Graves
- 1:50 INOR 107.** Electrospun composite nanofibers for enhanced photocatalytic degradation of environmental toxins. D.L. McCarthy, J. Troiano, J. Tollin, J. Liu, J.B. Decoste, W.E. Bernier, W.E. Jones
- 2:10 INOR 108.** Dehydrofluorination of 1,1,1,2,3-pentafluoropropane to produce eco-friendly refrigerant 2,3,3,3-tetrafluoropropene (HFO-1234yf) using Cr-based catalysts. S. Lim, J. Ha, H. Kim
- 2:30 INOR 109.** Electrochemical reduction of carbon dioxide with group 6 metal complexes. K.A. Grice, C. Saucedo, M. Sovereign
- 2:50** Intermission.
- 3:00 INOR 110.** Redox-active pincer ligands on chromium: Efforts toward reductive coupling of carbon dioxide. N.S. Labrum, C. Chen, K.G. Caulton
- 3:20 INOR 111.** Surface attachment of homogeneous CO_2 reduction catalysts: $\text{Re}(\text{bpy-CN})(\text{CO})_2\text{Cl}$ on gold. M.L. Clark, C.W. Machan, S.A. Chabolla, T. Dang, C.P. Kubiak
- 3:40 INOR 112.** Hydrocarbon oxidation by bimetallic late transition metal complexes with dual active sites. C. Hess, S. Lindsay
- 4:00 INOR 113.** Multinuclear palladium oxygen species related to aerobic oxidation catalysis. A.J. Ingram, K.L. Walker, R.N. Zare, R.M. Waymouth
- 4:20 INOR 114.** Iron-catalyzed synthesis of unprotected complex N-heterocycles via direct amination of primary, secondary, and activated C-H bonds. A. Mikhailine, T. Betley
- 4:40 INOR 115.** Facile microwave synthesis and catalytic properties of cobalt (II) porphyrinyl compounds. C.J. McElroy, P. Jairo, S. Amorello, P.D. Voegel

Section D

Boston Convention & Exhibition Center
Room 160C

Metalloenzyme Mechanisms

G. Ghirlanda, I. V. Korendovych, *Organizers*,
Presiding

- 1:30 INOR 116.** Using designed enzymes for mechanistic investigation of heme-copper oxidase and nitric oxide reductase. Y. Lu, A. Bhagi, I.D. Petrik, Y. Yu, J. Reed, S. Chakraborty, A. Mukherjee

- 2:00 INOR 117.** Short peptides self-assemble in the presence of metals to produce catalytic amyloids. I.V. Korendovych
- 2:30 INOR 118.** Binding of nitrogenase substrates to an iron complex with sulfur and carbon ligands. I. Coric, A.M. Brosnahan, B.Q. Mercado, P.L. Holland
- 3:00** Intermission.
- 3:10 INOR 119.** Kinetics and mechanisms of oxygen and peroxide activation with non-heme iron enzyme models. E. Rybak-Akimova
- 3:40 INOR 120.** Redox mechanisms of metalloenzymes, studied with protein electrochemistry. S.J. Elliott, E.T. Judd, K. Walsh, B. Levin
- 4:10 INOR 121.** Water oxidation by photosystem II. G.W. Brudvig

Section E

Boston Convention & Exhibition Center
Room 162A

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

C. Mottillo, E. Tsvion, *Presiding*

- 1:30 INOR 122.** Chemistry of CH_4 adsorption on MOFs with open metal sites. E. Tsvion, M.P. Head-Gordon
- 1:50 INOR 123.** Tailoring the nucleophilic character of metal-organic frameworks for the reactive removal of chemical threats. J.B. DeCoste, M.A. Browe, G.W. Wagner, G.W. Peterson
- 2:10 INOR 124.** Novel quick approach to tethering amine on metal-organic frameworks for selective CO_2 capture from air and flue gas. H. Li, K. Wang, H. Zhou
- 2:30 INOR 125.** Dioxygen activation in a cobalt metal-organic framework for O_2/N_2 separations and catalysis. D.J. Xiao, M. Gonzalez, J.R. Long
- 2:50 INOR 126.** DFT modeling of metal-organic frameworks for oxygen-nitrogen separation: Effect of temperature and metal. M.V. Parkes, J.A. Greathouse, T.M. Nenoff
- 3:10 INOR 127.** First-principles molecular dynamics simulations on hydrogen storage in metal-organic framework. K. Koizumi, K. Nobusada, M. Boero
- 3:30** Intermission.
- 3:40 INOR 128.** Functionalized metal-organic frameworks bearing flexible side chains: A way to tune gas sorption properties. I. Schwedler, S. Henke, A. Schneemann, P. Llewellyn, R.A. Fischer
- 4:00 INOR 129.** New Ca-based metal organic framework selectively absorbing Xe over Kr. X. Chen, A.M. Plonka, D. Banerjee, R. Krishna, H.T. Schaef, S. Ghose, P.K. Thallapally, J.B. Parise
- 4:20 INOR 130.** Light gas separations and storage with MOFs via modeling, synthesis, and pressurized induced structural changes. T.M. Nenoff, D.F. Sava Gallis, M.V. Parkes, J.A. Greathouse, M. Rodriguez, K.W. Chapman
- 4:40 INOR 131.** Stability analysis of microporous zeolitic imidazolate frameworks in carbon dioxide-rich atmospheres. C. Mottillo, T. Friscic
- 5:00 INOR 132.** Functionalized MOFs for hydrocarbon separation. A. Schneemann, E.D. Bloch, S. Henke, P. Llewellyn, J.R. Long, R.A. Fischer
- 5:20 INOR 133.** Structural changes in $M[(\text{bdc})(\text{tdc})_n]$ ($M = \text{Zn}, \text{Ni}$ or Cu) metal organic frameworks upon thermal dispersion of LiCl and adsorption of carbon dioxide. J. Guerrero-Medina, G. Mass-Gonzalez, L. Pacheco-Londoño, S.P. Hernandez-Rivera, R. Fu, A.J. Hernandez-Maldonado

Section F

Boston Convention & Exhibition Center
Room 161

Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*

K. G. Caulton, E. Tomat, *Presiding*

- 1:30 INOR 134.** Heteroleptic formazan complexes of cyclometallated platinum. T.S. Teets, E. Kabir

- 1:50 INOR 135.** Synthesis and reactivity of monoanionic pincer N-heterocyclic carbene iron complexes. B. Jackson, A. Fout

- 2:10 INOR 136.** Synthesis and characterization of aluminum, gallium, tin, and chromium complexes with a non-innocent bulky diimine ligand. R.A. Zarkesh, M. Anstey
- 2:30 INOR 137.** Fullerenes functionalized with piperazine: Building blocks for supramolecular architectures. A. Aghabali, A.L. Balch, M.M. Olmstead

- 2:50 INOR 138.** Cooperative activation of carbon dioxide by a nucleophilic ligand backbone an oxophilic metal. B.J. Cook, C. Chen, M. Pink, R.L. Lord, K.G. Caulton
- 3:10 INOR 139.** Ru-NHDC complexes from an abnormal Ru-NHC carbene. M.J. Bitzer, A. Pothig, J. Kueck, C. Jandl, F.E. Kuehn, W. Baratta

- 3:30 INOR 140.** Intramolecular C-C coupling reactions in rhenium complexes triggered by ligand methyl group deprotonation. R. Arevalo, J.A. Perez, L. Riera
- 3:50 INOR 141.** Hydroaminoalkylation of olefin catalyzed by silica supported metallaziridine. B. Hamzaoui, J.M. Basset

- 4:10 INOR 142.** Synthesis, characterization, and reactivity of ruthenium nitrosyl complexes in oxygen-rich ligand environments. Z.J. Tonzetich, V.M. Krishnan
- 4:30 INOR 143.** Dinuclear metallocycles with single anion bridges: Unusual magnetic and NMR properties. D.L. Reger, A.E. Pascui, M.D. Smith, J. Jerierska, A. Ozarowski

- 4:50 INOR 144.** Can polynuclear metal clusters behave as "extended" organometallic complexes? M. Nielsen, T. Betley
- 5:10 INOR 145.** Synthesis and photophysical properties of near-infrared Zn_{16}Ln metallacrown complexes. T.N. Nguyen, S.V. Elseva, I. Martinic, C. Chow, S. Petoud, V.L. Pecoraro

Section G

Boston Convention & Exhibition Center
Room 160A

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

M. L. Neidig, *Presiding*

- 1:30 INOR 146.** Electronic structure and bonding in iron(II)-bisphosphine complexes of relevance to iron catalyzed cross-coupling. J.L. Kneebone, S.L. Daifuku, V.E. Fleischauer, J.A. Bailey, M.L. Neidig

- 1:50 INOR 147.** C-H bond amination mediated by high-spin iron complexes. T. Betley, M.J. Wilding, D. Iovan, A. Mikhailine
- 2:10 INOR 148.** Spectroscopic investigation of in situ formed phenylated iron-bisphosphines and their reactivity in iron-catalyzed cross-coupling. S.L. Daifuku, J.L. Kneebone, B.E. Snyder, M.L. Neidig

- 2:30 INOR 149.** Structure, bonding, and mechanism in iron-catalyzed cross-coupling. M.L. Neidig

- 2:50 INOR 150.** Iron-NHC catalyzed C-C coupling by radical mechanism. J.A. Przyojski, Z.J. Tonzetich
- 3:10** Intermission.

- 3:15 INOR 151.** Mechanistic insights into C-H activation using (phebox)Ir compounds. S.I. Johnson, R.J. Nielsen, M. Zhou, A.S. Goldman, W.A. Goddard

- 3:35 INOR 152.** Borylation chemistry with pincer complexes of iridium. O. Ozerov, L.P. Press, C. Lee, J. Zhou, N. Bhuvanesh

- 3:55 INOR 153.** Rh(III) and Ir(III) complexes bearing protic NHCs: Synthesis and applications. F. Aznarez, M. Iglesias, L.A. Oro, E.F. Hahn

- 4:15 INOR 154.** Iridium catalyzed base-free hydrogenation of esters and lactones. T. Brewster, N.M. Rezaeeyeh, Z. Culaikova, M.S. Sanford, K.I. Goldberg

- 4:35 INOR 155.** Pincer (phebox) Ir(III) complexes in the C-H activation and oxidation of mesitylene. M. Zhou, S. Johnson, R.J. Nielsen, T. Emge, W.A. Goddard, A.S. Goldman

- 4:55 INOR 156.** Liberation of hydrogen from formic acid using homogeneous palladium complexes supported by N-heterocyclic carbene ligands. J. Eddy, P.G. Ariyananda, G.P. Yap, J. Rosenthal

- 5:15 INOR 157.** Selective heterogeneous C-H activation/halogenation reactions catalyzed by Pd@MOF composites. V. Pascanu, F. Carson, M. Vico Solano, M.J. Johansson, X. Zou, B. Martin-Matute

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Technical Session

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SUNDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Bioinorganic Chemistry: DNA, RNA and Inorganic Drugs

S. A. Koch, *Organizer*

6:00 - 8:00

INOR 158. In vitro biological structure-activity relationship of novel dithiocarbamate phosphine gold(I) complexes: DNA binding and molecular docking studies. **A.A. Isab**

INOR 159. Withdrawn.

INOR 160. Synthesis of an enzyme-activated prochelator for combating antibiotic resistance. **D. Besse, K.J. Franz**

INOR 161. Cytotoxic and DNA-binding properties of organorhenium-coordinated non-steroidal anti-inflammatory drugs (NSAIDs). **S. Azemati, S. Pramanik, S.K. Mandal, A.J. Winstead**

INOR 162. Iron complex PzPy: Triggering apoptosis from DNA intercalation. **A. Mokdad, G. Zoppellaro, R. Zboril**

INOR 163. Antiparasitic activity of copper(II) complexes of metronidazole. **J. Wu, J.H. Palmer, R.K. Upmacis**

Section B

Boston Convention & Exhibition Center
Hall C

Building Innovative Solid State Materials Through Solution Chemistry

J. R. Neilson, A. J. Norquist, C. M. Oertel,
Organizers

6:00 - 8:00

INOR 164. Role of noncovalent interactions templated vanadium oxides. **M. Wenny, A.J. Norquist, J. Schrier**

INOR 165. Solution chemical syntheses of solid state nanoelectronic device components. **A.J. Biacchi, A.R. Hight Walker**

INOR 166. Heterogenous frustrated Lewis pairs for small molecule activation. **J. Xing, J. Buffet, D. O'Hare**

INOR 167. Synthesis of metal-organic frameworks containing organophosphine linkers. **R. Sternberg, C.R. Wade**

INOR 168. Synthesis of single crystals and nanostructures of lead oxide carboxylates with halogenated benzoate ligands. **C. Gang, V.S. Mandala, M. Zeller, C.M. Oertel**

INOR 169. Rational synthesis of dimensionally reduced TiS₂ phases. **R.A. Morasse, T. Li, Z. Baum, J.E. Goldberger**

INOR 170. Ultrasonic spray synthesis as a route to shape controlled LaTiON nanoparticles. **E. Rugen, S.E. Skrabalak**

INOR 171. Thermodynamic investigations of actinide and lanthanide complexation: From fundamentals to applications. **P. Dau, L. Rao**

Section C

Boston Convention & Exhibition Center
Hall C

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

6:00 - 8:00

INOR 172. Electrocatalytic reduction of carbon dioxide to carbon monoxide by manganese carbonyl complexes containing diimines: The need for greater conjugation in the dypyrromethane vs. dypyrromethene system. **N.R. Wheeler, B. Dhakal, R.J. Hulme, G.A. Felton**

INOR 173. Photochemistry and redox non-innocence of electron rich fac-Re(I) tricarbonyl β-diketonate and oxyquinolate complexes: A fundamental study toward the application of CO₂ reduction. **K. Ngo, B. Mahantii, N. Lee, J.J. Rochford**

INOR 174. Flow synthesis of magnetic metal-organic frameworks. **K. He, C. Tsui, K.L. Yeung**

INOR 175. Electrocatalytic CO₂ reduction and redox non-innocence of Mn(I) tricarbonyl oxyquinolate complexes. **M.E. McKinnon, K. Ngo, R.P. Narayanan, J.J. Rochford**

INOR 176. Photoelectrochemical characterization of ruthenium flavanoid complexes in a dye-sensitized solar cell. **N. Lee, K. Ngo, G.E. Gilligan, A. Zachary, M. Lamberto, J.J. Rochford**

INOR 177. Recent developments for new Hg²⁺-fluorescence chemosensors based on 2-[4-(2-aminoethylsulfanyl)butylsulfanyl]ethanamine. **N. Wanichacheva, T. Puangsamlee, S. Watpathomsub, S. Kraithong**

INOR 178. Bis(aldimino)pyridine nickel complexes as electrocatalysts for the reduction of CO₂. **R.P. Narayanan, K. Ngo, B.R. Reed, S. Groysman, J.J. Rochford**

INOR 179. Highly sensitive and selective chemosensor based on cyclic fluorescein for Hg²⁺ detection in aqueous solution. **P. Piyanuch, S. Watpathomsub, H. Nienaber, N. Wanichacheva**

INOR 180. Structure-activity properties of curcuminoid ruthenium polypyridyl photosensitizers in dye sensitized solar cells. **G.E. Gilligan, N. Lee, S. Bag, J.J. Rochford**

INOR 181. Electrochemistry of cytochrome c from a cold-adapted microorganism. **N. Dalchand, M.C. Buzzeo, J.S. Magyar**

INOR 182. Synthesis and characterization of a dimanganese Schiff-base complex as an artificial water oxidation catalyst. **S. Kal, J.R. Buchwald, P.H. Dinolfo**

INOR 183. 59Co-NMR studies of Co compounds with O-donor ligands for WOC. **J. Weber, M. Youmans, L. Doerren**

Section D

Boston Convention & Exhibition Center
Hall C

Nanoscience

R. M. Richards, *Organizer*

6:00 - 8:00

INOR 184. Synthesis of polymer ligand stabilized fluorescent platinum nano-clusters and their applications as metal ions sensor and bio-imaging fluorophore. **X. Huang, H. Ishitobi, Y. Inouye**

INOR 185. Surface chemistry and composition manipulation of germanium nanocrystals. **K. Tabatabaei**

INOR 186. Highly fluorinated high-k hybrid dielectric nano materials for solution-processed electronic devices. **Y. Kim, J. Son, J. Lee**

INOR 187. Synthesis of ceria-doped titanate nanosheets and nanotubes. **Y. Fam, S.A. Ferdousi, C. Tsui, K.L. Yeung, Y. Du**

INOR 188. Synthesis and processing of core/alloy nanoparticles with stainless interfaces. **L. Pathade, T.L. Doane, R.D. Slaton, P. Lutz, M.M. Maye**

INOR 189. Synthesis and characterization of hollow Mn₃O₄ nanoparticles. **S. Varapragasam, C. Balasanthiran, J.D. Hoefelmeyer**

INOR 190. Bioresorbable smart stent incorporated with therapeutic nanoparticles for endovascular diseases. **D. Lee, T. Hyeon**

Section E

Boston Convention & Exhibition Center
Hall C

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

6:00 - 8:00

INOR 191. Multi-electron charging of π-bowls: Structural transformations, supramolecular assembly, and metal binding trends. **S.N. Spisak, C. Dubceac, N.J. O'Neill, Z. Zhou, A.S. Filatov, A. Zabula, M.A. Petrukhina**

INOR 192. Unsymmetrical pincer-type palladium complexes containing novel pyrazolyl aminophosphine ligands. **E. Cook, K. Iwasaki, J.D. Masuda, A. Xia**

INOR 193. Withdrawn.

INOR 194. Functionalized triazaphospholes: Intriguing phosphorus heterocycles with many perspectives. **J. Sklorz, C. Mueller**

INOR 195. Synthesis, characterization, and reactivity studies of a boron-nitrogen-containing isostere of tri-*o*-tolylphosphine. **C. McConnell, P. Memmel, C. Fristoe, P. Campbell, S. Liu**

Section F

Boston Convention & Exhibition Center
Hall C

Synthetic Chemistry Approaches to Magnetic Materials

D. E. Freedman, D. Harris, E. E. Rodriguez,
Organizers

6:00 - 8:00

INOR 196. Azamacrocyclic transition metal complexes for MR imaging and spectroscopy. **P.B. Tsitovich, J.R. Morrow**

INOR 197. Hydride reductions to control the magnetic properties of the double perovskite Sr₂FeMoO₆. **N.J. Schreiber, D.D. Taylor, E.E. Rodriguez**

Section G

Boston Convention & Exhibition Center
Hall C

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

6:00 - 8:00

INOR 198. One-step synthesis of hydrophilic up-conversion nanoparticles. **T. Wang, L. Wang, Z. Feng, N. He, Z. Chen**

INOR 199. New heteronuclear lanthanide-niobium oxide clusters. **B. Yan, D. Herrington, B. Garabato**

INOR 200. Influence of the aryl carbonyl group in CMPO ligands for the sensitization of lanthanide luminescence. **E.G. Leach, A.A. Kulesza, S.M. Biros**

INOR 201. Experimental and computational study of lanthanide-CMPO ligand complexes. **A.I. Vanderweide, R.L. Lord, S.M. Biros**

INOR 202. Series of rigid, bidentate ligands with varying degrees of hardness for the selective extraction of actinides from aqueous solutions. **J.A. Cunningham, S.M. Biros**

INOR 203. Synthesis and characterization of multidentate CMPO ligands for use in the complexation and extraction of f-elements. **A.R. Lear, S.M. Biros**

INOR 204. Withdrawn.

INOR 205. Synthesis, characterization, and the near-infrared luminescence properties of Nd^{III} and Yb^{III} complexes containing terpyridine derivative ligand and 3d-4f type conjugated terpyridine-alkyne bridging Yb^{III}-Co⁰ carbonyl cluster complex. **B. Zhu, Y. Liu, Y. Han**

INOR 206. Effect of rotational correlation time and magnetic field strength on the relaxivity of Eu(II)-containing complexes. **C.U. Lenora, M.J. Allen**

INOR 207. Exploration of multifunctional behavior of a metallacrown 21-MC-7 species. **J.C. Lutter, S.V. Eliseeva, J.W. Kampf, V.L. Pecoraro**

INOR 208. Carbazole-based coordination polymers of lanthanides and actinides. **C.E. Bien, D.R. Manke**

INOR 209. Doped hydroxyapatite nanoparticles as scaffolds for multimodal imaging. **D. SantaLucia, A. Washburn, L. Chapman, R. Tan, S. Lapi, A.L. Eckermann**

INOR 210. Electronic structure and thermodynamic studies of actinide and lanthanide complexation. **A. Dinescu, T. Weaver**

Section H

Boston Convention & Exhibition Center
Hall C

Main Group Chemistry

T. W. Hudnall, *Organizer*

6:00 - 8:00

INOR 211. Diels Alder cycloadditions catalyzed by aluminum based Lewis acids. **D. Vidovic, Z. Liu**

INOR 212. Building a Lewis acidic phosphorus. **D. Vidovic, M. Tay, D. Carmichael**

INOR 213. C-F bond activation by transient phosphonium dications. **D. Vidovic, N. Dordevic, M. Tay, D. Dimic, S. Muthaiah**

INOR 214. Intramolecular P-C bond oxidation. **D. Vidovic, G. Ilic**

INOR 215. Boron based nucleophilic ligands. **D. Vidovic, B. Murugesapandian**

INOR 216. m-Terphenyl-stabilized boron (bis)triflates. **D. Vidovic, D. Do, B. Tombling, S. Koo**

INOR 217. Preparative chemistry of potential B-N polymeric precursors. **K. Hauger, J. Cui, R.H. Neilson**

INOR 218. Synthetic efforts toward diamidocarbene-supported terminal borylenes. **A. Ledet, T.W. Hudnall**

INOR 219. Synthesis and characterization of carbene-stabilized arsenic(II) cations. **K.M. Melancon, A.J. Torres, T.W. Hudnall**

INOR 220. Coordination of N-heterocyclic phosphonium (NHP) cations to late transition metals: NHPs as sterically and electronically tunable nitrosyl analogues. **M. Bezpalko, C. Thomas**

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

INOR 221. 2-Trimethylsilylphosphine derivatives: Synthesis, reactivity, and coordination chemistry. **M.H. Habicht, C. Mueller**

INOR 222. Complete dehydrogenation of saturated BN-heterocycles. **Z. Giustra, L. Chou, B. Li, D.A. Dixon, C. Tsung, S. Liu**

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 160A

Inorganic Chemistry Lectureship

W. B. Tolman, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR 223. Semiconductor nanocrystals: Photophysics and technology. **M.G. Bawendi**

9:05 INOR 224. In situ phase transformation of colloidal nanocrystals. **P. Radovanovic**

9:35 INOR 225. Quantum dot–corrole conjugates for optical oxygen sensing. **D.G. Nocera, C. Lemon**

10:05 Intermission.

10:20 INOR 226. Determining band-edge potentials of colloidal quantum dots. **J.L. Dempsey, K.J. Hammon, R.R. Knauf**

10:50 INOR 227. Shining light on metal phosphide quantum dots: Understanding nucleation, growth, and photoluminescence enhancement. **B.M. Cossairt, D. Gary, J. Stein**

11:20 INOR 228. Doped semiconductor nanocrystals: An inorganic perspective. **D.R. Gamelin**

Section B

Boston Convention & Exhibition Center
Room 159

Synthetic Chemistry Approaches to Magnetic Materials

D. Harris, E. E. Rodríguez, *Organizers*

D. E. Freedman, *Organizer, Presiding*

8:30 INOR 229. New polar and magnetic corundum - type oxides, A2BB'O6: High pressure synthesis. **M.K. Greenblatt, M. Li, M. Retuerto, Z. Deng, M. Croft, D. Vanderbilt, M. Ye, P.W. Stephens, J. Hadermann, D. Walker, J. Hemberger, C.P. Grams, C. Jin, W. Li, J.I. Jang, F.O. Saouma, V. Gopalan, H. Akamatsu**

9:00 INOR 230. Nitrogen atom transfer for the assembly of magnetic molecules. **M. Ding, H. Lin, M. Pink, Y. Lozovsky, C. Mathoniere, R. Clerac, J.M. Smith**

9:20 INOR 231. Bottom-up approach to building layered iron chalcogenides for magnetism and superconductivity. **X. Zhou, C. Borg, E.E. Rodriguez**

9:40 INOR 232. New single-molecule magnets with high blocking temperatures. **K.R. Meihaus, S. Demir, J. Zadrozny, P. Bunting, J.D. Rinehart, J.R. Long**

10:10 Intermission.

10:20 INOR 233. Accurate experimental determination of magnetic anisotropy for a rational design of single-molecule magnets. **M. Perfetti, E. Lucaccini, G. Cucinotta, M. Serrì, L. Sorace, R. Sessoli**

10:50 INOR 234. Ca₂Mn₂O₇: A new family of frustrated materials? **D.C. Arnold**

11:10 INOR 235. Strategies for room temperature multiferroic magneto-electric oxides. **M.J. Rosseinsky**

11:40 INOR 236. Synthesis of benzoquinonoid radical-containing materials with strong magnetic exchange coupling. **I. Jeon, J. DeGayner, A. Gaudette, J. Park, A. Banisafar, A. Willis, D. Harris**

Section C

Boston Convention & Exhibition Center
Room 162B

Industrial Inorganic Chemistry: Innovation from Discovery to Applications

N. S. Radu, J. Walzer, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 INOR 237. Development of high functioning, durable smart windows. **H. Turner**

9:35 INOR 238. Homoleptic iridium complexes of 1,2,4-riazolones as blue emitters for OLED solid-state lighting. **G.D. Vo**

10:05 INOR 239. Synthesis and reactivity of backfluorinated NHC carbene complexes. **R. Blanski, R.H. Grubbs**

10:35 Intermission.

10:50 INOR 240. Industrial water treatment chemistry. **C. McInnis**

11:20 INOR 241. Controlling ethylene/ α -olefin selectivity with molecular olefin polymerization catalysts. **J. Klosin**

11:50 INOR 242. Ethylene to 1-hexene: From HTE to continuous unit operations with cyclometallated pyridyl amine chromium catalysts. **S. Brown, J.F. Walzer**

Section D

Boston Convention & Exhibition Center
Room 160C

Metalloenzyme Mechanisms

G. Ghirlanda, I. V. Korendovych, *Organizers, Presiding*

8:30 INOR 243. Controlling biological radical reactions: Lessons from radical SAM. **J.B. Broderick, M. Horitani, A. Byer, K. Shisler, T. Chandra, B.M. Hoffman**

9:00 INOR 244. Role of manganese in streptococcal virulence. **O. Makhlynets, D. Rhodes, A.K. Boal, K. Crump, A.C. Rosenzweig, T. Kitten, J. Stubbe**

9:30 INOR 245. De novo designed [2(4Fe-4S)] ferredoxin mimics: Modulation of redox and ET properties. **G. Ghirlanda, D.J. Sommer**

10:00 Intermission.

10:10 INOR 246. Spectroscopy of nitrogenase and CO — new spectroscopy of enzyme intermediates. **S.P. Cramer, L.B. Gee, A. Scott, P. Nack-Lehman, C. Dapper, W. Newton**

10:40 INOR 247. Discovery of a novel bacterial nitric oxide sensor. **E.M. Boon**

11:10 INOR 248. Snapshots of S-adenosylmethionine radical enzymes. **C.L. Drennan**

Section E

Boston Convention & Exhibition Center
Room 161

Molecular Water Oxidation Catalysis

S. Bernhard, *Organizer*

M. Albrecht, *Organizer, Presiding*

8:00 INOR 249. Iridium(III) bis-pyridine-2-sulfonamide complexes as efficient and durable catalysts for homogeneous water oxidation. **S. Bernhard, M. Li, J.I. Goldsmith, K. Takada**

8:30 INOR 250. Earth abundant metal-based catalysts for artificial photosynthesis. **L. Tong, L. Kohler, R. Zong, R. Zhou, L. Wickramasinghe, A. Kopecky, R.P. Thummel**

9:00 INOR 251. Crafting transition metal water oxidation catalysts. **A.D. Lobet**

9:30 INOR 252. In search for organic catalytic motifs for solar water splitting. **K. Glusac**

10:00 Intermission.

10:30 INOR 253. Studies of the pathways open to copper water oxidation catalysts containing proximal hydroxy groups during basic electrocatalysis. **D.L. Gerlach, S. Bhagan, A. Cruce, M.K. Bowman, S. Pan, E.T. Papish**

11:00 INOR 254. Molecular iron catalysts for water oxidation: Structural basis and reaction mechanism. **M. Costas, Z. Codola, J. Lloret-Fillol, L. Gomez**

11:30 INOR 255. Co-based molecular water oxidation catalysts. **K. Sakai**

Section F

Boston Convention & Exhibition Center
Room 160B

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

M. M. Maye, P. Radovanovic, *Presiding*

8:30 INOR 256. Coordination complexes in carbon nanotube composites for chemiresistive sensing. **S. Liu, L. Moh, G.T. Sazama, A.R. Petty, T.M. Swager**

8:50 INOR 257. Withdrawn.

9:10 INOR 258. Halide passivated colloidal PbS nanocrystals for application in hybrid solar cells. **H. Lu, R.L. Brutchey**

9:30 INOR 259. Using phase behavior and oxidation rates to control symmetry, composition, and internal microstructure in stainless nanomaterials. **M.M. Maye, L. Pathade, T.L. Doane, P. Lutz, R.D. Slaton**

9:50 INOR 260. Gold diazonium reduction on unusual substrates. **I. Bakas, K. Jlassi, D. Aswal, M. Chehimi, M. El Naggari, I. Shehadi, A. Mohamed**

10:10 INOR 261. Withdrawn.

10:30 Intermission.

10:40 INOR 262. Sustained quenching of rotational diffusional motion of catalytic Janus colloids. **S. Das, A. Garg, A. Campbell, D. Velegol, A. Sen, R. Golestanian, S. Ebbens**

11:00 INOR 263. Mechano luminescence and aggregation induced emission of bromine and methoxy substituted naphthyl conjugated β -diketonate compounds. **T.P. Butler, W.A. Morris, J. Samonina-Kosicka, C. Fraser**

11:20 INOR 264. Centimeter long metallic nanowires: Superconductive properties and applications. **J.L. Bischof, W. Zhao, T. Fitzgibbons, P.J. Sazio, M.H. Chan, J.V. Badding**

11:40 INOR 265. Dendritic growth of Pd on Au nanocubes examined by in situ liquid cell scanning transmission electron microscopy. **R.G. Weiner, D. Chen, R.R. Unocic, S.E. Skrabalak**

12:00 INOR 266. Morphology-controlled synthesis of W₁₈O₄₉ nanostructures for highly-efficient photocatalysis. **Z. Huang, J. Song, Z. Wang, X. Zhang, L. Pan, J. Zou**

12:20 INOR 267. Facile approach for the synthesis of sub-micron sized hollow and multiporous organosilica spheres. **M. Segers, M. Sliepen, N. Arlsten, P. Buskens, M. Moller**

Section G

Boston Convention & Exhibition Center
Room 162A

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

E. Borbas, T. Sorensen, *Presiding*

9:00 INOR 268. Advanced microscopy applications of lanthanide centred emission. **T.J. Sorensen**

9:20 INOR 269. Zinc responsive MRI contrast agents for in vivo imaging. **A.F. Martins, J. Yu, C. Preihls, V. Clavijo, P. Zhao, Y. Wu, A.D. Shery**

9:40 INOR 270. Tuning of the triplet-state energy of new highly luminescent Ln(III) complexes. **A. Duerrbeck, A.T. Hor, N.J. Long**

10:00 INOR 271. Development of volatile rare earth containing single-source precursors with proper metal ratios for low-temperature preparation of up- and down-conversion fluoride materials. **M.C. Barry, Z. Wei, A.S. Filatov, E. Dikarev**

10:20 Intermission.

10:30 INOR 272. Synthesis and evaluation of a series of lanthanide chelates that act as T2ex MRI contrast agents. **I. Daryaei, M. Moïnpour, M. Pagel**

10:50 INOR 273. Multiplex imaging with luminescent lanthanide complexes. **E. Borbas**

11:10 INOR 274. Molecular recognition of spermine by LnDOTP³⁻: Toward a noninvasive staging of prostate cancer. **A.O. Olatunde, L.L. Cheng, P.Z. Sun, P. Caravan**

2015 ACS Catalysis Lectureship

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Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Technical Session

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MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 162A

Building Innovative Solid State Materials Through Solution Chemistry

A. J. Norquist, *Organizer*

J. R. Neilson, C. M. Oertel, *Organizers, Presiding*

1:00 INOR 275. Towards multicomponent chalcogenide aerogels: Effect of chalcogenide, capping agent, and crystal structure on the kinetics of assembly. **J. Davis, S. Brock**

1:20 INOR 276. Control over phase and plasmonic behavior of copper sulfide nanoparticles through solution chemistry. **K. Plass**

1:50 INOR 277. Atomic-scale derivatives of transition metal chalcogenides. **J.E. Goldberger, T. Li, R. Morasse**

2:20 INOR 278. Three-phase co-assembly: Tunable, highly-ordered, porous silica films for photonics and sensing applications. **J. Aizenberg, I. Burgess, T. Shirman, K. Phillips, M. Duffy, N. Koay, T. Kay, G. England**

2:50 INOR 279. Low temperature synthesis of (noncentrosymmetric) oxide-fluoride material. **K.R. Poeppelmeier, K. Chang**

3:10 Intermission.

3:20 INOR 280. Functional nanostructured systems through solution chemistry. **M. Aksit, R.D. Robinson**

3:50 INOR 281. Towards magnetic or luminescent halide materials synthesized under hydrothermal conditions. **R. Gautier**

4:10 INOR 282. Photoelectrochemical characteristics of catalyst-modified WO₃ and CuWO₄ synthesized by solution-based methods. **B.M. Bartlett, C.R. Lhermitte, J.G. Verwer**

4:30 INOR 283. New ferrites from hydrofluxes: From zeolite to hexaferrite related structures. **H. Zur Loye**

5:00 INOR 284. Hybrid inorganic-organic materials with an aromatic cation and charge transfer: (C₇H₇)₂SnI₃ and C₇H₇PbI₃. **A. Maughan, J. Kurzman, J.R. Neilson**

Section B

Boston Convention & Exhibition Center
Room 159

Synthetic Chemistry Approaches to Magnetic Materials

D. E. Freedman, D. Harris, *Organizers*

E. E. Rodriguez, *Organizer, Presiding*

1:30 INOR 285. Synthetic approaches to magnetically ordered organic-based magnets With T_cs as high as 400 K (127 °C) and coercive fields as high as 27,000 Oe. **J.S. Miller**

2:00 INOR 286. Magnetism in mixed-anion systems. **E. McCabe, J.S. Evans, C. Stock**

2:20 INOR 287. Strong exchange coupling in radical-bridged dlanthano complexes. **S. Demir, M. Gonzalez, J. Zadrozny, M. Nippe, J.R. Long**

2:40 INOR 288. Synthetic routes to new homo- and heterometallic magnetic molecules and single-molecule magnets. **G. Christou**

3:10 Intermission.

3:20 INOR 289. Modular molecular magnets: Investigation of coupling, anisotropy, and electronic factors on magnetic bistability. **K.R. Dunbar**

3:50 INOR 290. Application of coordination chemistry to the design and synthesis of molecular qubits. **J. Zadrozny, J. Niklas, O. Poluektov, D.E. Freedman**

4:10 INOR 291. Consideration of electronic structure in transition metal complexes for the design of MRI thermometers and magnets. **I. Jeon, D. Harris**

4:30 INOR 292. Synthetic approaches for high-blocking temperature single-molecule magnets. **M. Murugesu**

Section C

Boston Convention & Exhibition Center
Room 162B

High-Energy Organometallic Complexes: Reactivity Driving New Synthesis and Catalysis

C. C. Cummins, M. R. Smith, *Organizers*

R. Waterman, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 INOR 293. Molecular Fe-mediated nitrogen fixation catalysis: Improving turnover and mechanistic insights. **J.C. Peters, S.E. Creutz, T.J. Del Castillo, J. Rittle, N.B. Thompson**

2:00 INOR 294. Chemical transformations with two-coordinate, first-row metal complexes. **T. Tilley**

2:20 INOR 295. New insights on electrochemically-promoted catalytic asymmetric hydrogenation. **B.T. Donovan-Merkert**

2:40 INOR 296. Photohydrides: Visible light-triggered hydride transfer as a strategy in catalysis. **A.J. Miller, C.L. Pitman, S. Barrett, K.R. Brereton, S.A. Slattery**

3:00 INOR 297. Small, but not so innocent, the redox non-innocence of multiply bonded ligands: Implications for catalysis. **T.R. Cundari**

3:20 Intermission.

3:30 INOR 298. Investigation of the reactivity of low-coordinate Ni complexes stabilized by NHC ligands. **S.M. Baldwin, S.A. Del Ciello, R. Witzke, J. Teesdale, G.L. Hillhouse**

3:50 INOR 299. Mechanistic investigations of quantum dot nucleation and growth. **M.P. Campos, L. Hamachi, M.P. Hendricks, I. Jen-La Plante, J.S. Owen**

4:10 INOR 300. Modeling aspects of hydrodeoxygenation: C–O and C–C bond cleavage by electron-rich molybdenum and tungsten trimethylphosphine compounds. **A. Sattler, A.A. Zuzek, D. Buccella, G. Parkin**

4:30 INOR 301. Redox-active M[SNS]₂ cofactors for heterobimetallic catalysis. **A.F. Heyduk, K.E. Rosenkoetter, M. Wojnar, J.W. Ziller**

4:50 INOR 302. Palladium complexes: An umpolung on transition metal carbenes. **P. Cui, C.C. Comanescu, V.M. Iluc**

Section D

Boston Convention & Exhibition Center
Room 160C

Metalloprotein Inhibitors: Drugs, Drug Candidates, and New Targets at the Interface of Medicinal and Inorganic Chemistry

S. Cohen, Z. Sweeney, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 INOR 303. Design and optimization of potent, selective fungal CYP51 inhibitors. **W.J. Hoekstra, E. Garvey, C. Yates, R. Schotzinger**

2:15 INOR 304. Specificity and regulation of metal-dependent deacetylases: Implications for biological function. **C.A. Fierke, C.A. Pitcain, B. Kim, E.D. Sullivan, N.A. Wolfson, J.E. Lopez**

2:50 INOR 305. Structural studies on metal-binding pharmacophores for metalloprotein inhibitors. **S. Cohen**

3:25 Intermission.

3:35 INOR 306. Novel inhibitors of iron and zinc-containing enzymes. **C. Schofield**

4:10 INOR 307. Drug discovery strategies toward a once daily HIV integrase strand transfer inhibitor. **A.M. Walji**

4:45 INOR 308. Recent advances in the development of influenza endonuclease inhibitors. **J. Bauman, H. Sagong, D. Patel, S. Baker, R. Vijayan, A.K. Parhi, K. Das, L. Martinez-Sobrido, E. Arnold, E.J. LaVoie**

Section E

Boston Convention & Exhibition Center
Room 161

Molecular Water Oxidation Catalysis

M. Albrecht, *Organizer*

S. Bernhard, *Organizer, Presiding*

1:30 INOR 309. Translating nature's principles of water oxidation to successful man-made catalysts. **G.C. Dismukes, P. Smith, G. Gardner, C. Cady, K. Galvino, H. Chen, D.A. Case, M.K. Greenblatt**

2:00 INOR 310. Layered calcium manganese oxides (birnessites) as bio-inspired water-oxidation catalysts. **P. Kurz**

2:30 INOR 311. Natural born catalysts: The great beauty of molecular photosynthesis. **M. Bonchio**

3:00 INOR 312. Water oxidation with metal-organic frameworks. **W. Lin**

3:30 Intermission.

4:00 INOR 313. Electrochemically driven water-oxidation catalysis beginning with cobalt-polyoxometalates: Determination of the true, homogeneous vs. heterogeneous catalyst. **R.G. Finke, S. Folkman**

4:30 INOR 314. Bioinspired photochemical water oxidation with cobalt catalysts. **G.R. Patzke, S. Luber**

5:00 INOR 315. Low-temperature syntheses of amorphous mixed-metal oxide electrocatalysts. **C.P. Berlinguette**

Section F

Boston Convention & Exhibition Center
Room 160B

Chemistry of Materials: Materials for Energy and Catalytic Applications

C. G. Lugmair, *Organizer*

A. I. Carrillo Gomez, *Presiding*

1:30 INOR 316. Examining the role of imidazolium ionic liquids in the proton-coupled electron transfer promoted conversion of CO₂ to CO on bismuth based materials. **J.L. DiMeglio, J. Medina-Ramos, R.C. Pupillo, J. Rosenthal**

1:50 INOR 317. Mixed-metal nanosheet water oxidation catalysts made by pulsed-laser ablation in liquids — Part 1: Synthesis, characterization, and electrocatalysis. **B.M. Hunter, J.D. Blakemore, H.B. Gray, J.R. Winkler, A.M. Mueller**

2:10 INOR 318. Hybrid luminescent mesoporous silica with catalytic properties. **A.I. Carrillo Gomez, A. Lanterna, M.L. Marin, J. Scaiano, O. Reiser**

2:30 INOR 319. DFT study on a 2D, π-conjugated, nickel metallo-organic framework for ethylene purification. **S. Moncho Escriva, E.N. Brothers, M.B. Hall**

2:50 INOR 320. Transition metal selenide nanostructures as highly efficient catalysts for oxygen evolution reaction. **A. Swesi, J. Masud, M. Nath**

3:10 INOR 321. Design of silica-based hybrid catalysts and their application in alkane oxidation. **M. Yadav, A.J. Karkamkar**

3:30 Intermission.

3:40 INOR 322. Mixed-metal nanosheet water oxidation catalysts made by pulsed-laser ablation in liquids — Part 2: Mechanistic insights gained by novel in-situ spectroscopies. **B.M. Hunter, H.B. Gray, J.R. Winkler, A.M. Mueller**

4:00 INOR 323. Improving catalytic activity of copper-based inorganic materials for water oxidation. **X. Liu, S. Cui, P. Du**

4:20 INOR 324. Metal organic frameworks as crystallized capping agent for metal nanoparticle synthesis. **L. Chou, A.P. Young, C. Tsung**

4:40 INOR 325. Flexible ion-conducting composite membranes for lithium batteries. **R.D. Miller, S. Kitajima, C. Scott, K. Virwani, D. Bethune, H. Kim, L. Thompson, M. Reich, M. Schneider, W. Schmidbauer, M. Kunze, E. Jung, W. Wilcke, N. Aetukuri**

5:00 INOR 326. Electrochemically driven mechanical energy harvesting. **S. Kim, S. Choi, K. Zhao, H. Yang, G. Gobbi, S. Zhang, J. Li**

5:20 INOR 327. Solution speciation and stability of cobalt-polyoxometalate water oxidation catalysts by X-ray scattering. **M.D. Nyman, S. Goberna-Ferrón, J. Galan-Mascaros**

Section G

Boston Convention & Exhibition Center
Room 160A

Bioinorganic Chemistry: Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

M. I. Galinato, *Presiding*

1:30 INOR 328. Fast unimolecular multiple-site CPET over a large temperature range. **M.A. Bowring, L.R. Bradshaw, D.R. Gamelin, J.M. Mayer**

1:50 INOR 329. Effect of heme enzyme electronic structure modification on their nitrite reductase functionality. **M.I. Galinato, E. Luteran**

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

2:10 INOR 330. Electronic and steric influence on the biomimetic copper(I)-nitro complexes. S.C. Hsu, Y. Chang, W. Chuang

2:30 INOR 331. Biochemical characterization of enzymes involved in sulfur assimilation from dimethylsulfone. D.K. Wicht

2:50 INOR 332. Superoxide dismutase mimicry by a zinc(II) complex with a redox-active organic ligand. C.R. Goldsmith, M. Yu, D.D. Schwartz, J.D. Gordon

3:10 Intermission.

3:20 INOR 333. Imine-functionalized tris(pyrryl)amine ligands: A highly tunable platform for iron oxidation chemistry. Z. Gordon, A. Fout

3:40 INOR 334. Modeling NO signaling: Reversible interaction of NO at a Copper(II) thiolate. S. Zhang, T.H. Warren

4:00 INOR 335. Crystallographic studies of the immune-response, metal chelating protein calprotectin. S.E. Bowman, M. Baker, E.M. Nolan, C.L. Drennan

4:20 INOR 336. Bioinspired aminopyridine transition-metal complexes derived from piperidine for epoxidation catalysis. G. Yang, S. Thompson, E.A. Mikhalyova, E. Rybak-Akimova

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MONDAY EVENING

Section A

Boston Convention & Exhibition Center Hall C

Sci-Mix

S. A. Koch, *Organizer*

8:00 - 10:00

164, 166, 171, 174, 179, 183, 185, 196, 200, 211, 212. See previous listings.

INOR 337. Characterization and reactivity of iron and cobalt bimetallic tris(phosphinoamide) complexes. K.M. Gramigna, S. Kuppuswamy, R. Mathialagan, C.M. Thomas

INOR 338. Lanthanide complexes for environmental and biological imaging. P.S. Barber, M.A. Mendez, S.L. Worters, A.M. McAdams, M. Cendejas, J.P. Guyot, L.D. Jaramillo

497, 499, 500-502, 506, 514, 516, 524-525, 527, 532, 534-536, 540-542, 547, 550-551, 553-554, 560, 567, 573-576, 580-582, 584, 737, 741, 744-747, 750-751, 755, 759, 763, 765-766, 769, 773-776, 779-780, 786. See Subsequent Listings.

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center Room 157B

Inorganic Nanoscience Award

S. L. Stoll, *Organizer, Presiding*

8:20 Introductory Remarks.

8:30 INOR 339. Solution-based synthesis and applications of multifunctional nanomaterials. S.S. Wong

9:00 INOR 340. Nature of the DNA bond. C.A. Mirkin

9:30 INOR 341. Nanoelectronics meets biology: From new tools to electronic therapeutics. C.M. Lieber

10:00 INOR 342. Precise chemical, physical, and electronic nanoscale contacts. P.S. Weiss

10:30 Intermission.

10:45 INOR 343. Zinc oxide nanocrucible arrays for magnetic nanodot synthesis via ALD-assisted block polymer lithography. W.L. Gladfelter, C. Lin, S. Polissetty, L. O'Brien, A. Baruth, M.A. Hillmyer, C. Leighton

11:15 INOR 344. Electrodeposited nanowire photonics. R.M. Penner

11:45 INOR 345. Modeling the effect of carbon nanotube functionalization on mechanical and optical properties. G.C. Schatz

12:15 Concluding Remarks.

Section B

Boston Convention & Exhibition Center Room 159

Synthetic Chemistry Approaches to Magnetic Materials

D. E. Freedman, E. E. Rodriguez, *Organizers*

D. Harris, *Organizer, Presiding*

8:30 INOR 346. Magnetic properties of low-dimensional intermetallic materials. S.M. Clarke, D.E. Freedman

8:50 INOR 347. Synthetic elucidation of design principles for long-lived electronic spin-based qubits. M. Graham, J. Zadrozny, M. Shiddiq, J.S. Anderson, M. Fataftah, S. Hill, D.E. Freedman

9:10 INOR 348. Synthetic strategies for manipulating magnetic properties in microporous manganese oxides. A. Larson, P. Motakef, E.E. Rodriguez

9:30 INOR 349. Superconducting CuSe₂ polymorph selection through kinetically-controlled solid-state metathesis. A. Martinlich, J. Kurzman, J.R. Neilson

Section C

Boston Convention & Exhibition Center Room 162B

High-Energy Organometallic Complexes: Reactivity Driving New Synthesis and Catalysis

M. R. Smith, R. Waterman, *Organizers*

C. C. Cummins, *Organizer, Presiding*

9:00 INOR 350. Synthesis and reactivity of titanium nitrides. From dimers and monomers to discrete salts. D.J. Mindiola

9:20 INOR 351. New nickel(0) complexes supported by chelating N-heterocyclic carbene ligands: Unusual structures and small molecule activation. M. Reineke, M. Sampson, A.L. Rheingold, C.P. Kubiak

9:40 INOR 352. Metal nitrenes and amides in catalytic C-H functionalization. T.H. Warren

10:00 INOR 353. Transition-metal catalyzed reactions that form bonds to phosphorous. R. Waterman

10:20 INOR 354. Small molecule activation by low valent nickel complexes. C.G. Riordan

10:40 Intermission.

10:50 INOR 355. Reduction chemistry of rare-earth metal complexes supported by ferrocene diamide ligands. P. Diaconescu

11:10 INOR 356. M-M interaction in low-valent Ni(II)-Ni(II) species and their use in small molecule activation. F. Olechnowicz, G.L. Hillhouse, R.F. Jordan

11:30 INOR 357. Tandem catalytic processes for light alkane upgrading and ethylene polymerization. J.E. Bercaw, D.C. Leitch, A. Sattler, J.A. Labinger

11:50 INOR 358. Generation of late metal imido and carbene fragments via cooperative reactions across metal-metal bonds in early/late heterobimetallics. C.M. Thomas, S.L. Marquard, B. Wu, J. Krogman, K.M. Gramigna

12:10 INOR 359. Characterization and reactivity of a series of macrocyclic cobalt-Mabiq compounds. C. Hess

12:30 INOR 360. When three's a crowd: Reactivity of low-coordinate Ni-NHC polyfluorometalacycles. R. Baker

Section D

Boston Convention & Exhibition Center Room 160C

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

M. Emmert, *Presiding*

8:00 INOR 361. Structural requirements for interfacial proton-coupled electron transfer. M. Jackson, Y. Surendranath

8:20 INOR 362. Withdrawn.

8:40 INOR 363. Green chemistry design for rare earth recycling. M. Emmert

9:00 INOR 364. Activation of challenging C-O bonds through anion catalysis. M. Emmert

9:20 INOR 365. High-performance aqueous redox flow battery using nontoxic organic-inorganic electrolyte. K. Lin, Q. Chen, M.P. Marshak, M.R. Gerhardt, L. Tong, L. Eisenach, R.G. Gordon, M.J. Aziz

9:40 INOR 366. Photoelectrochemical characterization of non-innocent ligand ruthenium β -diketonate complexes in dye-sensitized solar cells. N. Lee, K. Ngo, G.E. Gilligan, A. Zachary, J.J. Rochford, M. Lamberto

10:00 Intermission.

10:10 INOR 367. Selective carbon dioxide reduction on rhenium grafted to a glassy carbon surface. S. Oh, Y. Surendranath

10:30 INOR 368. Copper(II) bis-perfluoropinacolate complex for electrochemical reduction of nitrate in water. S.F. Hannigan, L. Doerrer, L. Tahsini

10:50 INOR 369. Elucidating biological energy transduction from ammonia: Electronic structure studies of ammonia monooxygenase and hydroxylamine oxidoreductase. K.M. Lancaster, J. Caranto, M. Smith, A. Vilbert, R. Walroth

11:10 INOR 370. Effects of solvent on the ionic liquid mediated electrocatalytic conversion of CO₂ to CO at a Bi-based electrode. T.P. Keane, J.L. DiMeglio, J. Rosenthal

11:30 INOR 371. Investigating the interface between nanostructured black silicon and hydrogen-evolution reaction catalysts: Mapping the semiconductor/metal junction. N.C. Anderson, J. Aguiar, N.R. Neale

11:50 INOR 372. Selective electrocatalytic CO₂ reduction by a polypyridyl-iron complex. D.Z. Zee, M. Nippe, A.E. King, C.J. Chang, J.R. Long

Section E

Boston Convention & Exhibition Center Room 161

Molecular Water Oxidation Catalysis

M. Albrecht, *Organizer*

S. Bernhard, *Organizer, Presiding*

8:30 INOR 373. Cp*Ir and Ir(CO)₂ precatalysts for water oxidation. R.H. Crabtree, G.W. Brudvig, U. Hentermar, J.D. Blakemore, D.M. Tiede, S.W. Sheehan, J. Thomsen, S. Hashmi, M. Zhou, D. Huang

9:00 INOR 374. In situ characterization of molecular water oxidation catalysts. D. Hettterscheid

9:30 INOR 375. From molecular-defined to nanostructured catalysts for water-splitting. M. Beller

10:00 Intermission.

10:30 INOR 376. Computational models applied to homogeneous water oxidation catalysis: What's the value proposition? C.J. Cramer

11:00 INOR 377. Chemical and light-driven oxidation of water catalyzed by iridium complexes. A. Macchioni, A. Bucci, I. Corbucci, L. Fagioli, G. Pastori, C. Zuccaccia

11:30 INOR 378. Molecular water oxidation catalysis with iridium triazolylidene complexes -- enhancing catalytic performance. M. Albrecht, A. Petronilho

Section F

Boston Convention & Exhibition Center Room 160B

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

R. S. Forgan, A. B. Thompson, *Presiding*

8:30 INOR 379. Kinetically tuned dimensional augmentation (KTDA) method to synthesize robust Fe-MOFs with various applications. K. Wang, H. Zhou

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8:50 INOR 380. Synthesis, structure, magnetic and nonlinear optical (NLO) properties of Mn(II), Cu(II), and Ni(II) complexes of 3-(2-pyridyl)-5,6-diphenyl-1,2,4-triazine-4, 4'-disulfonate. **O.A. Odunola, O.A. Ibrahim, E.O. Onawumi, M. Hong**

9:10 INOR 381. Defect Engineered mixed valence Ru-MOFs: Study on the influence of defect metal sites. **W. Zhang, M. Kauer, R. Wagner, D.J. Xiao, K. Epp, O. Kozachuk, Y. Wang, R.A. Fischer**

9:30 INOR 382. Stability through flexibility: Mechanical properties of Zr and Hf MOFs from single crystal techniques. **R.S. Forgan, R. Marshall, C. Hobday, C. Morrison, T. Bennett, S. Moggach**

9:50 INOR 383. Derivatives of MOF-5 via solvothermal and cation exchange techniques. **A.W. Stubbs, C. Brozek, M. Dinca**

10:10 Intermission.

10:20 INOR 384. Synthesis of metal-organic materials (MOMs) using a microwave reactor. **C.V. Gauthier, J.J. Flanagan**

10:40 INOR 385. Synthesis of freestanding metal-organic-framework (MOF) aerogels. **Z. Liu, W. Han, K.L. Yeung**

11:00 INOR 386. Design and synthesis of metal-organic frameworks from bipyrazole ligands. **Q. Jia, Q. Li**

11:20 INOR 387. Grafting heterobimetallic complexes onto the metal organic framework NU-1000. **A.B. Thompson, T. Wang, J.T. Hupp, O.K. Farha, R. Penn, A. Stein, C. Lu**

11:40 INOR 388. Quantitative direct and indirect mapping of linker distributions in mixed linker MOFs via STEM-EDX. **C. Wiktor, M. Meledina, S. Turner, G. van Tendeloo, R.A. Fischer**

Section G

Boston Convention & Exhibition Center
Room 160A

Electrochemistry

B. L. Lucht, Organizer, Presiding

8:30 INOR 389. Optimizing the electrocatalytic reduction of CO₂ by Re- and Mn-based bipyridine complexes with supramolecular assembly. **C.W. Machan, S.A. Chabolla, C.P. Kubiak**

8:50 INOR 390. Low cost electrocatalysts with pendant functionality: The mechanism of enhanced electrocatalytic activity for CO₂ reduction. **G. Neri, C. Wilson, J.J. Walsh, A.J. Cowan**

9:10 INOR 391. Quinone electrochemistry in acidic and alkaline solutions and its application in large-scale energy storage. **M.R. Gerhardt, C. Chen, K. Lin, M.P. Marshall, L. Tong, C. Galvin, R.G. Gordon, M.J. Aziz**

9:30 INOR 392. Graphene as a protective layer for silicon in an aqueous PEC cell. **A. Nielander, N.S. Lewis**

9:50 INOR 393. Mechanistic insights into proton coupled electron transfer activation of CO₂ catalyzed by pure metal surfaces. **A. Wuttig, Y. Surendranath**

10:10 INOR 394. Role of 1, 3-propane sultone and vinylene carbonate in solid electrolyte interface (SEI) formation and gas generation.

B. Zhang, B.L. Lucht, M. Metzger, S. Solchenbach, H. Gasteiger, S. Meini

10:30 INOR 395. Improved performance of graphite/LiNi_{0.5}Mn_{1.5}O₄ cells cycled to high voltage (4.8 V) with electrolyte additives. **Y. Dong, B.L. Lucht, M. Xu, L. Zhou, F. Chesneau**

Section H

Boston Convention & Exhibition Center
Room 162A

Chemistry of Materials: Synthesis and Properties

C. G. Lugmair, Organizer

P. J. Cappillino, Presiding

8:30 INOR 396. Anion sensing using a platinum(II) complex. **A.E. Norton, J.A. Krause, W.B. Connick**

8:50 INOR 397. Synthesis and characterization of tungsten nitrido precursors for deposition of WN_x films. **A. Koley, K. McClain, M. Nolan, C. O'Donohue, T. Anderson, L. McElwee-White**

9:10 INOR 398. Effects of alpha substitution and strapped structure on the mechanochromic luminescence and aggregation-induced emission behavior of difluoroboron β-diketonate dyes. **W.A. Morris**

9:30 INOR 399. Effect of nitrate concentration on the properties of solution-processed Al₂O₃ thin films. **C. Perkins, J.C. Ramos, D. Park, B. Fulton, D.W. Johnson, D.A. Keszler**

9:50 INOR 400. Synthesis of nanostructured, bimetallic, noble metal powders using Atomic Layer Electroless Deposition (ALED). **P.J. Cappillino, J.D. Sugar, F. el Gabaly, T.Y. Cai, Z. Liu, J.D. Stickle, D.B. Robinson**

10:10 INOR 401. InP quantum dots with tunable emission by post-synthetic modification with Lewis acids. **J. Stein, B. Cossairt**

10:30 Intermission.

10:40 INOR 402. Supercritical fluid electrodeposition of germanium. **P. Bartlett, C. Cummings, M. Hasan, A.L. Hector, W. Levason, D. Pugh, G. Reid, D. Smith, J. Spencer**

11:00 INOR 403. Porous carbon coated metal nanoparticles for electrocatalysis. **M. Sheehan, M. Rudden, C. Tsung**

11:20 INOR 404. Dual electrically conducting spin-crossover bifunctional molecular materials based on cobalt-TCNQ radical salts. **X. Zhang, Z. Wang, H. Xie, K.R. Dunbar**

11:40 INOR 405. Smectic A mesophases from luminescent sandic platinum(II) mesogens. **M. Krikorian, C. Voll, M. Yoon, K. Venkatesan, T.M. Swager**

12:00 INOR 406. Two synthetic systems of nonlinear optical crystals with disparate phase matchabilities. **M.D. Donakowski, H. Lu, R. Gautier, K.R. Poeppelmeier**

12:20 INOR 407. Addressing challenges in nanocrystal synthesis using substituted thiourea and selenourea precursors. **M.P. Campos, M.P. Hendricks, L. Hamachi, I. Jen-La Plante, R. Swain, G. Cleveland, A. Graham, J.S. Owen**

Section I

Boston Convention & Exhibition Center
Room 158

Organometallic Chemistry: Synthesis and Characterization

N. S. Radu, Organizer

G. L. Powell, Presiding

8:30 INOR 408. Stabilizing unusual oxidation state of heterometallic complexes by coordination of low valent group 13 organyls ECp* (E = Al, Ga, In). **J. Kim, C. Gemel, R.A. Fischer**

8:50 INOR 409. Bis-cyclometalated iridium complexes supported by β-ketiminato (acNac) and β-diketiminato (NacNac) ligands. **T.S. Teets, A. Maity, Y. Radwan**

9:10 INOR 410. Synthesis and reactivity of PBP-type pincer iridium and rhodium complexes. **W. Shih, W. Gu, M.C. MacInnis, O. Ozerov**

9:30 INOR 411. Aqueous hydride transfer thermodynamics of a bime-tallic iridium ruthenium complex. **K.R. Brereton, C.L. Pitman, A.J. Miller**

9:50 Intermission.

9:55 INOR 412. Synthesis, characterization, and reactivity of a novel Ru(0)-NHCP complex. **T. Wang, L. Pan, E. Mosafari, D.W. Stephan**

10:15 INOR 413. Multinuclear osmium carbonyl complexes with dicarboxylate ligands. **G.L. Powell**

10:35 INOR 414. Understanding electronic structure requirements for iron-catalyzed C-H bond hydroxylation. **C. Kleinlein, T. Betley**

10:55 INOR 415. Withdrawn.

11:15 INOR 416. New paramagnetic rhodium(II) dimers without Rh-Rh bonds. **D. Zhu, P. Budzelaar**

Section J

Boston Convention & Exhibition Center
Room 157C

Inorganic Spectroscopy

S. A. Koch, Organizer

I. S. Butler, Presiding

9:00 INOR 417. Variable-temperature and high-pressure Raman spectra of the group 8 metallocenes (η⁵-C₅H₅)₂M (M = Fe, Ru, Os). **I.S. Butler, Y. Desjardins-Langlais**

9:20 INOR 418. Two-photon absorption spectroscopy of inorganic compounds. **K. Takematsu, S. Wehlin, W. Sattler, J.R. Winkler, H.B. Gray**

9:40 INOR 419. Spectroscopic monitoring of proton transfer and proton-coupled electron transfer reactions. **T.T. Eisenhart, W.C. Howland, J.C. Lennox, J.L. Dempsey**

10:00 Intermission.

10:10 INOR 420. Electronic coupling studies in quadruply bonded Mo₂ and W₂ complexes. **C. Ziehm, M.H. Chisholm**

10:30 INOR 421. Electronic and spectroscopic properties of avo-benzene derivatives attached to M₂ quadruple bonds (M = Mo and W). **M.H. Chisholm, C.B. Durr, T.L. Gustafson, W. Kender, T. Spilker, P.J. Young**

10:50 INOR 422. Probing molecular magnetism by inelastic neutron scattering. **S.E. Stavretis, S. Hunter, A.A. Podlesnyak, L. Chen, X. Chen, Z. Xue**

2015 ACS Catalysis Lectureship

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International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Technical Session

Sponsored by PMSE, Cosponsored by INOR†

TUESDAY AFTERNOON

Section B

Boston Convention & Exhibition Center
Room 159

Organometallic Chemistry: Applications to Materials and Polymer Science

N. S. Radu, Organizer

J. A. Byers, Presiding

1:30 INOR 423. On the mechanism of the regio- and stereoselective cyclopolymerization of 1,6-hepta- and 1,7-octadiynes by mo-imido alkylidene N-heterocyclic carbene catalyst. **M. Buchmeiser, K. Herz, J. Haenle, W. Frey**

1:50 INOR 424. Withdrawn.

2:10 INOR 425. Mechanistic insights into the stereoselective ring opening polymerization of poly(lactic acid) catalyzed by achiral iron(II) based complexes. **A. Kaur, C.M. Manna, F. Haeffner, J.A. Byers**

2:30 INOR 426. Controlling stereochemistry, architecture, and composition in ring opening polymerization reactions using a versatile iron-based catalyst. **J.A. Byers, A.B. Biernesser, K.R. Delle Chiaie, A. Kaur, J.A. Kehl, J.B. Curley**

2:50 INOR 427. Hysteretic adsorption of CO₂ onto a Cu₂(pzdc)₂(bpy) porous coordination polymer and concomitant framework distortion. **K. Riascos-Rodríguez, A.J. Schroeder, M.R. Arend, P.G. Evans, A.J. Hernandez-Maldonado**

3:10 INOR 428. General mechanism for the synthesis of group II-VI and IV-VI nanocrystals. **H. Liu, R. Garcia-Rodríguez**

Section C

Boston Convention & Exhibition Center
Room 162B

High-Energy Organometallic Complexes: Reactivity Driving New Synthesis and Catalysis

C. C. Cummins, R. Waterman, Organizers

M. R. Smith, Organizer, Presiding

1:30 INOR 429. Self-assembled multinuclear palladium catalysts for olefin polymerization. **R.F. Jordan, J. Wei**

1:50 INOR 430. Secondary coordination sphere effects promote chlorine photoelimination from monomeric Ni(III) complexes. **D.G. Nocera, B. Anderson, S. Hwang, D.C. Powers, A. Maher, R. Hadd**

2:10 INOR 431. Importance of making molecules in catalysis. **M.R. Smith**

2:30 INOR 432. Gold diazomethyl and gold ketenylidene clusters: Reactive carbide precursors? **J.P. Sadighi, N.T. Daugherty, J. Bacsa**

2:50 INOR 433. Electronic and reactivity effects of N-heterocyclic carbene and functionalized diphosphine ligands on tungsten-benzylidene complexes. **C. Hansen, M.D. Hopkins**

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

3:10 Intermission.

3:20 INOR 434. Reactivity of nitrene/imido complexes of $\{bis-(1-N(DIP-P)_2-2-phenyl)diimine\}M$ (1-M; M = Ti, Cr, Fe). P.T. Wolczanski, S.P. Heins, W.D. Morris, E.B. Lobkovsky, T. Cundari

3:40 INOR 435. New rhodium complexes for the activation and functionalization of strong bonds. T.B. Gunnoe, W.A. Goddard, T. Cundari, R.J. Nielsen, M.S. Webster-Gardiner, M.E. O'Reilly, B.A. Vaughan, R. Fu, D. Pahls, M. Sabat

4:00 INOR 436. Joys of nickel(0) chemistry: C–CN bond activation of aromatic nitriles, h^2 -arene intermediates, and the effect of Lewis acids. W.D. Jones, T. Li, J.J. Garcia, B.D. Swartz

4:20 INOR 437. High-energy organometallics featuring encumbering isocyanides. J.S. Figueroa, C.C. Mokhtarzadeh, A. Carpenter

4:40 INOR 438. Macrobicyclic hexacarboxamide cryptand coordination chemistry. J. Stauber, E.D. Bloch, C.C. Cummins, D.G. Nocera, K.D. Vogiatzis, L. Gagliardi

5:00 Concluding Remarks.**Section D**

Boston Convention & Exhibition Center Room 160C

Coordination Chemistry**Macrocycles and More**

D. C. Crans, *Organizer*

E. Rybak-Akimova, *Presiding*

2:00 Introductory Remarks.

2:05 INOR 439. From reversible oxygen binding with synthetic macrocycles to oxygen activation and catalytic oxidations. E. Rybak-Akimova

2:25 INOR 440. Not so sticky side of sugars: Metal complexes interaction with monosaccharides in aqueous media. G.T. Musie, C. Stewart, M.A. Pedraza, H. Arman

2:45 INOR 441. Rhenium chalcogenide clusters containing N-heterocyclic carbene ligands. L.F. Szczepura, W. Wilson, D. Huh

3:05 INOR 442. Imaging gene expression in mammals: A coordination chemistry solution. T.J. Meade, S.M. Kamper

3:30 INOR 443. Macrocyclic metal complexes designed for enhanced protein binding: Biological activity and molecular imaging. B. Burke, G. Clemente, C. Cawthorne, S.J. Archibald

3:55 INOR 444. Reprogramming EF-hands for design of catalytically amplified lanthanide sensors. I.V. Korendovych, K. Mack, O. Moroz, Y. Moroz, A. Olsen, J. McLaughlin

4:15 INOR 445. Heterobimetallic complexes: Structure and function. A. Borovik

4:40 INOR 446. Glimpses into the power of synthetic macrocycles in transition metal and supramolecular coordination chemistry. K. Bowman-James

Section E

Boston Convention & Exhibition Center Room 161

Bioinorganic Chemistry: Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

D. Rokhsana, D. K. Wicht, *Presiding*

1:30 INOR 447. Mimicking [FeFe] hydrogenase by covalent linkage of a synthetic diiron cluster to polymer scaffolds. C.A. Tooley, E.B. Berda, S. Pazić

1:50 INOR 448. Lewis acid-induced valence tautomerism of a manganese(V)-oxo porphyrinoid complex results in dramatic inhibition of oxygen atom transfer reactivity. J. Zaragoza, R.A. Baglia, M. Siegler, D.P. Goldberg

2:10 INOR 449. Streptavidin artificial metalloproteins for asymmetric catalysis. C. Chen, C. Chang, C. Yang, S.C. Hsu, J. Carey

2:30 INOR 450. Porphyrin-containing polymer nanoparticles for modeling heme proteins iron coordination. K. Rodriguez, S. Pazić

2:50 INOR 451. Constrained peptides: Investigating metal binding and catalytic activity. A.R. Aldous, K.P. Neupane, M.R. Eshelman, J. Kritzer

3:10 Intermission.

3:20 INOR 452. Old cofactor in a new light: Adenosylcobalamin in light-dependent gene regulation. M. Jost, S. Padmanabhan, M. Elias-Armanz, C.L. Drennan

3:40 INOR 453. Insights from QM and QM/MM models of carbon monoxide dehydrogenase containing a unique Mo-Cu center. D. Rokhsana, T. Large, M. Dienst, M. Retegan, F. Neese

4:00 INOR 454. Geometrical and electronic structure of the nitrosyl adduct of the non-heme iron active site in anthranilate 1,2-dioxygenase revealed through 14 , 15 N and 12 H ENDOR spectroscopy. V. Hoeke, D.M. Kurtz, B.M. Hoffman

4:20 INOR 455. Functional bioinorganic peptide assemblies. H.C. Fry, L.A. Solomon

4:40 INOR 456. Spontaneous carbon dioxide activation by bimetallic nickel complexes. F. Möller, U. Apfel

Section F

Boston Convention & Exhibition Center Room 160B

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

J. A. Byers, C. R. Wade, *Presiding*

1:30 INOR 457. Variable-temperature in situ powder X-ray diffraction monitoring of mechanosynthesis of metal-organic frameworks. K. Uzarevic, I. Halasz, C. Mottillo, A. Puškaric, P. Julien, V. Strukil, T. Friscic

1:50 INOR 458. Synthesis of nanoscale zirconium porphyrin MOFs for biomedical applications. M. Ketty, W. Morris, D. Harris

2:10 INOR 459. Molecular encapsulation beyond the aperture size limit in metal-organic framework crystals. C. Tsung

2:30 INOR 460. In situ monitoring of a mechanochemical reaction reveals a metastable polymorph of the archetypal framework ZIF-8. A.D. Katsenis, A. Puškaric, C. Mottillo, P. Julien, K. Uzarevic, S.A. Kimber, P. Lazic, R. Dinnebier, I. Halasz, T. Friscic

2:50 INOR 461. Mechanochemistry: An excellent approach to bulk, clean and high-yielding synthesis of metal-organic frameworks. T. Friscic

3:10 Intermission.

3:20 INOR 462. Mechanistic features of linker exchange in ZIF-8 and UiO-66. J.A. Byers, C. Tsung, J.V. Morabito, Z. Li, R. Kyada, M. Nero

3:40 INOR 463. polyMOFs: A new class of interconvertible polymer-MOF hybrid materials. Z. Zhang, S. Cohen

4:00 INOR 464. Metal-organic framework supported pincer complexes: At the interface of homogeneous and heterogeneous catalysis. C.R. Wade, S.A. Burgess, S. Baranowski

4:20 INOR 465. Basic post-synthetic modification approach of Cr derived metal-organic frameworks (MIL-101) for the efficient promotion of Knoevenagel condensation reaction. Y. Luan

4:40 INOR 466. Metal-organic frameworks as platform to arrange and protect single-molecule magnets in multidimensional arrays. M. Wriedt, D. Aulakh, J.B. Pyser

Section G

Boston Convention & Exhibition Center Room 160A

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

M. Buchmeiser, *Presiding*

1:30 INOR 467. New methods for the construction of highly-encumbered C–C bonds using a simple cobalt catalyst. M.R. Brennan, A. Fout

1:50 INOR 468. New molecular ruthenium and iron electrocatalysts for the reduction of carbon dioxide. C.W. Machan, M.D. Sampson, C.P. Kubiak

2:10 INOR 469. Molybdenum and tungsten imido alkylidene N-heterocyclic carbene complexes: Activity, immobilization, and functional group tolerance in olefin metathesis. M. Buchmeiser, S. Sen, R. Schowner, D. Imbrich, W. Frey

2:30 INOR 470. Challenges in optimizing alkyne metathesis catalysts. Ó. Arias i Burguera, K. Brandhorst, M. Freytag, P.G. Jones, M. Tamm

2:50 INOR 471. Molecular iridium complexes for applied water oxidation electrocatalysis. S.W. Sheehan, U. Hintermair, J. Thomsen, G.W. Brudvig, R.H. Crabtree, C.A. Schmuttenmaer

3:10 Intermission.

3:20 INOR 472. Insights into redox cooperativity between cocatalysts: Mechanistic studies of aerobic alcohol oxidation by Cu and redox-active organic cocatalysts. S.D. McCann, S.S. Stahl

3:40 INOR 473. Homogeneous catalysis for signal enhancement in NMR: From catalyst design to analytical applications. B. van Weerdenburg, N. Eshuis, N. Herkmens, S. Wijmenga, M. Tessari, M. Feiters, F.P. Rutjes

4:00 INOR 474. (NHC)₂Pd(0)-catalyzed *cis*-bis-silylations of internal alkynes with unactivated disilanes. O. Navarro, J. Spencer, M.B. Ansell, G. Cloke, M. Roe

4:20 INOR 475. Hydrosilylation of internal C–C multiple bonds – insights on mechanism and kinetics. T.K. Zimmermann, K. Riener, F.E. Kuehn

4:40 INOR 476. Metal-ligand multiple bonds in iron complexes competent for ppm-loading C–H amination. M.J. Wilding, T. Betley

5:00 INOR 477. Ring-opening polymerization of lactides and lactones by an indium alkoxide salen complex. S. Quan, P. Diaconescu

Section H

Boston Convention & Exhibition Center Room 162A

Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*

C. T. O'Hara, *Presiding*

1:30 INOR 478. Iron catalyzed α -C–H oxidation of tertiary amines inspired by cytochrome P450. C.J. Legacy

1:50 INOR 479. Developing a complementary metalation strategy to directed *ortho*-metalation: Directed *meta-meta'*-dimetalations of polyaromatics. C.T. O'Hara, A. Martinez-Martinez, R.E. Mulvey

2:10 INOR 480. Template base directed metallations in arene and metallocene chemistry. R.E. Mulvey, C.T. O'Hara

2:30 INOR 481. Competitive C–N and C–O reductive elimination from an isolated Pd(IV) hydroxo alkyl amido complex. E. Abada, A.N. Vedernikov

2:50 Intermission.

3:00 INOR 482. PCN pincer complexes of Pd^{II}: Hydrogenolysis of mono- and dinuclear hydroxides. W.D. Bailey, L. Luconi, A. Rossin, S.E. Flowers, W. Kaminsky, R.A. Kemp, G. Giambastiani, K.I. Goldberg

3:20 INOR 483. Catalysis with low-valent cobalt bis(carbene) pincer complexes. A. Ibrahim, A. Fout

3:40 INOR 484. In the quest for new highly active and versatile catalysts for Pd-catalyzed allylic substitution reactions. O. Pamies, M. Diéguez

4:00 INOR 485. Photoredox catalytic trifluoromethylation of non-prefunctionalized alkenes and heterocycles using cyclometalated Pt(II) complexes. Y. You

4:20 INOR 486. Mechanistic details for the acceptorless dehydrogenation of primary amines to nitriles with Ru-[NNN] pincer complexes. L. Hale, N.K. Szymczak, T. Malakar, A. Paul

4:40 INOR 487. Mechanistic studies on the reductive elimination of C(sp³)-X bonds from RhIII. T. Stevens, K.I. Goldberg

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Section I

Boston Convention & Exhibition Center
Room 158

**Organometallic Chemistry:
Synthesis and Characterization**

N. S. Radu, *Organizer*

C. R. Wade, *Presiding*

1:30 INOR 488. Intermetalloid transition metal-group 13 clusters: A novel approach on molecular congeners of Hume-Rothery phases. **J. Wessing**, C. Ganesamoorthy, C. Gemel, R.A. Fischer

1:50 INOR 489. Nickel complexes supported by a monoanionic bis(carbene) ligand: Reactivity and accessibility of higher oxidation states. **G. Espinosa Martinez**, A. Fout

2:10 Intermission.

2:15 INOR 490. Characterization of iron imido species relevant to *N*-group transfer chemistry. **D. Iovan**, T. Betley

2:35 INOR 491. Development of binuclear gold complexes for reductive coupling. **B. Reiner**, C.R. Wade

2:55 INOR 492. Synthesis of group VI carbonyl species bearing bis-tetrazinyl pyridine (btzp) ligand. **N.A. Maciulis**, S.M. Curtis, C. Chen

3:15 INOR 493. Alkene and alkyne activation in a bisphosphine monoxide gold(I) complex. **C. Hahn**

3:35 INOR 494. Synthesis and characterization of heptacoordinate amidinate complexes. **T. Callaway**, Z. Xue

3:55 INOR 495. Actinide metal fluorides: Synthesis, characterization, and chemistry. **A.G. Lichtscheidl**, M.J. Monreal, K. Browne, D.E. Morris, B. Scott, A.T. Nelson, J.L. Kiplinger

**International Entrepreneurship:
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TUESDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Chemistry of Materials

C. G. Lugmair, *Organizer*

6:00 - 8:00

INOR 496. Synthetic approaches to iron selenide nanostructures. **S.E. Ingram**, S.L. Stoll

INOR 497. Effects of calcination on rutile white pigment via short sulfate process. **C. Tian**

INOR 498. Tryptophan as fluorescent guest in metal-organic framework. **N. Fedorka**, B. Yan

**Technical program information
known at press time.**

**The official technical program
for the 250th ACS National
Meeting is available at:
www.acs.org/boston2015**

INOR 499. Precursor synthesis and atomic layer deposition of CoO, thin films. **J. Kim**, R.A. Fischer, A. Devi

INOR 500. Mechanochromic luminescence and mechanochromic luminescence quenching of iodine-substituted difluoroboron β -diketonate dyes with varying alkyl chain lengths. **W.A. Morris**

INOR 501. Superacidic mesoporous materials. **A. Vasiliev**, O. Adetola

INOR 502. Pattern formation observed during the flow-driven precipitation of calcium oxalate and calcium carbonate. **B. Bohner**, G. Schusztar, D. Horvath, A. Toth

INOR 503. Multicomponent metal-organic frameworks and their controlled defect structures. **S.J. Lee**, L. Liu, J.J. Pak, S.G. Telfer

INOR 504. Oxygen reduction reaction using MnO₂ and ordered mesoporous carbon composites as electrocatalysts for Li-O₂ battery applications. **J. Chen**, C. Chin, H. Yang

INOR 505. Synthesis of novel PEG-2000/Fe-MIL-101 composite phase change material and study of its thermal properties. **Y. Qi**, Y. Luan, M. Yang, G. Wang

INOR 506. Tuning non-covalent interactions between substituted sphenylcyanines with C₆₀ and C₇₀ fullerenes. **H.M. Rhoda**, M. Kayser, Y. Wang, A.Y. Nazarenko, R. Belosludov, P. Kiprof, D.A. Blank, V. Nemykin

INOR 507. Carbonized metal organic frameworks for electrocatalysis and electrochemical energy storage. **M. Sheehan**, H. Cai, C. Tsung

INOR 508. Synthesis of functionalized of Co- and Zn-dipyrazolate metal-organic frameworks. **S.O. Gunther**, C.R. Wade

INOR 509. Synthesis of novel porous coordination polymer material for smart antenna application. **H. Wang**

INOR 510. Mechanical and thermal properties study of silica aerogel insulation material and its property prediction using big data. **H. Wang**

INOR 511. Magnetic behavior of conductive 2D metal-organic frameworks. **T. Soejima**, M.G. Campbell, M. Dinca

INOR 512. General approach to robust, freestanding MOF-polymer composite membranes. **M.S. Denny**

INOR 513. Palladium detection and sorption by sulfur-laced MOFs: Implications for heterogeneous catalysis and nuclear wastes. **Z. Xu**, M. Zha, J. Liu

INOR 514. Graphene-polypyrrole composite materials as counter electrodes in dye sensitized solar cells. **K. Devarapaly**

INOR 515. Size dependence of metal-insulator transition in stoichiometric Fe₃O₄ nanocrystals. **J. Lee**, T. Hyeon

Section B

Boston Convention & Exhibition Center
Hall C

**Coordination Chemistry:
Characterization and Applications**

D. C. Crans, *Organizer*

6:00 - 8:00

INOR 516. Calixarene compounds and their use as molecular materials. **J.F. Ferreira**, I.A. Bagatin

INOR 517. Terpyridine-based metal complexes incorporating secondary sphere hydrogen bonding. **E.W. Dahl**, N.K. Szymczak

INOR 518. Characterization of oxometalates interactions with interfaces. **I. Sanchez Lombardo**, S. Alvarez, K.R. Werst, N.A. Segaline, N.E. Levinger, D.C. Crans

INOR 519. Bipyridine-supported zinc flavonolate photoCORMs. **M. Popova**, S.A. Sorenson, A. Arif, L.M. Berreau

INOR 520. Further explorations in Cu-O₂ interactions with perfluorinated O-donor ligands. **S. Neville**, L. Doerrer

INOR 521. Spontaneous thermal dispersion of LiCl in [Zn(bdc)(ted)₃]: A study of structural changes and pure component equilibrium adsorption of carbon dioxide, methane, and hydrogen. **G. Mass-Gonzalez**, J. Guerrero-Medina, L. Pacheco-Londoño, S.P. Hernandez-Rivera, R. Fu, A.J. Hernandez-Maldonado

INOR 522. Single-ion magnetic properties in a new heterobimetallic complex. **M. Ding**, M. Pink, R. Clerac, Y. Lozovyy, J.M. Smith

INOR 523. Chemical tools for detecting Mn²⁺ in live cells. **S. Bakthavatsalam**, A. Sarkar, A. Rakshit, A. Datta

INOR 524. Metalloporphyrin-based dual mode colorimetric sensors. **D.J. Miller**, M.J. Gunsch, K.A. Leamy, C.L. Bablin, L.J. Tucker, J.L. O'Donnell

INOR 525. Non-toxic and water-soluble CO-releasing molecule for medicinal applications. **R. Mede**, M. Klein, H. Görls, G. Gessner, R. Claus, M. Schmitt, M. Bauer, S. Heinemann, J. Popp, M. Westerhausen

INOR 526. Luminescent lanthanide complexes containing Schiff base ligands. **C. Lau**, P.K. Yuen

INOR 527. Synthesis and characterization of novel nickel complexes and their application in electrocatalysis. **S. Sobottka**, M. van der Meer, B. Sarkar

Section B

Boston Convention & Exhibition Center
Hall C

**Coordination Chemistry: Synthesis
and Characterization**

D. C. Crans, *Organizer*

6:00 - 8:00

INOR 528. Fe(II), Co(II), and Ni(II) complexes of macrocycles with benzimidazole and imidazole pendants for ParaCEST MRI applications. **P.J. Burns**, P.B. Tstivovich, A. Olatunde, J.R. Morrow

INOR 529. Assignment of ¹H resonances in *cis*-(dichloro)ruthenium(II) complexes containing bidentate heterocyclic ligands based on 2,2'-bipyridine

D. Rillema, H. Nguyen

INOR 530. Varying binding mode and electronic structural aspects of ruthenium coordinated Nindigo ligand. **P. Mondal**

INOR 531. Coordination chemistry of sulfur and selenium oxidized derivatives of tris(2-pyridyl)phosphine with select lanthanide salts. **A.R. Bevan**, C. Fairfield, A.K. Frampton, D. Pericic, N.A. Piro, W.S. Kassel

INOR 532. Synthesis, characterization, and the coordination chemistry with select lanthanide nitrates of di(2-pyridinyl)phenylphosphonate and oxide derivatives. **C. Fairfield**, D. Pericic, A.K. Frampton, N.A. Piro, W.S. Kassel

INOR 533. Synthesis, characterization, and coordination chemistry of tris(3,5-dimethylpyrazolyl)phosphine oxide and bis(3,5-dimethylpyrazolyl)phenylphosphine oxide. **A.K. Frampton**, D. Pericic, C. Fairfield, W.G. Dougherty, N.A. Piro, W.S. Kassel

INOR 534. Synthesis and characterization of novel Cu(I) and Ag(I) azolate/phenanthroline and azolate/terpyridine complexes. **A.R. Hinkle**, A. Siller, K. Reyes, T. Nguyen, M. Omary

INOR 535. Synthesis, characterization, and reactivity of Cl-Nb(PrNPh₂)₃M-Br complexes (M = Co, Fe). **G. Culcu**, C. Thomas

INOR 536. Novel ruthenium(II) complexes with polythiamacrocycles. **A.Y. Nazarenko**, E. Rybak-Akimova

INOR 537. Induction of E/Z azobenzene isomerization as a pendant moiety of Re(CO)₃ diimine complexes. **A. Hasheminasab**, L. Wang, M. Dawadi, R.S. Herrick, J. Rack, C.J. Ziegler

INOR 538. Intermolecular nucleophilic attack to coordinated 1,10-phenanthroline. **J.A. Perez**, R. Arevalo, L. Riera

INOR 539. Mid- to late- transition metal complexes with a new NNN pincer ligand. **H. Lin**, S. Nguyen, W. Lee

INOR 540. Mimicking the secondary coordination sphere of metalloproteins using a pyrrole-imine ligand scaffold. **M.J. Drummond**, Z. Gordon, A. Fout

INOR 541. Synthesis and self assembly of a bis-bidentate secondary [hoshine oxide metal complex for small molecule activation. **N.I. Rinehart**, A. Kendall, D. Tyler

INOR 542. Mixed ligand complexes of bis(2,2'-bipyridine)copper(II) perchlorate with selected pseudohalides: Synthesis, characterization, and X-ray structures. **O. Adekunle**, R. Butcher, O. Bakare, O.A. Odunola

INOR 543. Spectroscopic and solid state evaluation of tetra-aza macrocyclic cobalt complexes with solution behavior that parallels the classic cobalt(II) chloride equilibrium. **H.M. Johnston**, K.M. Lincoln, K.N. Green

INOR 544. Metal-metal bonding in heterobimetallic Ti/IV complexes. **B. Wu**, C. Thomas

INOR 545. Reduction and hydrogenation processes on polynuclear titanium nitrido complexes. **M. Gonzalez-Moreiras**, M. Greño, M. Mena, A. Perez-Redondo, C. Yelamos

INOR 546. Toward the synthesis of metal-epoxide coordination complexes. **A.S. Braegelman**, N.L. Fackler

INOR 547. Towards structural-functional mimics of *Acetyl/ene hydratase*: Reversible activation of acetylene with biometric tungsten alkyne-complexes. **L.M. Peschel**, F. Belaj, N.C. Möschen-Zanetti

INOR 548. Synthesis and structural characterization of zinc complexes with 1,3-bis(diphenylphosphinomethyl)benzene. **M. Young**, T. Siddiquee

Section C

Boston Convention & Exhibition Center
Hall C

Electrochemistry

B. L. Lucht, *Organizer*

6:00 - 8:00

INOR 549. Electrochemical rectification of molecular multilayered films towards redox mediators for dye-sensitized solar cells. **M.R. Civic**, P.H. Dinolfo

INOR 550. Direct and stable attachment of a molecular iridium catalyst for water oxidation to electrode surfaces. **S.W. Sheehan**, J. Thomsen, U. Hintermaier, R.H. Crabtree, G.W. Brudwig, C.A. Schmuttenmaer

INOR 551. Withdrawn.

- INOR 552.** AlCl₃ based ionic liquid with a neutral substituted pyridine ligand for electrochemical deposition of aluminum. **Y. Fang, X. Jiang, X. Sun, S. Dai**
- INOR 553.** Transition metal chalcogenide nanofilms: Oxygen reduction reaction catalysts prepared by E-ALD. **B. Yan, J. Falkowski, Y. Surendranath**
- INOR 554.** Metal-coordinating molecular catalyst grafted onto carbon electrodes. **R.S. Kim, T. Fukushima, Y. Surendranath**
- INOR 555.** Cyclic voltammetric studies of singly-bridged lanthanum, europium and gadolinium polyoxometalates in the presence of potassium. **J.F. Kirby, D.K. Ampadu**

Section D

Boston Convention & Exhibition Center
Hall C

Inorganic Spectroscopy

S. A. Koch, *Organizer*

6:00 - 8:00

- INOR 556.** Effect of metal-remote amino-groups on metal center in ruthenium (II) complexes with terpyridine ligands. **H. Li, Y.A. Jellani, J. Melnyczuk, H. Lisa, J. Wu, T. Yerokun, C.W. Ingram, J. Harruna**
- INOR 557.** Investigating the photophysical properties of dendrimeric fluorophore-labeled palladium catalysts using single-molecule fluorescence spectroscopy. **K. Lupo, S. Upadhyay, A. Marquard, R.H. Goldsmith**

Section E

Boston Convention & Exhibition Center
Hall C

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

6:00 - 8:00

- INOR 558.** Insight into the active species and mechanism of alkyl-alkyl cross-coupling with iron. **V. Fleischauer, M.L. Neidig**
- INOR 559.** Iridium-catalyzed hydrogenation of electron-deficient carbonyls under acidic conditions. **T. Brewster, N.M. Rezaee, Z. Culaikova, A.J. Miller, D.M. Heinekey, M.S. Sanford, K.I. Goldberg**
- INOR 560.** New iridium pincer complexes for the aldehyde-water shift reaction. **J.M. Goldberg, T. Brewster, G.W. Wong, T. Lekich, J.C. Tran, K.I. Goldberg, D.M. Heinekey**
- INOR 561.** Catalytic dehydroaromatization of alkanes via an iridium pincer complex: Toward a mechanistic understanding and control of product distribution. **A.M. Steffens, A.S. Goldman**
- INOR 562.** Synthesis and reactivity of pincer-supported rhenium. **A.J. Kosanovich, O. Zherov**
- INOR 563.** CNN-pincer complexes of ruthenium for the catalytic hydrogenation of esters. **A.R. Chianese, D. Kim, M. Barnard, L. Le, T. Cervarich, K. Bogdanovski, M.J. Drance, K.H. Jensen**
- INOR 564.** Methyl JohnPhos as a new ligand for cross-coupling catalysis. **A.J. Kendall, D.T. Seidenkranz, D. Tyler**
- INOR 565.** Stoichiometric and catalytic reactivity of hexamethyldisilane at an (*N*-heterocyclic carbene)₂-palladium centre. **M.B. Ansell, G. Cloke, J. Spencer, O. Navarro**
- INOR 566.** Mechanistic study of catalyst initiation in Suzuki coupling using single-molecule and NMR spectroscopy. **A. Marquard, K. Lupo, J. Ng, S. Upadhyay, D. Hinton, R.H. Goldsmith**

- INOR 567.** High yielding and selectivity in the solventless telomerisation of isoprene with alcohols using NHC-Pd catalysts at room temperature. **I. Maluenda, M. Chen, D. Guest, M. Roe, M.L. Turner, O. Navarro**
- INOR 568.** Ambiphilic phosphine boronate esters by the iridium-catalyzed C-H borylation of phosphines. **S. Wright, K.M. Crawford, N. Hlynch, T.R. Ramseyer, E. Albitz, T.B. Clark**

- INOR 569.** Bimetallic hafnium pyridyl-amido olefin polymerization catalysts. **Y. Gao, A.R. Mouat, A. Motta, A. Macchioni, C. Zuccaccia, M. Delferro, T.J. Marks**

- INOR 570.** Rapid, regioconvergent, solvent-free alkene hydroisilylation with a cobalt catalyst. **C. Chen, M.B. Hecht, A. Kavara, W.W. Brennessel, B.Q. Mercado, D.J. Weix, P.L. Holland**

- INOR 571.** Activation of monohalogenated substrates using photo initiated copper catalyzed atom transfer radical addition (ATRA). **G.J. Pros, T. Pintauer**

- INOR 572.** Boryl cyclopentadienyl transition metal complexes for C-H functionalization of pyridines. **A. Carl, J.R. Andrea**

- INOR 573.** Mechanistic investigations of the concerted-metalation deprotonation reaction with [Cp*RhCl]₂. **A.P. Walsh, W.D. Jones**

- INOR 574.** Silica-supported tungsten-oxo alkylidene catalysts for use in phase-separated tandem alkane metathesis. **P.E. Sues, V. Mougél, C. Cooper, R.R. Schrock**

- INOR 575.** Kinetic studies on the formation of alternating *trans*-AB copolymers through ring-opening metathesis polymerization using molybdenum alkylidene initiators. **H. Jeong, J.M. John, R.R. Schrock, A.H. Hoveyda**

- INOR 576.** *Z*-to-*E* isomerization processes in reactions catalyzed by cyclometalated ruthenium alkylidenes. **T. Ahmed, J.M. Grandner, M.B. Herbert, B.L. Taylor, K.N. Houk, R.H. Grubbs**

- INOR 577.** Homogeneous copper catalysts for the hydrogenation of carbonyl compounds at room temperature. **A. Chakraborty, M.E. Healey, J.A. Krause, H. Guan**

- INOR 578.** Microwave assisted formation of binuclear rhodium paddlewheel complexes. **O. Serrano, O.F. González-Belman, M. Flores-Alamo**

Section F

Boston Convention & Exhibition Center
Hall C

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

6:00 - 8:00

- INOR 579.** Microporous titanates with band gaps in the visible range for photocatalytic splitting of water. **B.C. Hodges, P. Moetakef, E.E. Rodriguez**
- INOR 580.** Large electric-field-induced strain in La-doped Bi-perovskite ceramics. **J. Lee, J. Kang, T. Dinh**
- INOR 581.** Electrodeposition and nucleation studies of vanadium oxide polymorphs. **Z.M. Chan, C.R. Cox, D.G. Nocera**
- INOR 582.** Synthesis and characterization of Mn²⁺ doped Ni₂(BO₃)₂ nanopowder. **A.U. Morkan, E. Gul**
- INOR 583.** Synthesis and characterization of rare earth metal doped magnesium borates. **A.U. Morkan, I.A. Morkan, E. Gul, G.O. Kahveci**

- INOR 584.** Preparation and characterization of new borophosphates of PrB(PO₃)₂ and TbB(PO₃)₂. **A.U. Morkan, I.A. Morkan, G.O. Kahveci, E. Gul**

- INOR 585.** Structural and photoluminescent characterization of anti-perovskite phosphors: Sr₃AlO₄F:P⁵⁺ and Sr_{3-x}Na_xAl_{1-2x}PxZnxO4F (0 ≤ x ≤ 1). **S. Keil, E.C. Sullivan**

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 160A

Coordination Chemistry

Characterization and Applications

D. C. Crans, *Organizer*

N. Gerasimchuk, *Presiding*

- 8:00 INOR 586.** Extreme service lubrication: Synthesis and characterization of trimeric silyl(II) 3,5-dimethyl-4-n-hexylpyrazolate complex and its tribological implementation. **A.M. Seyam, B.A. Johnson, M. Desanker, D. Jin, H.S. Bazzi, Y. Chung, Q. Wang, M. Delferro, T.J. Marks**

- 8:20 INOR 587.** Mechanistic studies of oxidative aliphatic carbon-carbon bond cleavage in Cu(II) chlorodiketionate complexes. **S. Saraf, D. Tierney, C. James, T. Borowski, L.M. Berreau**

- 8:40 INOR 588.** Reactivity and cation exchange of MOF-5. **C. Brozek**

- 9:00 INOR 589.** Flash photolysis of C₃ symmetric first-row transition metal azides: A photochemical investigation of the preparation of high-valent nitrido complexes. **A.S. Kinne, K.G. Caulton, J.M. Smith, J.M. Zaleski**

- 9:20 INOR 590.** Regulation of primary geometry in pincer complexes bearing secondary sphere hydrogen bonds. **E.W. Dahl, N.K. Szymczak**

- 9:40 INOR 591.** Design of a macrocyclic self-assembled secondary phosphine oxide metal complex for dinitrogen rejection from natural gas. **N.I. Rinehart, A. Kendall, D. Tyler**

10:00 Intermission.

- 10:10 INOR 592.** Heterobimetallic Ti-Co complex featuring a metal-metal multiple bond and its application to the reductive coupling of ketones to alkenes. **B. Wu, C. Thomas**

- 10:30 INOR 593.** Hydrogen activation by iridium(III) complexes bearing a bidentate protic NH₂NH-C⁺phosphine ligand. **S. Cepa, E.F. Hahn**

- 10:50 INOR 594.** Vanadium(IV) complexes with nuclear spin-free ligands: Application of coordination chemistry principles to quantum information processing. **J. Zadrozny, J. Niklas, O. Poluektov, D.E. Freedman**

- 11:10 INOR 595.** New strategy for the NIR emitters beyond 900 nm: Preparation of self-assembled luminescent 1D Pt-cyanoximates. **N. Gerasimchuk, M.Y. Berezin**

- 11:30 INOR 596.** Fluorescent ratiometric Cu(II) sensor based on Poly(N-isopropylacrylamide). **L. Nyiranshuti**

- 11:50 INOR 597.** Modeling the ligand tuning effect over the transition temperature in spin-crossover systems using density functional methods. **J. Cirera Fernandez**

Section B

Boston Convention & Exhibition Center
Room 159

Organometallic Chemistry: Synthesis and Characterization

N. S. Radu, *Organizer*

C. C. Cummins, *Presiding*

- 8:30 INOR 598.** Electrochemical and computational studies of (bisimino)pyridine ruthenium complexes. **M. Noss, D.H. Berry**

- 8:50 INOR 599.** Study of low-valent nickel chemistry supported by a series of PEP pincer-type ligands. **Y. Lee**

- 9:10 INOR 600.** Reversible P-S bond formation/cleavage reactions at a nickel center supported by an anionic PPP ligand: A mechanistic view of a new type of metal-ligand cooperation. **S. Oh, Y. Lee**

9:30 Intermission.

- 9:35 INOR 601.** CO₂ activation with uncommon metal-ligand cooperation. **Y. Kim, S. Oh, S. Kim, J. Kim, Y. Lee**

- 9:55 INOR 602.** CO activation at a low-valent nickel center. **C. Yoo, Y. Lee**

- 10:15 INOR 603.** Silane-cobalt interaction in stepwise formation of a silyl cobalt(II) complex. **J. Kim, S. Kim, Y. Lee**

- 10:35 INOR 604.** Molybdenum hydride and dihydride complexes bearing diphosphine ligands with a pendant amine: Formation of complexes with bound amine. **S. Zhang, M. Bullock**

Section C

Boston Convention & Exhibition Center
Room 158

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

B. M. Bartlett, A. J. Norquist, *Presiding*

- 8:30 INOR 605.** Solid state chemistry of AMX₃ halide perovskites (X = I, Br, Cl). **P. Woodward, M. Linabug, E. McClure**

- 9:10 INOR 606.** Sodium and terbium chlorobismuthate(III) salts: Synthesis, structure, and photocatalytic behavior. **J. Ahern, A. Kelly, H.H. Patterson, R.D. Pike**

- 9:30 INOR 607.** Electronic and steric factors guiding the synthesis of magnesium-based battery electrolytes. **B.M. Bartlett, A.J. Crowe, E. Nelson**

- 9:50 INOR 608.** Exfoliation of layered perovskites through microwave assisted grafting with n-alkohols. **J. Boykin, L. Smith**

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10:10 INOR 609. Electronic paramagnetic resonance spectroscopy of transition metal ions in Sr_2TiO_4 and chemically reduced Sr_2TiO_4 powders. K.A. Lehuta, A. Haldar, K.R. Kittilstved

10:30 Intermission.

10:45 INOR 610. Materials discovery in templated metal oxides. A.J. Norquist

11:05 INOR 611. $[\text{W}_{21}\text{O}_{72}]$ building block: A route to gigantic isopolyoxotungstates with pentagonal and double-stranded motifs. C. Zhan, D. Long, L. Cronin

11:25 INOR 612. Solid-state synthesis of bismuth-based metallo-drugs. D. Tan, F. Qi, T. Friscic

11:45 INOR 613. Synthesis of metal-organic architectures from metals by redox-promoted mechanochemical self-assembly. M. Glavinovic, F. Qi, A.D. Katsenits, T. Friscic, J. Lumb

12:05 Concluding Remarks.

Section D

Boston Convention & Exhibition Center Room 160C

Coordination Chemistry

Macrocycles and More

D. C. Crans, *Organizer*

K. J. Takeuchi, *Presiding*

9:00 INOR 614. Direct synthesis of non-stoichiometric nanocrystalline metal oxides and their composites: Impact on battery-relevant electrochemistry. K.J. Takeuchi, A.C. Marschilok, E.S. Takeuchi

9:25 INOR 615. Probing life limiting parasitic reactions in electrochemical energy storage. E.S. Takeuchi, A.C. Marschilok, K.J. Takeuchi

9:50 INOR 616. Reactions of boronic acids with tetrafluoroborate. J.J. Grzybowski, P. Smith, J. Korsan, D. Aleo

10:15 INOR 617. Science and technical arts collaborative teaching (STACT) project: Touching the third rail of chemical education. K.A. Goldsby, S.M. Ames

10:40 INOR 618. Hybrid active organic/inorganic materials: Impact of molecular ordering on charge transport performance. E. Reichmanis

11:05 INOR 619. Daryle Busch, supporter of inclusion and diversity. E.A. Nalley

11:30 INOR 620. Research-based strategies for enhancing student performance in introductory chemistry courses. J.A. Heppert, M. Barker, D. Pakhira, L. Myers

Section E

Boston Convention & Exhibition Center Room 161

Nanoscience: Applications

R. M. Richards, *Organizer*

D. Yablon, *Presiding*

8:30 INOR 621. Enantiomeric separations of chiral pharmaceuticals using chiral tetrahedral Au nanoparticles. N. Shukla, D. Yang, A.J. Gellman

8:50 INOR 622. Engineering of nanoparticles to achieve macroscopic functionality. D. Ha, H. Zhang, B. Hu, T. Ly, O. Otelaja, M. Fayette, A. Nelson, M. Islam, L. Sun, R. Hovden, F. Wise, D. Muller, R.D. Robinson

9:10 INOR 623. Mechanisms and behavior of gas permeation through single layer graphene membranes. L. Drahushuk, M. Strano

9:30 INOR 624. Light or heat? The origin of cargo release from nanopipette particles containing upconversion nanocrystals under IR irradiation. J. Dong, J.I. Zink, M. Strano

9:50 Intermission.

10:00 INOR 625. Advances in nanomechanical measurements with scanning probe microscopy based methods. D. Yablon

10:20 INOR 626. Cell uptake of boron-nitride nanotubes loaded with curcumin. J. Niskanen, Y. Wang, X. Zhang, I. Zhang, Y. Xue, D. Golberg, D. Maysinger, F.M. Winnik

10:40 INOR 627. Quantum dot luminescent concentrator cavity exhibiting thirty fold concentration. N. Bronstein, Y. Yao, L. Xu, E. O'Brien, A.S. Powers, V.E. Ferry, P. Alivisatos, R.G. Nuzzo

11:00 INOR 628. Absorption measurements of single plasmonic metal oxide nanocrystals reveal considerable peak heterogeneity hidden within ensemble spectra. R.W. Johns, D.J. Milliron, H. Bechtel

11:20 INOR 629. Understanding the effect of hydrogen passivation of impurities in solution processed metal oxide thin films. J.C. Ramos, Y. Huang, C. Perkins, D. Park, D.A. Keszler

11:40 INOR 630. Preparation and precise size control of metal oxide nanocrystals via a "living" growth synthesis. A.W. Jansons, B.M. Crockett, M.C. Sharps, L.K. Plummer, J.E. Hutchison

Section F

Boston Convention & Exhibition Center Room 160B

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

H. Liu, L. M. Wheeler, *Presiding*

8:00 INOR 631. Synthesis and structure of colloidal silica - polymethacryloxypolyloxane nanocomposite particles. H. Tu, M.J. Monello, R. Lewis, D. Fomitchev

8:20 INOR 632. Chemical transformations of semiconductor nanocrystals: Mechanism and role of defects and surfaces. S.L. White, P.K. Jain

8:40 INOR 633. Inorganic ligand exchange on germanium nanocrystals. L.M. Wheeler, B. Chernomordik, M.C. Beard, N.R. Neale

9:00 INOR 634. Formation of endohedral mono-metallofullerenes. P.W. Dunk, A.G. Marshall, H.W. Kroto

9:20 INOR 635. DNA-based nanofabrication of inorganic materials. H. Liu, F. Zhou, H. Kim

9:40 INOR 636. Electrospinning $\text{SiO}_2\text{-TiO}_2$ nanofibers using sol-gel chemistry. F. Huang, S. Das, M.T. Janish, P.G. Kotula, C. Carter, C.J. Cornelius

10:00 Intermission.

10:10 INOR 637. Nonplasmonic nanoparticles as extremely stable photothermal sources. R.J. Johnson, B. Lear

10:30 INOR 638. Synthesis of hollow Ge nanoparticles via electrodeless deposition. B. Nolan, E. Muthuswamy, E. Chan, S. Kauzlarich

10:50 INOR 639. Thermochemistry of reduced graphene oxide and its nitrogen-doped variants. E. Muthuswamy, J. Chen, A. Navrotsky

11:10 INOR 640. Iron(II) spin crossover nanoparticles in a block-copolymer matrix. O. Klimm, C. Stegelmeier, S. Rosenfeldt, S. Foerster, B. Weber

11:30 INOR 641. Generating efficient and tunable white light using hybrid transparent metal oxide-based nanoconjugates. P. Radovanovic

11:50 INOR 642. Solid-solid phase transformations and 2D heterostructures in copper sulfide nanoparticles. D. Ha, A.H. Caldwell, M. Ward, S. Honrao, K. Mathew, R. Hovden, M. Koker, D. Muller, R. Hennig, R.D. Robinson

Section G

Boston Convention & Exhibition Center Room 162A

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

D. T. de Lill, D. A. Penchoff, *Presiding*

9:00 INOR 643. Synthesis, structure, and electronic spectroscopy of actinide complexes and materials. H.S. La Pierre, E.F. Batista, E.D. Bauer, D.L. Clark, S.A. Kozimor, M. Loeble, R.L. Martin, S.G. Minasian, D.K. Shuh, P. Yang

9:20 INOR 644. Selective and sustainable separation of rare earth elements. K.D. Field, M. Emmert

9:40 INOR 645. Spectator ion-directed synthesis of lanthanide-organic frameworks. D.T. de Lill

10:00 INOR 646. Actinide and lanthanide complexes: What the CSD and structural informatics can tell us about their complexation. K. Moyle, S. Vyas, S. Wiggan, P.C. Sanschagrin, J. Brennan

10:20 Intermission.

10:30 INOR 647. Optimizing ligand design for extraction of low concentration uranyl from aqueous media: An integrated theoretical and experimental study. D.A. Penchoff, C. Peterson, J.P. Camden, D.M. Jenkins, A.K. Wilson

10:50 INOR 648. Generation of uranium(IV) bis(imido) intermediates in the synthesis of U(VI) bis(imido) complexes. J.M. Boncella, N.C. Tomson, A.M. Tondreau, B. Scott

11:10 INOR 649. Precision design of new multidentate ligands for f-elements. I. Yakovlev, R.J. Abergel

Section H

Boston Convention & Exhibition Center Room 157C

Main Group Chemistry

T. W. Hudnall, *Organizer*

J. D. Protasiewicz, D. Vidovic, *Presiding*

8:30 INOR 650. Activation of robust bonds by aluminum(I). T. Chu, Y.D. Boyko, G.I. Nikonov

8:50 INOR 651. Complexation and activation of silanes with a strongly Lewis acidic alane: Isolation, structural characterization, and diverse catalysis. J. Chen, E.Y. Chen

9:10 INOR 652. Homo- and hetero-aryl Lewis acidic boranes: H_2 activation by an electrochemical-frustrated Lewis pair approach. R.J. Blagg, G. Wildgoose

9:30 INOR 653. Reactions between compounds containing protonic and hydridic hydrogens. X. Chen, H. Li, X. Chen, Q. Yang

9:50 Intermission.

10:00 INOR 654. C-C coupling reactions catalyzed by a Pd(II) complex with the amphiphilic ligand 8-quinoyldimethylborane. S.R. Tamang, J.D. Hoefelmeyer

10:20 INOR 655. Coordination of N-heterocyclic phosphonium cations to nickel using a chelating ligand framework. M. Bezpalko, C. Thomas

10:40 INOR 656. Coordination chemistry of Group 1 cations with soft donor macrocycles. M. Champion, M. Everett, A. Jolleys, W. Levason, D. Pugh, G. Reid

11:00 INOR 657. Competition between ligation and solvation in heavy alkaline earth metal tetraarylborates. C.M. Lavin, A.G. Goos, D.G. Allis, K. Ruhlandt-Senge

11:20 INOR 658. Calcium arylphosphonates for bone therapy. V. Lopez, M.D. Lijewski, V.N. Bampoh, K. Ruhlandt-Senge

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WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center Room 160A

Nanoscience: Semiconductors

R. M. Richards, *Organizer*

M. zamkov, *Presiding*

1:30 INOR 659. Quantitative theory of adsorptive separation for the electronic sorting of single-walled carbon nanotubes. R. Jain, K.C. Tvrdy, R. Hari, Z. Ulissi, M. Strano

1:50 INOR 660. Titanium nitride etching in the semiconductor industry: Mechanistic considerations. J. Hoogboom, D. Yu, M. Shen, S. Braun, Y. Burk, A. Klipp

2:10 INOR 661. Liquid contacting of PbS quantum dot solids. E. Johansson, V. Dereviankin, V. Uzunov

2:30 INOR 662. Hole transfer from photoexcited quantum dots to molecular species: Understanding the relationship between driving force and rate. J.H. Olshansky, T. Ding, Y. Lee, P. Alivisatos

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

2:50 INOR 663. Quantum confined semiconductor nanoshells. **M. Zamkov**, N. Razgoniaeva, D. Burchfield

3:10 INOR 664. Insights on the solution syntheses of 0D and 2D tin chalcogenide semiconductors. **A.J. Bianchi**, A.R. Hight Walker

3:30 INOR 665. Heavily transition metal doped semiconductor nanocrystals using magnetic molecular clusters as single source precursors. **S. Pittala**, K.R. Kittilstved

3:50 INOR 666. Mastering the seed-mediated synthesis of gold nanorods. **N.D. Burrows**, S. Harvey, C.J. Murphy

4:10 INOR 667. Biaxially stretchable Ag NW-based transparent conductors. **J. Pyo**, B. Kim, T. Kim, H. Park, J. Park, J. Lee, S. Lee

4:30 INOR 668. Using conduction electron spin resonance to probe the degree of interfacial mixing between chemisorbed aromatic thiols and gold nanoparticles. **A. Cirri**, B. Lear

4:50 INOR 669. Temperature dependence of the nanocrystal nucleation revealed through plasmon resonance of bimetallic nanoparticles. **N. Razgoniaeva**, A. Acharya, N. Sharma, P. Adhikari, M. Zamkov

5:10 INOR 670. Assembly of well-defined nanomaterials from transition metal clusters: Emergence of new properties at the nano/small-molecule boundary. **A. Beecher**, J.S. Owen

Section B

Boston Convention & Exhibition Center Room 159

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

T. Betley, L. Do, *Presiding*

1:30 INOR 671. Synthesis, characterization, and reactivity of a nonclassical dihydride cobalt bis(carbene) complex. **K. Tokmic**, M.R. Brennan, D. Kim, A. Fout

1:50 INOR 672. Carbodicarbene ruthenium complexes: Highly active catalysts for the chemoselective hydrogenation of olefins. **C. Franckevicius**

2:10 INOR 673. Pd-catalyzed selective hydrosilylation of allylamines. **H. Tafazolian**, J.A. Schmidt

2:30 INOR 674. Reactivity of the low-coordinate bis(alkoxide) metal complexes in N-N and C-N bond formation reactions. **M. Yousif**, J. Bellow, R. Lord, S. Groysman

2:50 INOR 675. Phosphine-directed C-H borylation of arenes: Synthesis and utility of phosphine boronate esters. **T.B. Clark**, K.M. Crawford, N. Huynh, S. Wright, T.R. Ramseyer

3:10 Intermission.

3:15 INOR 676. JohnPhos palladium catalysis: How structure affects kinetics. **A.J. Kendall**, D.T. Seidenkranz, D. Tyler

3:35 INOR 677. Withdrawn.

3:55 INOR 678. Activation of chlorohydrocarbons by a rhodiumtrispyrazolylborate complex. **Y. Jiao**, W.D. Jones

4:15 INOR 679. Redox active ligand design on a surface: Synthesis and characterization of tetrazine complexes of Pt, V, and Nb from metal atoms. **D. Skomski**, C. Tempas, A.V. Polezhaev, B.J. Cook, J. Man, S.L. Tait, **K.G. Cautlon**

4:35 INOR 680. Tuning nickel for catalytic olefin hydrogenation via dative bonds to Lewis acidic metalloligands. **R. Cammarota**, C. Lu, P.A. Radd

4:55 INOR 681. Selective alcohol hydrogenation and dehydrogenation catalysis and their potential applications inside living systems. **L. Do**

5:15 INOR 682. Selective formation of n-butanol from ethanol with iridium-based homogeneous catalysts. **S. Chakraborty**, W.D. Jones

Section C

Boston Convention & Exhibition Center Room 162A

Inorganic Catalysts

S. A. Koch, *Organizer*

A. M. Angeles Boza, S. C. Marinescu, *Presiding*

1:30 INOR 683. Ethylene addition to cobalt bis(thiooxolene): A DFT study. **D. Sredojevic**, E.N. Brothers

1:50 INOR 684. Synthesis and reactivity of peroxide and oxide bridged cofacial bimetallic complexes. **E.D. Bloch**, J. Stauber, C.C. Cummins, D.G. Nocera

2:10 INOR 685. H₂ oxidation by cobaloximes: Mechanistic insight into hydrogen evolution catalysis. **S.A. Del Ciello**, J.R. Winkler, J.C. Peters, H.B. Gray

2:30 INOR 686. Heavy atom isotope effects as probes of CO₂ activation. **A.M. Angeles Boza**

2:50 INOR 687. Rational design of photochemical super-reductants based on tungsten-alkylidyne chromophores. **H.B. Vibbert**, M.D. Hopkins

3:10 Intermission.

3:20 INOR 688. Gas generation from simple carboxylic acids and diphosphine-supported first-row transition metals. **A.M. Tondreau**, J.M. Boncella, B. Scott

3:40 INOR 689. Synthesis, properties, and water oxidation activity of a novel dinuclear Ru(II) polypyridine complex. **N. Nair**, R. Zhou, R.P. Thummel

4:00 INOR 690. Efficient proton reduction from water by cobalt dithiolene metal-organic surfaces (MOS). **S.C. Marinescu**

4:20 INOR 691. DNA-hosted gold nanocluster enhances enzymatic electroreduction of oxygen by mediating efficient electron transfer. **S. Chakraborty**, S. Babanova, R.C. Rocha, A. Desireddy, K. Artyushkova, P.B. Atanassov, J.S. Martinez

4:40 INOR 692. Determination of the relative acidity of binary HCl/MCl_n superacids that involve Lewis acids from groups 13 & 15. **J. Stiel**, Z. Tun, C. Tessier

5:00 INOR 693. Metal complexes for fixation, electrocatalytic, photocatalytic and chemical CO₂ reduction. **I. Ivanovic-Burmazovic**

Section D

Boston Convention & Exhibition Center Room 160C

Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*

T. Betley, R. C. Scarrow, *Presiding*

1:30 INOR 694. Vapochromic materials that don't incorporate vapors. **M. Karimi Abdolmaleki**, S. Chatterjee, M. Olen Bovee, J.A. Krause, W.B. Connick

1:50 INOR 695. Transition metal single-molecule magnet in a nuclear spin-free ligand field environment. **M. Fataftah**, J. Zadrozny, D. Rogers, D.E. Freedman

2:10 INOR 696. Synchrotron-based methods to study metal-metal bonded complexes of the first-row transition metals. **R.J. Eisenhart**, L.J. Clouston, Y. Chen, V.G. Young, C. Lu

2:30 INOR 697. Strong magnetic coupling in dinuclear transition-metal complexes bridged by a 2,5-diamino-1,4-benzoquinonediimine radical. **J. DeGayner**, I. Jeon, D. Harris

2:50 INOR 698. High-spin ground state and single-molecule magnet behavior in octahedral iron clusters [M₆]. **R. Hernandez Sanchez**, T. Betley

3:10 INOR 699. Strong magnetic exchange in high-dimensional networks of transition metal ions bridged by benzosemiquinonoid ligands. **I. Jeon**, D. Harris

3:30 INOR 700. Emergent single molecule magnetism in highly symmetric clusters. **T. Betley**, R. Hernandez Sanchez

3:50 INOR 701. Synthesis and magnetic properties of 1,2,4,5-benzenetetrathiolate-bridged dinuclear complexes. **A. Banisafar**, I. Jeon, D. Harris

4:10 INOR 702. Synthesis, structural and spectroscopic characterization of thiocyanate ligated heterobimetallic lantern complexes. **J.L. Guillet**, C.J. Daley, J.A. Golen, A.L. Rheingold, L. Doerrer

4:30 INOR 703. Excited state charge distribution in Mo₂L₄ paddlewheel compounds indicated by CEC stretch. **C. Jiang**, P.J. Young, M.H. Chisholm

4:50 INOR 704. Influence of environmental factors on quantum decoherence in mononuclear transition metal complexes. **M. Graham**, J. Zadrozny, M. Shiddiq, J.S. Anderson, M. Fataftah, S. Hill, D.E. Freedman

Section E

Boston Convention & Exhibition Center Room 161

Bioinorganic Chemistry: Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

J. P. Caradonna, *Presiding*

1:30 INOR 705. H₂S and metal mediated HNO generation as new signaling mechanisms. **I. Ivanovic-Burmazovic**

1:50 INOR 706. Diiron μ -thiolate complexes that bind N₂ across multiple oxidation states: Towards new structural/functional models of nitrogenase. **S. Creutz**, J. Peters

2:10 INOR 707. Stabilization of reactive species within a metal organic framework. **J.S. Anderson**, A. Gallagher, J. Park, D. Harris

2:30 INOR 708. Mechanistic insights into the N-N reductive coupling of NO by low coordinate Cu and Ni complexes. **S. Kundu**, T.H. Warren

2:50 INOR 709. Modeling halogen bonding and protein dynamics in iodothyronine deiodinase. **C.A. Bayse**

3:10 INOR 710. Activation of oxygen at an iron(II) center: Coupling α -keto acid decarboxylation with alkane to alcohol conversion. **J.P. Caradonna**, L. Gregor, J. McNally, P. Tarves

3:50 Intermission.

3:30 INOR 711. Novel thermodynamic cycle to determine the reduction potential and reduction enthalpy and entropy of azurin. **M.L. Croteau**, D. Wilcox

4:10 INOR 712. Delivery of active large proteins using mesoporous silica nanoparticles. **G. Deodhar**

4:30 INOR 713. Biomimetic roles as heme protein cofactors. **M. Hoffmann**, K. Kleeberg, B. Wolfram, P. Schweyen, U. Papke, M. Bröring

4:50 INOR 714. Thermodynamics of Cu(I), Ag(I), and other d¹⁰ metal ions binding to the metallochaperone HAH1, and the effect of glutathione on this binding. **M. Stevenson**, J. Schuster, D. Wilcox

5:10 INOR 715. Ruthenium dihydroxypyridine complexes are tumor activated prodrugs due to low pH and blue light induced ligand release. **E.T. Papish**, M. Lockart, K. Jernigan, D.J. Charboneau, K.D. Hughes, S.E. Brown, F.S. Thowfek, D. Dozier, E.J. Merino, Y. Kim, J.J. Paul

Section F

Boston Convention & Exhibition Center Room 160B

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

M. G. Campbell, *Presiding*

1:30 INOR 716. New rare-earth-free hybrid phosphor for efficient solid-state lighting. **Z. Hu**, G. Huang, W.P. Lustig, F. Wang, H. Wang, S.J. Teat, D. Banerjee, D. Zhang, J. Li

1:50 INOR 717. Functionalizing polymer fibers with UiO-66-NH₂ using ALD oxide nucleation layers. **J. Zhao**, P.S. Williams, W. Xie, D.T. Lee, G.W. Peterson, G.N. Parsons

2:10 INOR 718. Porphyrinic metal-organic frameworks for photodynamic therapy. **J. Park**, D. Feng, H. Zhou

2:30 INOR 719. Electrochemical investigations of conductive metal-organic frameworks. **E. Miner**, D. Sheberla, M. Dinca

2:50 INOR 720. Electrically conductive 2D metal-organic frameworks for chemiresistive sensing. **M.G. Campbell**, D. Sheberla, S. Liu, T.M. Swager, M. Dinca

3:10 INOR 721. Molecular-level characterization of the guest effect on the transition temperature in spin crossover metal-organic frameworks. **J. Cirera Fernandez**, F. Paesani

3:30 Intermission.

3:45 INOR 722. Electrically conductive metal-organic frameworks based on through-bond charge transport design principle. **S. Lei**, T. Miyakai, C.H. Hendon, S. Seki, A. Walsh, M. Dinca

4:05 INOR 723. Cation-dependent intrinsic electrical conductivity in tetrafluorovalene-based microporous metal-organic frameworks. **S.S. Park**, E. Hontz, L. Sun, C.H. Hendon, A. Walsh, T.A. Van Voorhis, M. Dinca

4:25 INOR 724. Thermochemistry of multiferroic organic-inorganic hybrid perovskites. **N. Gowdaiana pallya puttaiah**, A. Navrotsky

4:45 INOR 725. Leach-free catalysis and electroactive materials from metal-thiolate-enabled porous frameworks. **Z. Xu**, K. Yee, M. Zeller

5:05 INOR 726. Imparting functionality to biocatalysts via embedding enzymes into nanoporous materials by a de novo approach: Size-selective sheltering of catalase in metal-organic framework microcrystals. **W. Chang Cheng**

5:25 INOR 727. Lanthanide-based nano-MOFs as multimodal bioimaging agents. **D.T. de Lill**

Section G

Boston Convention & Exhibition Center
Room 158

Coordination Chemistry: Synthesis and Characterization

D. C. Crans, *Organizer*

L. Doerrer, G. T. Musie, *Presiding*

1:30 INOR 728. Rational design: Programming small molecule reactivity in a multinuclear iron cluster. **B. Malbrecht, T. Betley**

1:50 INOR 729. Synthesis and structure of $(\text{dpp-BIAN})\text{V}(\mu_2\text{-Cl})_2(\mu_3\text{-Cl})_2\text{Mg}_2(\text{thf})_4$: A trinuclear vanadium(II)-magnesium species with a radical anion dpp-BIAN ligand coordinated to the vanadium(II) center. **D.A. Nadelman, R.V. Nadelman, S. Leed, J. Niklas, J.D. Gordon, C.D. Abernethy**

2:10 INOR 730. Mononuclear and terminally bound titanium nitride complexes formed via reductive denitrogenation of a titanium azide. **M. Carroll, P.J. Carroll, D.J. Mindiola**

2:30 INOR 731. Structure correlation of square-planar metal complexes with pendant nucleophiles. **J. Ringo, T. Green, J.A. Krause, W.B. Connick**

2:50 INOR 732. 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**

3:10 Intermission.

3:20 INOR 733. Biomimetic coordination chemistry of bi- and tridentate thiol ligands. **N.C. Möscher-Zanetti, L.M. Peschel, S. Holler, M. Tüchler, F. Belaj**

3:40 INOR 734. Multidentate pyrrole-based phosphine, polypyrazolyl, and Schiff base ligands for transition metal complexes: Catalysis and fluxional properties. **G. Mani, S. Kumar, D. Ghorai, R. Kumar**

4:00 INOR 735. Withdrawn.

4:20 INOR 736. Tunable spin equilibria in four-coordinate iron trisphosphine phosphinimato complexes. **S. Creutz, J. Peters**

International Symposium on Mesoporous Zeolites

Sponsored by ENFL, Cosponsored by CATL, I&EC and INOR

Polymer Concepts in Inorganic Chemistry Courses

Sponsored by CHED, Cosponsored by INOR, PMSE and POLY

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

WEDNESDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Bioinorganic Chemistry: Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

6:00 - 8:00

INOR 737. Mössbauer studies of multi-metallic assemblies of complexes with different spin states. **V.C. Popescu, M. Cohara, P. Ghosh, M.Y. Darensbourg**

INOR 738. Secondary coordination sphere effects in copper macrocyclic complexes. **B.D. Neisen, W.B. Tolman**

INOR 739. Magnetic circular dichroism studies of iron binding in wild-type and mutant calprotectin. **T.M. Woodruff, T.G. Nakashige, E.M. Nolan, M.L. Neidig**

INOR 740. Modeling reversible S-NO bond formation and S-S disulfide cleavage at copper and zinc sites. **A. Gee, S. Zhang, T.H. Warren**

INOR 741. Release of NO from nitrite at copper(I) via electrophilic activation. **Z. Sakhaei, S. Kundu, T.H. Warren**

INOR 742. Determination of the reactivity of Fe^{3+} -1,2-dihydroxibenzenes complexes in the Fenton reaction. **D. Contreras, Y. Duran, D. Carmona, H.D. Mansilla, L. Cornejo**

INOR 743. Withdrawn.

INOR 744. Reaction pathway prediction and differentiation in the TBP geometries found in vanadium-phosphatase protein complexes using shape analysis. **I. Sanchez Lombardo, S. Alvarez, C. McLaughlan, D.C. Crans**

INOR 745. Discrimination of nitroxyl and biological thiols with modular, lysine-based fluorophores. **A. Loas, R.J. Radford, A.D. Liang, S.J. Lippard**

INOR 746. Reaction of bis-(1,4,7-triazacyclononane)nickel(III) with L-cystinesulfonic acid. **D.M. Stanbury, R. Chan, N. Payne**

INOR 747. Synthetic modeling of the sMMO diiron active site with a preorganized macrocyclic ligand framework. **F. Wang, M. Minier, A. Loas, S.J. Lippard**

INOR 748. Interaction of the heme protein cytochrome c with negatively-charged lipid membranes. **X. Chen, Y. Liu, E.V. Pletneva**

INOR 749. Vanadium phosphatase inhibitors favor the trigonal bipyramidal transition state geometry. **D.C. Crans, B. Peters, C.C. McLaughlan, G.R. Willsky**

INOR 750. Preparation of metal-substituted myoglobin to promote new reactivities. **K.L. Stone**

INOR 751. Efforts toward the synthesis of catalytic antibiotics via attachment of a metal binding domain to Vancomycin. **J. Gray, J.A. Lundeen, P.J. Loll, E.T. Papish**

INOR 752. Degradation of aromatic hydrocarbons by functional and structural models of iron-containing dioxygenases. **M. Molenda, J. Li, M. Panda, W.W. Brennessel, F.A. Chavez**

Section C

Boston Convention & Exhibition Center
Hall C

Inorganic Catalysts

S. A. Koch, *Organizer*

6:00 - 8:00

INOR 753. Low-temperature precursors for vanadium oxide nanomaterials for catalytic application. **A.A. Alothman, A.W. Apblett**

INOR 754. Terminal alkene isomerization using the bifunctional ruthenium catalysts: Stability study. **D. Vidovic, A. Smarun**

INOR 755. Mechanistic studies of O-O bond formation in cobalt-catalyzed water oxidation. **C. Brodsky, A. Ullman, D.G. Nocera**

INOR 756. Pyridine-aza macrocycles (PyMACs) with appended functionalities for hydrogen peroxide activation and oxidation catalysis. **T. Palluccio, S.G. McKenzie, E. Rybak-Akimova**

INOR 757. Biomimetic chemistry of Ttz relevant to copper nitrite reductase: The influence of protonated Ttz^{RI, R2} in copper complexes toward electrochemical behavior and reactivity (Ttz=tris(1,2,4-triazolyl)hydroborate). **S. Siek, N. Dixon, E.T. Papish**

INOR 758. Mechanistic investigation of non-heme iron-aminopyridine oxidation catalysts. **M. Piquette, O. Makhlynets, D. Bowen, E. Rybak-Akimova**

INOR 759. Diastereoselective binding of bis(secondary phosphines) in $[\text{Cu}(\text{I-Pr-DuPhos})(\text{PhHP-PPH})][\text{PF}_6]$ complexes: Synthesis, structure, and dynamic processes. **S. Gibbons, J.L. Peltier, C.R. Valleau, D.S. Glueck, J.A. Golen, A.L. Rheingold**

INOR 760. Development of novel iron complexes for catalytic C-H bond activation and amination. **C. Giberson-Chen, A. Mikhailine, T. Betley**

INOR 761. Withdrawn.

INOR 762. Homogeneous hydrogenation of carbon dioxide to methanol through cascade catalysis. **N.M. Rezayee, C.A. Huff, M.S. Sanford**

Section D

Boston Convention & Exhibition Center
Hall C

Organometallic Chemistry: Applications to Materials and Polymer Science

N. S. Radu, *Organizer*

6:00 - 8:00

INOR 763. Synthesis and radiation chemistry of phosphonium hexatungstate compounds for the precursor of metal oxide thin films. **S. Saha, J.M. Amador, S.R. Decker, L.N. Zakharov, D.A. Kesler**

INOR 764. Application of achiral, sterically constrained bis(imino)pyridine iron complexes for the stereoregular polymerization of lactide, a mechanistic study. **J.A. Kehl, J.A. Byers, C.M. Manna, L. Yablou**

INOR 765. Withdrawn.

Section E

Boston Convention & Exhibition Center
Hall C

Organometallic Chemistry: Synthesis and Characterization

N. S. Radu, *Organizer*

6:00 - 8:00

INOR 766. Synthesis and reactivity of a new class of frustrated Lewis pairs. **A.C. McQuilken, T.H. Warren**

INOR 767. One pot synthesis of arene-based PCP/PNP ligands and corresponding nickel complexes. **W. Shih, O. Ozerov**

INOR 768. Water-soluble organogold(III) complex: Luminescence, self-assembly, and photochemistry in water. **F. Wang, C. Che**

INOR 769. Low-valent, neutral, and isocarbonyl complexes of iron with multidentate carbene ligands. **A. Hickey, C. Chen, J.M. Smith**

INOR 770. Synthesis, characterization, and photophysical properties of dendrimeric fluorophore-labeled palladium catalysts for single-molecule spectroscopy. **S.P. Upadhyay, K. Lupo, A. Marquard, R.H. Goldsmith**

INOR 771. Reactivity of carbene transfer reagents with high-spin iron dipyrin complexes. **A. Wrobel, M.J. Wilding, T. Betley**

INOR 772. Effects of a pyrene substituent on indium containing porphyrins. **C. Holstrom, H.M. Rhoda, E. Mailgaspe, V. Nemykin**

INOR 773. Rutheniumtetraphenylporphyrin axially coordinated with bisferrocenylisocyanides: A synthesis, spectroscopic, electrochemical, and theoretical study. **M. Fathi-Rasekh, S. Dudkin, M.V. Barybin, V. Nemykin, A.D. Spaeth**

INOR 774. Conformational dynamics control selectivity for two-electron chemistry in three-coordinate Co(II) amide complexes. **M.R. Brennan, H. Patel, A. Fout**

INOR 775. High-spin cobalt dipyrin complexes featuring metal-ligand multiple bonds. **Y. Baek, M.J. Wilding, T. Betley**

INOR 776. Synthesis and reactivity of low-valent, low-coordinate Co(II) and Fe(II) complexes. **J.A. Killion, M.R. Brennan, A.R. Fout**

INOR 777. Competition between the formation of seven-membered and five-membered cyclometalated platinumacycles. **C.M. Anderson, M.W. Greenberg, J. Tanski**

INOR 778. Synthesis and characterization of neutral bis-PTA pincer ligands for catalysis in water. **K. Zielinski, J.R. Andreatta**

INOR 779. Insertion of transition metal carbonyls into the dimetallates of germanium and tin. **M.L. McCreah-Hendrick, P.P. Power**

INOR 780. Reversible transformation between a phosphinite-Ni(0) and a phosphide-Ni(II) alkoxide via unique metal-ligand cooperation. **S. Kim, Y. Kim, S. Oh, Y. Lee**

INOR 781. C-C bond formation between CO and iodoalkanes at a nickel(II) center and its mechanistic study. **C. Yoo, Y. Lee**

INOR 782. Syntheses of silyl cobalt(II) complexes via SiH-cobalt interaction. **J. Kim, S. Kim, Y. Lee**

INOR 783. Photophysical properties of a series of copper complexes. **Y. Kim, J. Kim, S. Kim, Y. Lee**

INOR 784. Reversible P-S bond formation/cleavage: PPP vs. PNP. **S. Oh, Y. Lee**

Section F

Boston Convention & Exhibition Center
Hall C

Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*

6:00 - 8:00

INOR 785. Development of Ru(II) complexes for the activation of covalent bonds. **K.H. Taylor, T.B. Gunnoe, M. Sabat**

INOR 786. New chemistry of high-valent nickel fluoroalkyl complexes. **S. Yu, D. Vicio**

INOR 787. Stepwise conversion of a platinum dimethyl complex to a perfluorometallacyclobutane derivative. **L. Xu, D. Soloway, D.A. Vicio**

INOR 788. High oxidation state molybdenum imido complexes for the catalytic preparation of haloalkenes. **J.K. Lam**, J. Hvil, R.R. Schrock, A.H. Hoveyda

INOR 789. Fast "Wittig-like" reactions as a consequence of the inorganic enamine effect. **S. A. Gonsales**, M. Pascualini, I. Ghiviriga, K. Abboud, A.S. Veig

MEDI

Division of Medicinal Chemistry

W. Young and S. Plumlee, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits (see *CHED, Monday*)

Metalloprotein Inhibitors: Drugs, Drug Candidates, and New Targets at the Interface of Medicinal and Inorganic Chemistry (see *INOR, Monday*)

International Entrepreneurship: How to Start a Business and Thrive in Global Marketplace (see *IAC, Tuesday*)

Computational Toxicology: From QSAR models to Adverse Outcome Pathways (see *CINF, Wednesday*)

SOCIAL EVENTS:

Reception, 5:30 PM: Tuesday

BUSINESS MEETINGS:

Business Meeting, 8:30 AM: Sunday

Business Meeting, 6:00 PM: Monday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 210B

NeuroInflammation

S. Runyon, *Organizer*

B. T. Shireman, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 MEDI 1. Discovery of novel, selective brain penetrant P2X7 antagonists for the treatment of depression.

M.A. Letavic, B.M. Savalli, C. Chrovian, B.T. Shireman, A. Bhattacharya, J.M. Ziff, D.M. Swanson, A. Soyode-Johnson

9:35 MEDI 2. From natural product to the first oral treatment of multiple sclerosis: The discovery of FTY720 (Gilenya™). **F. Zecri**

10:05 MEDI 3. CHDI-00340246, a potent and selective kynurenine monooxygenase inhibitor as potential therapeutic agent for the treatment of Huntington's disease. **L.M. Toledo-Sherman**, M. Prime, L. Mrzljak, D. Winkler, V. Khetarpal, I. Munoz-SSanjuan, C. Dominguez

10:35 MEDI 4. Imaging neuroinflammation in the human brain via TSPO. **J.M. Hooker**

11:05 MEDI 5. Azetidine carbamate irreversible inhibitors of monoacylglycerol lipase (MAGL). **C. Butler**

11:35 MEDI 6. FPR2/ALXR agonists: Discovery, characterization, and application in a mouse model of AD. **O. Corminboeuf**, X. Leroy, L. Piali, S. Cren, S. Richard-Bildstein, C. Grisostomi, S. Froidevaux, D. Bur, S. Delahaye

Section B

Boston Convention & Exhibition Center
Room 210A

Evolution of Natural Product Research in Drug Discovery

R. Li, A. J. Peat, E. Velthuisen, *Organizers, Presiding*

8:55 MEDI 7. Current and future perspectives on natural products in antibacterial research. **D.G. Brown**

9:25 MEDI 8. Natural products as a source for the discovery of Hsp90 inhibitors. **B. Blagg**

9:55 MEDI 9. Role of innovative technologies for discovery of novel natural products: Platensimycin and kibdelomycin story. **S.B. Singh**

10:25 MEDI 10. Microbial genomics and strain prioritization to streamline natural product discovery. **B. Shen**

10:55 MEDI 11. Re-emergence of natural products in drug discovery and development. **D.H. Sherman**

11:25 MEDI 12. Future of natural products in anti-infective drug discovery: Treasure hunt or industrial engine? **J. Silverman**

Section C

Boston Convention & Exhibition Center
Room 210C

General Orals

W. B. Young, *Organizer*

J. B. Schwarz, *Presiding*

8:30 MEDI 13. Discovery of a novel sulfone series of BACE1 inhibitors for Alzheimer's disease. **W. Wu**, C. Bennett, D.A. Burnett, P. Chen, J. Cumming, M.S. Domalski, E.J. Gilbert, J. Hao, D. Kaelin, A.W. Stamford, B. Taoka, S. Walsh, J.L. Duffy, R.P. Nargund, A.E. Weber, P. Orth, H. Wang, J.P. Caldwell, J.D. Scott, Y. Yu, B. Simmons, Y. Xu, J. Kuethe, R. Ruck, D. Rindgen, G. Wang, R. Anstatt, H. Mei, A. Pavlovsky, M. Cartwright, B. Smith, M. Michener, G. Agnihotri, X. Chen, S. Gold, R. Hodgson, L. Hyde, R. Kuvellkar, S. Lu, R. Mayer-Ezell, E. Parker, L. Stahl, B. Werner, Q. Zhang, M. Kennedy

8:50 MEDI 14. Identification of pyridazinone analogs as selective P2X3 antagonists for pain management. **X. Wang**, B.D. Wakefield, B. Liu, B. Brown, T. Li, P. Kym, V. Scott, Y. Fan, T. Vortherm, W. Niforatos, C. Mills, S. Joshi, M.R. Schrimpf, C. Lee, J. Brioni

9:10 MEDI 15. Delivering safety and efficacy in kinase inhibitor programs. **K.L. Lee**, R. Naven, N. Greene, F. Shah, C.A. Northcott, M. Dowty, T. Smeal, S. Yamazaki, D. Hepworth

9:30 MEDI 16. Design of novel orally efficacious liver X receptor (LXR) β agonist. **Y. Zheng**, L. Zhuang, K. Fan, C.M. Tice, W. Zhao, C. Dong, S.D. Lotesta, K. Leftheris, Z. Liu, D. Lala, B.M. Mckeever, G.M. McGeehan, R.E. Gregg, D.A. Claremont, **S.B. Singh**

9:50 MEDI 17. Inhibition of ER stress-associated IRE-1/XBP-1 pathway with small molecules. **S. Ranatunga**, C. Tang, C. Kang, C. Kriss, B. Kloppenburg, C. Hu, J. Del Valle

10:10 MEDI 18. Discovery of the first, designed for inhalation, prostacyclin receptor agonist for pulmonary arterial hypertension. **M. Healy**

10:30 MEDI 19. Discovery and evaluation of selective, orally available and brain penetrant inhibitors of leucine rich repeat kinase 2 (LRRK2). **D. DeMong**, K. Basu, J.D. Scott, M.W. Miller, G. Agnihotri, M. Baptista, B. Cheewatrakoolpong, J. Columbus, X. Dai, X. Duan, M. Fell, E. Frank, A. Frassetto, T.J. Greshock, J. Harris, A. Hruza, Z. Hu, W. Li, S. Lin, H. Liu, M. Macala, H. Mei, C. Mirescu, J. Morrow, M. Poirier, G. Scapin, B. Sherborne, M. Smith, H. Stevenson, C. Strickland, P. Tempest, M.L. Vicarel, P.L. Walsh, L. Xiao, H. Zhang, X. Zhou, J.L. Duffy, M. Kennedy, J. McCauley, R.P. Nargund, E. Parker, R. Ruck, A.W. Stamford, A.E. Weber

10:50 MEDI 20. Discovery and pharmacology of a novel class of DGAT2 inhibitors. **J. Imbriglio**, H. Youm, Z. Feng, R. Liang, Y. Xiong, J. Tata, A. Taggart, S. Pinto

11:10 MEDI 21. Discovery and optimization of quinazolinone-pyrrolo-dihydro-pyrrolones as potent, selective, and orally bioavailable Pim1,2,3 kinase inhibitors. **L.H. Pettus**

11:30 MEDI 22. Withdrawn.

11:50 MEDI 23. Discovery of small molecule utrophin modulators for the therapy of Duchenne muscular dystrophy (DMD). **N. Araujo**, A. Vuorinen, R. Fairclough, S. Guiraud, J.R. Donald, C. Cairnduff, D. Hewings, F. Martinez, K. Csatayova, N. Willis, S. Squire, A. Babbs, B. Edwards, N. Shah, J. Tinsley, F.X. Wilson, S.G. Davies, G.M. Wynne, K.E. Davies, **A. Russell**

Integrated Approaches in Structure-Based Drug Design

Sponsored by COMP, Cosponsored by CINF and MEDI

Advances in Oligonucleotide Therapeutics

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SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 210B

General Orals

W. B. Young, *Organizer, Presiding*

1:30 MEDI 24. Discovery of potent inhibitors of the antiapoptotic proteins Bcl-2 and Bcl-x_l, resulting in the identification of a clinical candidate for the treatment of cancer (AZD4320). **E.J. Hennessy**, S. Ioannidis, A. Adam, P. Brassil, K. Byth, E. Clark, R.B. Diebold, K. Dillman, T. Gero, P. Grover, S. Huang, P. Lewis, T. MacIntyre, C. Ogoe, F. Powell, G. Repik, D.J. Russell, J.C. Saeh, P. Schroeder, P. Secrist, M. Su, J.G. Varnes, W. Zhang

1:55 MEDI 25. Medicinal chemistry discovery of the clinical candidate AZD9496: A potent and orally bioavailable selective estrogen receptor down-regulator and antagonist. **C. De Savi**, R. Bradbury, A. Rabow, R. Norman, D. Buttar, G. Currie, C. Donald, B. Hayter, P. MacFaul, P. Ballard, S. Pearson, T. Moss, S. Lamont, L. Feron, S. Glossop, C. Davies

2:20 MEDI 26. BMS-933043, a novel α 7 nicotinic acetylcholine receptor partial agonist active in pre-clinical models of schizophrenia. **D. King**, J. Cook, C. Iwuagwu, I. McDonald, A. Easton, R. Miller, K. Jones, Y. Li, R. Pieschl, D. Sivarao, P. Chen, C. Daly, D. Post-Munson, N. Lodge, Y. Benitez, W. Clarke, D. Morgan, R. Denton, K.A. Lentz, R. Zaczek, L. Bristow, J.E. Macor, R.E. Olson

2:45 MEDI 27. Discovery and characterization of an indole acid direct AMPK activator for the treatment of diabetic nephropathy. **K.O. Cameron**, S.K. Bhattacharya, N. Bodycombe, K.A. Borzilleri, J.A. Brown, M. Calabrese, E. Cokorinos, E.L. Conn, M.S. Dowling, D. Fernando, R. Frisbie, A.S. Kalgutkar, D.W. Kung, R.G. Kurumbail, Y. Mao, R. Miller, F. Rajamohan, A. Reyes, C. Rose, C.T. Salatto, A. Shavnya, A.C. Smith, B. Thuma, M. Tu, J. Ward, J.M. Withka, A. Wolford, J. Xiao

3:10 MEDI 28. Optimization of 1,2,4-triazolopyridines as inhibitors of human 11 β -hydroxysteroid dehydrogenase Type 1 (11 β -HSD-1): Discovery of clinical candidate BMS-823778. **J. Li**, L.J. Kennedy, H. Wang, J. Li, S.J. Walker, Z. Hong, S.P. O'Connor, X. Ye, S.Y. Chen, S. Wu, D.S. Yoon, A. Nayeem, D.M. Camac, P. Morin, S. Sheriff, M. Wang, T. Harper, R. Golla, R. Seethala, T. Harity, R. Ponticciello, N. Morgan, J.F. Taylor, R. Zebo, D. Gordon, J.A. Robl

3:35 MEDI 29. Discovery of AZD1979: An MCH1r antagonist with a beneficial safety pharmacology profile and predictable free exposure in the brain. **A. Johansson**, C. Löfberg, M. Fredenwall, S. von Unge, R. Bergman, J. Peranson, R. Judkins, L. Li, A. Hogner, M. Antonsson, M. Hayes, K. Ploj, L. Benthem, D. Lindén, P. Johnström, M. Schou

4:00 MEDI 30. Discovery of TAK-659, an orally available investigational inhibitor of spleen tyrosine kinase (SYK). **B. Lam**

4:25 MEDI 31. Discovery of AMG 333: A potent, orally bioavailable TRPM8 antagonist for the treatment of migraine. **D.B. Horne**, K. Biswas, J. Brown, V.K. Gore, S. Harried, M.R. Kaller, V. Ma, H. Monenschein, T. Nguyen, W. Zhong, M.D. Bartberger, C. Davis, M. Rose, M. Horner, T. Wu, R. Sandrock, S. Lehto, S. Rao, B. Youngblood, M. Zhang, D. Zhu, N. Gava, J.J. Chen

4:50 MEDI 32. Discovery of BMS-929075 an HCV NS5B replicase allosteric inhibitor advanced to phase 1 clinical studies. **K. Yeung**, K.E. Parcella, B.R. Beno, J.A. Bender, K. Grant-Young, K. Rigat, Y. Wang, M. Liu, J. Lemm, K. Mosure, U. Hanumegowda, X. Zhuo, D. Parker, M. Sinz, K. Santone, D. Smith, J. Li, K.J. Fraunhoffer, A. Delmonte, E. Colston, C. Pasquinelli, M. Gao, N.A. Meanwell, S. Roberts, J. Knipe, J.F. Kadow

Section B

Boston Convention & Exhibition Center
Room 210A

Protein-Protein Interactions

J. j. Chen, J. E. Gestwicki, *Organizers, Presiding*

2:00 MEDI 33. Current state and future of drug discovery for PPI. **M. Arkin**

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- 2:35** **MEDI 34.** Selective BCL-2 family inhibitors: Potential therapeutics and powerful research tools. **A.J. Souers**
- 3:10** **MEDI 35.** Structure-based discovery of novel indolizines as potent and orally bioavailable Bcl-2 antagonists. **A. Letiran, T. Le Diguarher, J. Starck, J.B. Murray, J.E. Davidson, J.M. Henlin, C. Graham, I. Chen, O. Geneste, J. Hickman, M. Nyerger, G. De Nanteuil**
- 3:45** **MEDI 36.** Targeting protein-protein interactions for new cancer therapeutics. **S. Wang**
- 4:20** **MEDI 37.** From de novo design to the clinic: The discovery of AMG 232, an inhibitor of the MDM2-p53 interaction. **S.H. Olson**

Innovation from Discovery To Application Plenary Session

Sponsored by MPPG, Cosponsored by BIOT, MEDI, PMSE and POLY

Integrated Approaches in Structure-Based Drug Design

Sponsored by COMP, Cosponsored by CINF and MEDI

Advances in Oligonucleotide Therapeutics

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SUNDAY EVENING

Section A

Westin Boston Waterfront
Galleria

General Posters

W. B. Young, Organizer

7:00 - 9:00

- MEDI 38.** Photocleavable mass-tag encoded protein bead-arrays for proteome-scale drug-protein screening by MALDI-MS imaging. **Y. Zhou, Z. Liu, K. Rothschild, M. Lim**
- MEDI 39.** Design and synthesis of conjugates of trityl tags with targeting molecules: Applications to imaging mass spectrometry. **Y. Zheng, L. Wang, C. Dai, B. Wang**
- MEDI 40.** Discovery and structure-activity relationship (SAR) of BRD7539, a small molecule inhibitor of *Plasmodium falciparum* dihydroorotate dehydrogenase (PfDHODH). **M. Maetani, N. Kato, L. Ross, E.J. Comer, C. Scherer, D. Wirth, S.L. Schreiber**
- MEDI 41.** 4-Amidinoquinolines and 10-amidinobenzonaphthridines as new classes of antimalarials with high potency in vitro and in vivo. **V.N. Korotchenko, R. Sathunuru, L. Gerena, D. Caridha, Q. Li, T. Luong, D. Hettithantrige, R. Olmeda, L. Zhang, S. Marcissin, V.E. Zottig, M. Kreishman Deltrick, P. Smith, A. Lin**
- MEDI 42.** Hit-to-lead optimization of a new class of compound to treat human African trypanosomiasis. **L. Ferrins, R. Rahmani, S. Russell, A. Jones, N. Nguyen, H. Newson, M. Sykes, V. Avery, M. Piggott, J. Baell**
- MEDI 43.** Highly water-soluble benzimidazole derivatives useful for the treatment of fasciolosis. **R. Castillo-Bocanegra, M.A. Flores-Ramos, F.O. Ibarra, A. Hernandez Campos, Y. Vera-Montenegro, H. Jung-Cook, G.J. Cantó-Alarcón**
- MEDI 44.** Hit-to-lead optimization efforts of HTS hits for human African trypanosomiasis. **D. Klug, R. Diaz, C. Cordon-Obras, D. Rojas-Barros, M. Navarro, M.P. Pollastr**
- MEDI 45.** Synthesis, inhibitory activities and molecular modeling studies of pentacosenoic and pentacosynoic acids as novel HIV-1 reverse transcriptase inhibitors. **N.M. Carballera, L. Giménez Moreira, E. Orellano, K. Rosado, R. Guido, A.D. Andricopulo**
- MEDI 46.** Withdrawn.
- MEDI 47.** Exploring HIV-1 tropism using synthetic mimics of co-receptors CXCR4 and CCR5. **C. Hashimoto, A. Gross, J. Eichler**
- MEDI 48.** Targeting the nucleocapsid protein of HIV-1 (NCp7) with nucleobase flexibility. **N. Steenrod, T. Ku, M. Mori, M. Botta, K.L. Seley-Radtke**
- MEDI 49.** Toward the synthesis of novel 1,3-azaborines as potential HIV-1 protease inhibitors. **K.M. Norris, K. Sigurjonsson, M.D. Frank, L. Fabry-Asztalos**
- MEDI 50.** β -Substituted fosmidomycin analogs targeting 1-deoxy-d-xylulose-5-phosphate reductoisomerase: Synthesis, structural biology, and antimicrobial properties. **R. Chofor, S. Sooriyaarachchi, M.D. Risseuw, T. Bergfors, T.A. Jones, S.L. Mowbray, S.P. Van Calenberg**
- MEDI 51.** Development of novel antagonists of PqsR as pathogen-blockers for *Pseudomonas aeruginosa*. **M.G. Zender, C. Lu, C. Maurer, B. Kirsch, M. Empting, A. Steinbach, R.W. Hartmann**
- MEDI 52.** Identifying a potent inhibitor of *Pseudomonas aeruginosa* through the Distributed Drug Discovery (D3) process. **W.L. Scott, R.E. Denton, G. Anderson, K. Marrs, J.G. Samaritoni, S. Colglazier, J. Lacombe, M. Phillips, M.J. Odonnell**
- MEDI 53.** Human acetylcholinesterase inhibition activity of some methyl pyridinium β -lactams. **S.N. Yasapala, A. Lodge, J.J. Topczewski, Q.M. Daniel**
- MEDI 54.** Development of novel anthrax toxin lethal factor inhibitors using synthetic, computational, X-ray crystallographic and high-throughput screening approaches. **E.K. Kurbanov, K.M. Maize, J. Solberg, R.L. Johnson, B. Finzel, J. Hawkinson, M.A. Walters, E.A. Amin**
- MEDI 55.** Biological evaluation of an in vivo-potent dual target PQS quorum sensing inhibitor that hinders biofilm formation. **R.W. Hartmann, A. Thomann, A.G. Martins, C. Brengel, E. Weidel, C. Boerger, M. Empting**
- MEDI 56.** Design and synthesis of bacterial biofilm inhibitors for *Salmonella enterica* serovar Typhi. **C. Hambira, M. Lautenschlager, J.S. Moshiri, J.S. Gunn, J. Fuchs**
- MEDI 57.** Rational design of potent and selective inhibitors of *Pseudomonas aeruginosa* virulence factor Cif. **S. Kitamura, K.L. Hvorecny, D.R. Madden, B.D. Hammock, C. Morisseau**
- MEDI 58.** Some antiplasmodial and antimycobacterial drug-metal complexes: Reactions, analysis, and biological properties. **J.A. Obaleye, N. Simon, U.B. Eke, A.C. Tella, J.O. Adebayo, M.O. Bamigboye, E.A. Balogun**
- MEDI 59.** Evaluation of the oxidation of enrofloxacin by permanganate and the antimicrobial activity of the products. **Y. Xu, S. Liu, F. Guo, B. Zhang**
- MEDI 60.** Synthesis, antifungal, and antiviral activity of N-benzyl derivatives of tetraene macrolide antibiotic luensomycin. **V. Belakhov, A. Garabadzhiu, V. Kolodyznaya, O. Topkova**
- MEDI 61.** In vitro and in vivo activity of multitarget inhibitors against *Trypanosoma brucei*. **Y. Wang, W. Zhu, G. Yang, G. Huang, S. Byun, G. Choi, K. Li, Z. Huang, R. Docampo, E. Oldfield, J. No**
- MEDI 62.** Design, synthesis, and modeling of potential di-metalloprotein inhibitors. **C. Reidl, M. Moore, A. Stewart, P.W. Thomas, W. Fast, D.P. Becker**
- MEDI 63.** Investigation of quorum sensing inhibition by phevallin and its derivatives. **S. Forschner-Dancause, M. Grande, S.M. Meschwitz**
- MEDI 64.** S. mutants GTF inhibitors for the prevention of dental biofilms. **S. Nijampatnam, Q. Zhang, T. Nguyen, H. Wu, S.E. Velu**
- MEDI 65.** Targeted antibiotics to bacteria with thiomaltose. **X. Wang, N. Murthy**
- MEDI 66.** Novel inhibitors of *M. tuberculosis* InhA: A little learning can go a long way. **T.P. Stratton, A.L. Perryman, X. Wang, S. Li, S.D. Paget, A.J. Olson, S. Ekins, J. Freundlich**
- MEDI 67.** Metabolomics-aided optimization of antitubercular thienopyrimidines. **S. Li, C. Vilchêze, S. Chakraborty, X. Wang, H. Kim, M. Anisetti, S. Ekins, K.Y. Rhee, W.R. Jacobs, J. Freundlich**
- MEDI 68.** Synthesis and evaluation of boronic acid inhibitors of the nonvalonate isoprenoid biosynthesis pathway. **J. Gamrat, S.J. Burke, D. Tomares, J.W. Tomsho**
- MEDI 69.** Modulation of repetitive behaviors in autism spectrum disorder: Design, synthesis, and biological evaluation of a potent and selective serotonin autoreceptor antagonist. **D. Keefe, S.W. Goldstein, A. Khalil, O.M. Ghoneim**
- MEDI 70.** Imidazobenzodiazepines for improving $\alpha 5$ -GABA_R subtype selectivity and their pharmacological relevance. **M.M. Poe, G. Gallos, R. Puthenkalam, M.M. Savic, C.W. Emala, M. Ernst, J.M. Cook**
- MEDI 71.** Development of highly potent, selective BET bromodomain inhibitors that are CNS penetrant and effective in rodent models of brain cancer. **J. Albert, S. Johnstone, M. Bayraktarian, A. Johnstone, C. Penas, V. Stathias, S. Brothers, N. Ayad, C. Wahlestedt**
- MEDI 72.** Identification, synthesis, and evaluation of novel botulinum neurotoxin serotype A inhibitors. **K.H. Raghunandan, Y. Teng, W.T. Berger, N. Nesbitt, K. Kumar, T. Balius, R.C. Rizzo, P.J. Tonge, I. Ojima, S. Swaminathan**
- MEDI 73.** Synthesis and biological evaluation of regioisomers of 3-(1-naphthyl)-1-pentylindole (JWH-018). **A.N. Thaxton, C.R. Clark, J. DeRuiter, F. Smith**
- MEDI 74.** Enantioselective synthesis of heterocyclic analogs of the CGRP receptor antagonist BMS-927711 for treating migraine. **G. Luo, L. Chen, C.M. Conway, W. Kostich, J.E. Maacor, G.M. Dubowchik**
- MEDI 75.** Further structure-activity relationships study of dithiolethiones: Correlation of electronic properties, glutathione induction, and neuroprotection. **D. Brown, S. Betharia, J. Yen, H. Mistry, Q. Tran**
- MEDI 76.** Imaging active amyloid plaques of Alzheimer's disease with near-infrared fluorescent probes capable of cascade signal amplification. **J. Yang, J. Yang, A. Moore, C. Ran**
- MEDI 77.** Discovery of small molecule insulin-degrading enzyme inhibitors. **H. Wang, T.D. Bannister, S. Abdul-Hay, M.A. Leissring, F. Madoux, S.C. Schurer, M. Cameron**
- MEDI 78.** Development of novel mGlu₁ PAMs: Chemical tools to improve functionality of mutant receptor isoforms found in a schizophrenic population. **P.M. Garcia-Barrantes, H.P. Cho, J. Brogan, M. Bures, C. Clawson, C.R. Hopkins, J. Conn, C.W. Lindsley**
- MEDI 79.** Preparation and characterization of novel, functionally selective mGlu₂ receptor agonists. **S.S. Henry, L. Prieto, L. Taboada, J. Hao, M. Reinhard, C. Beadle, L. Walton, T. Man, H. Rudyk, B. Clark, D. Tupper, S. Baker, C. Lamas, C. Montero, A. Marcos, J. Blanco, M. Bures, D. Clawson, S. Atwell, F. Lu, J. Wang, M. Russell, B.A. Heinz, X. Wang, J.H. Carter, B.G. Getman, J.T. Catlow, S. Swanson, B.G. Johnson, D.B. Shaw, D.L. McKinzie, J.A. Monn**
- MEDI 80.** Identification and optimization of mGluR2 NAM as novel drug candidates for Alzheimer's disease. **A. Blayo, S. Mayer, C. Amalric, L. Cardona, T. Catalain, F. Courvaud, G. Hommet, N. Lotz, B. Manteau, S. Mikidadi, E. Steinberg, L. Deshons, L. Baron, S. Scheffler, C. Franchet, M. Frauli, S. Schann**
- MEDI 81.** Discovery of highly potent, selective and brain-penetrant GluN2A-selective NMDA receptor positive allosteric modulators (PAMs). **E. Villemure, M. Volgraf, J.B. Schwarz, B.D. Sellers, C.Q. Ly, P.J. Lupardus, H. Wallweber, B.M. Liederer, G. Deshmukh, J. Hansson, D.H. Hackos, K. Scearce-Levie, P. Yuen, G. Wu, A. Liu, Y. Jiang**
- MEDI 82.** Synthetic enablement of bicyclic morpholinopyrimidones as mGluR5 negative allosteric modulators (NAMs). **M. Reese, S.V. O'Neil, B. Boscoe, M.M. Claffey, L.A. McAllister**
- MEDI 83.** Synthesis of a non-aversive non rewarding dual kappa-delta opioid receptor analgesic blocking cocaine reward behavior. **A. Varadi, G.F. Marrone, D. Afonin, J. Subrath, V. Le Rouzic, A. Hunkele, G.W. Pasternak, J. McLaughlin, S. Majumdar**
- MEDI 84.** Insight into opioid-opioid receptor binding through analysis of structural data, mutagenesis studies, and SAR of opioid peptides. **M.J. Ferracane, J.V. Aldrich**
- MEDI 85.** Asymmetric synthesis and evaluation of bifunctional μ/δ opioid peptidomimetics: Probing unexplored chemical space. **A. Nastase, N.W. Griggs, A. Harland, J.P. Anand, E.M. Jutkiewicz, J.R. Traynor, H.I. Mosberg**
- MEDI 86.** Structural modifications to the lactone of salvinorin A for the development of addiction therapies. **R.M. Saylor, T.E. Priszczano**
- MEDI 87.** Design, synthesis, and initial structure-activity relationship (SAR) study of novel multifunctional dopamine D₂/D₃ agonists with modulatory property against α -synuclein aggregation and toxicity. **D. Luo, H. Sharma, T. Antonio, M. Reith, A.K. Dutta**

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

- MEDI 88.** Discovery of bicyclic aminopyrazines and aminoquinazolines as potent and selective A2A antagonists for Parkinson disease. **G. Zhou, A. Ali**
- MEDI 89.** Identification of imidazotriazinone analogs as potent and selective PDE9 inhibitors demonstrating good drug-like properties and cognitive enhancement in a rodent cognition model. **A.J. McRiner, D.A. Burnett, M.G. Bursavich, S. Kapadnis, L. Leventhal, S. Nolan, A.S. Ripka, G. Shapiro, C. Tang, M. Wen, G. Koenig**
- MEDI 90.** Rapid technique for new scaffold generation II: What is the best source of inspiration? **T. Cheeseright, S. Tomasio, P. Tosco, M.D. Mackey**
- MEDI 91.** Probing synthetic lethality of PARP1 activities. **K. Sulier, J.S. Josan**
- MEDI 92.** Is this compound worth making. **T. Cheeseright, M.D. Mackey, G. Tedesco, P. Tosco, S. Tomasio**
- MEDI 93.** Withdrawn.
- MEDI 94.** Design, synthesis, and biological evaluation of thiophene-based heteroaryl derivatives as MEK5 inhibitors. **D. Shah, A. Motta, T. Wright, J. Cavanaugh, P.T. Fiherty**
- MEDI 95.** Computational approach for performing medicinal chemistry transformations within a 3D active site. **M.R. Goldsmith**
- MEDI 96.** Exploiting solvent effects in drug design and optimization. **C. Williams**
- MEDI 97.** Building a rational model for the prediction of allosteric sites. **C. Indey, N. Tomkinson**
- MEDI 98.** Novel dUTPase inhibitors for 5-fluorouracil-resistant cancers. **C.M. DeAngelo, M.A. Sainz, K.J. Gaffney, S.G. Louie, N.A. Petasis**
- MEDI 99.** Post-HTS structural alert: Promiscuous, non-selective 3-hydroxy-pyrrolidin-2-one hits triaged by ALARM NMR. **J.L. Dahlin, W. Nissink, Z. Zhang, M.A. Walters**
- MEDI 100.** Cell permeable ATP analog for kinase-catalyzed labeling. **A.E. Fouda, M.K. Pflum**
- MEDI 101.** Lead identification of novel tetrahydroisoquinolines as mineralocorticoid receptor antagonists. **P. Lan, Z. Sun, A.K. Ogawa, Z. Wu, P.J. Sinclair, J. Tata**
- MEDI 102.** Examination of the protective effects of berberine in thiol oxidative stress. **C. Lynch, S. Sadhu, T.M. Seefeldt**
- MEDI 103.** Optimization of amide-containing EP3 receptor antagonists. **E.C. Lee, K. Futatsugi**
- MEDI 104.** Synthesis of 17 β -N-arylcaramoylandrost-4-en-3-one derivatives and their in vitro and in vivo effect as potent 5 α -reductase inhibitors. **F. Cortes, M. Cabeza, B. Alvarez, M. Ramirez-Apan, R. Castillo-Bocanegra, E.A. Bratoeff**
- MEDI 105.** Synthesis of 17-triazolylehydroepiandrosterone derivatives with substituted cinnamates at C-3 and their in vitro and in vivo biological activity. **M. Mendoza Jasso, M. Cabeza, M. Ramirez-Apan, F. Cortes, E.A. Bratoeff**
- MEDI 106.** Design of 7-azaindole-based Rho kinase (ROCK) inhibitors. **U.K. Bandarage, J. Cao, J. Come, J.J. Court, H. Gao, M. Jacobs, C. Marhefca, T. Nakayama, D. Newsome, S. Nanthakumara, S. Rodems, S. Shah, M. Stewart, P. Taslimi, J. Green**
- MEDI 107.** Synthesis of neuroprotective agents against stroke in less than 10 steps. **G. Abu deaih, I. Hyatt, M.P. Croatt**
- MEDI 108.** Cytochrome P450 aromatic oxidation: A simple model for reactive metabolites prediction. **A. Tomberg, J. Pottel, Z. Liu, C.R. Corbeil, P. Labute, N. Moitessier**
- MEDI 109.** Microfibrous borate bioactive glass dressing sequesters bone-bound bisphosphonate in the presence of simulated body fluid. **C. Pramanik, T. Wang, S. Ghoshal, L. Niu, B.A. Newcomb, Y. Liu, C.M. Primus, H. Feng, D.H. Pashley, S. Kumar, F.R. Tay**
- MEDI 110.** Cytotoxicity and cellular uptake of metallic nanorods fabricated by electron beam physical vapor deposition and metallic nanospheres. **P. Favi, M.M. Valencia, P. Elliott, A. Restrepo, M. Gao, H. Huang, J. Pavon, T. Webster**
- MEDI 111.** Evaluating device design and cleanliness of orthopedic device models contaminated with a clinically relevant bone test soil. **A.D. Lucas, S. Nagaraja, E. Gordon, V. Hitchins**
- MEDI 112.** Isotopic-labeling of covalent modifiers to identify cellular mechanisms of action. **Z.V. Boskovic, S. Chattopadhyay, C. Huang, S.L. Schreiber**
- MEDI 113.** Novel liquid fiducial tissue marker with potential use in image-guided radiotherapy. **H. Schaarp-Jensen, R.I. Jolck, A.E. Hansen, A.I. Jensen, L.M. Bruun, A.E. Christensen, P. Bengtsson Scherman, A. Kjaer, M. Clausen, T.L. Andresen**
- MEDI 114.** Utilizing Rosette nanotubes for the delivery of siRNA for cancer therapeutics. **G. Delos Reyes, U. Ho, H. Fenniri**
- MEDI 115.** Cyclic penta- and hexa leucine peptides without N-methylation are orally absorbed. **W. Kok, T. Hill, R. Lohman, H. Hoang, D. Nielsen, C. Scully, C. Schroeder, B. Colless, P. Bernhardt, D.J. Edmonds, D.A. Griffith, C.J. Rotter, R.B. Ruggeri, D. Price, S. Liras, D. Craik, D.P. Fairlie**
- MEDI 116.** Oral peptide delivery through the vitamin B₁₂ dietary uptake pathway. **R. Bonaccorso**
- MEDI 117.** Methods for enhancing the solubility of the multifunctional curcumin molecule. **J. Hinaman, A.M. Smith, J. Hughes, L. Mielnicki, M.P. McCourt**
- MEDI 118.** Investigation of zeolite-MOF composite microneedle. **H.Y. Poon, B. Zhong, Z. Liu, S. Kwan, K.L. Yeung**
- MEDI 119.** Transdermal therapeutic systems for benzodiazepines. **A. Sosnov, V.N. Tohmakhchi, M.S. Krymchak, A.I. Korovyakovskaya, F.M. Semchenko**
- MEDI 120.** Withdrawn.
- MEDI 121.** Selective targeting of α 4 β 3 γ 2 GABA_A receptors on airway smooth muscle as a novel strategy to treat asthma. **M. Stephen, R. Jahan, G. Gallos, C.W. Emala, M. Ernst, W. Sieghart, J.M. Cook**
- MEDI 122.** In silico design and discovery of novel PDE-IV inhibitors. **F. Jabeen, G.G. Pillai, C.D. Hall, A. Katritzky**
- MEDI 123.** Identification of novel autotaxin inhibitors: Lead optimization through structure based drug design. **S. Jones, L. Pfeifer, B.H. Norman, N.E. Hughes, T. Bleisch, T.J. Beauchamp, C.J. Rito, Y. Dao, V.J. Klimkowski, J. Gruber, M. Chambers, C. Wwearingen, D. McCann, D.R. Mudra, J.D. Durbin, H. Bui, C. Lin, J. Oskins, S. Chandrasekar, K. Thirunavukkarasu**
- MEDI 124.** Synthesis of benzyl ((S)-1-((1S,2R,4R)-2-acetamido-4-(tertbutylamino)cyclohexyl)-2-oxopyrrolidin-3-yl)carbamate. **M. Yang, Z. Xiao, R. Zhao, B. Wang, J.V. Duncia, D.S. Gardner, J.B. Santella, R.J. Cherney, B. Chen, M. Cvijic, Q. Zhao, J.C. Barrish, P.H. Carter**
- MEDI 125.** Solid phase synthesis and biological screening of quinolinone library. **S. Kwak, Y. Jung, T. Kim, B. Son, J. Park, S. Choi, H. Ko, Y. Kim**
- MEDI 126.** Covalent chemical probes of APOBEC3 DNA cytosine deaminases. **M.E. Olson, A.L. Perkins, M. Li, R.S. Harris, D.A. Harki**
- MEDI 127.** Synthesis of α -truxillic acid derivatives as antinociceptive and anti-inflammatory agents, targeting fatty acid binding protein (FABP). **S. Tong, M. Kaczocha, M.J. Rebecchi, B.P. Ralph, Y. Teng, W.T. Berger, W. Galbavy, M.W. Elmes, S.T. Glaser, L. Wang, R.C. Rizzo, D.G. Deutsch, I. Ojima**
- MEDI 128.** Discovery and optimization of novel pyrazolopyrimidines as allosteric integrase inhibitors. **A. Pendri, G. Li, M.A. Walker, B. Naidu, D. Langley, H. Lewis, A. Ng, G.L. Trainor, I.B. Dicker, C. Cianci, M. Krystal, Z. Lin, T. Protack, L. Discotto, B. Minassian, S. Jenkins, N.A. Meanwell, S.W. Gerritz**
- MEDI 129.** Reverse amide pyrazolopyrimidines as potent HIV LEDGF inhibitors. **Z. Zheng, S. D'Andrea, D. Langley, N. Narasimhulu, M.M. Patel, B. McAuliffe, L. Discotto, B. Minassian, C. Cianci, J.F. Kadow, N.A. Meanwell, M.A. Walker**
- MEDI 130.** Synthesis and SAR of novel C2- pyrazolopyrimidine amides as allosteric integrase inhibitors. **M.M. Patel, B. Naidu, N.A. Meanwell, C. Cianci, M. Krystal, B. McAuliffe, B. Minassian, L. Discotto**
- MEDI 131.** 5,6,7,8-Tetrahydro-1,6-naphthyridine derivatives as potent non-catalytic site HIV-1 integrase inhibitors. **K. Peese, C. Allard, T. Connolly, B.L. Johnson, C. Li, M.M. Patel, M. Sorensen, N.A. Meanwell, C. Cianci, S. Jenkins, B. Naidu, M.A. Walker**
- MEDI 132.** Ruthenium-based self-regenerating antioxidant catalysts and materials. **A.G. Tennyson**
- MEDI 133.** Discovery of novel potent peripherally restricted PDE10a inhibitors. **S.K. Meegalla, C.R. Illig, H. Huang, D. Parks, J. Chen, Y. Lee, K. Wilson, S. Patel, W.S. Cheung, T. Lu, T. Kirchner, H. Askari, R.J. Patch, J. Geisler, M. Connelly, M.R. Player**
- MEDI 134.** Optimizing ligand efficiency of selective androgen receptor modulators (SARMs). **A.L. Handlon, R. Cadilla, L.M. Leesnitzer, R.V. Merrihew, C. Poole, J. Ulrich, J.W. Wilson, P. Turnbull**
- MEDI 135.** Antioxidant and hypoglycemic evaluation of 1,5-diarylpiperazine derivatives. **S. Salgado, E. Hernández-Vázquez, J. Ramirez-Espinosa, S. Estrada-Soto, F. Hernández-Luis**
- MEDI 136.** Design, synthesis, and biological evaluation of thienopyrimidine derivatives as DPP IV inhibitors for the treatment of type 2 diabetes. **J. Wang, H. Liu**
- MEDI 137.** Short hydrophobic peptides with cyclic constraints are potent GLP-1 receptor agonists. **T.A. Hill, H.N. Hoang, W. Kok, K. Song, D.J. Edmonds, D.R. Derksen, D.W. Piotrowski, J.M. Withka, C. Limberakis, R.V. Stanton, A.M. Mathiowetz, D. Price, S. Liras, D.A. Griffith, D.P. Fairlie**
- MEDI 138.** Discovery and SAR of benzofuran GPR120 agonists. **N.L. Subasinghe, J. Lanter, E.C. Lawson, Z. Sui, Y. Wang, J. Gunnet, H. Hua, A. Suckow, C. Jenkinson, P. Haug, J. Leonard, W.V. Murray**
- MEDI 139.** Novel xanthine oxidase inhibitors as a therapeutic agent or a preventive agent for gout and hyperuricemia. **A. Kawana, C. Kanazawa, Y. Takahashi, Y. Muroga, M. Imazeki, Y. nakada**
- MEDI 140.** Structure-activity relationships of amide and sulfonamide analogs of Omarigliptin (MK-3102), a novel, long acting DPP-4 inhibitor for treatment of type 2 diabetes. **P. Chen, D. Feng, X. Qian, J. Appgar, R. Wilkening, J. Cox, G. Doss, G. Eiermann, H. He, K. Lyons, J. Metzger, A. Petrov, J.K. Wu, S. Xu, B. Zhang, N.A. Thornberry, A.E. Weber, R. Sinha Roy, T. Biftu**
- MEDI 141.** Discovery of small molecule functional agonist leads of APJ receptor. **S. Narayanan, R. Maitra, J.R. Deschamps, K. Bortoff, J. Thomas, Y. Zhang, K. Warner, S. Runyon**
- MEDI 142.** Approaches to ring-fused 1,2,4-triazoles, a druggable drug scaffold. **E.P. Stevens, D.H. Robinson**
- MEDI 143.** Synthesis of new heterocyclic ring systems for use in molecular libraries. **T.A. Pfister, E.P. Stevens**
- MEDI 144.** Preparation and reactions of 2-functionalized-4, 5-diaryloxazoles: Synthesis of extended diaryloxazole scaffolds. **P.C. Patil, F.A. Luzzio**
- MEDI 145.** Salicylaldehyde ester-induced chemoselective peptide ligations: Enabling generation of natural peptidic linkages at the hydroxyproline site. **K. Ha, A. Katritzky, D. Hall**
- MEDI 146.** Natural product-inspired, DNA-programmed combinatorial library for targeting protein-protein interactions. **K.E. Denton, C.J. Krusemark**
- MEDI 147.** Dietary natural products as promising leads for antiprostaglandin cancer agents. **Q. Chen**
- MEDI 148.** Synthesis and characterization of 24-epiconicasterol. **R. Joseph, J.P. Giner**
- MEDI 149.** Evaluation of antibacterial activity of *Artemisia vulgaris* extracts against *Staphylococcus aureus*. **A.K. Addo-Mensah, G. Garcia, I. Maldonado, L. Lee, E. Anaya, G. Cadena**
- MEDI 150.** Total synthesis and biological evaluation of the C-11 epimer of ipomoeassin F. **E. Barber, G. Zong, H. Aljewari, W. Shi**
- MEDI 151.** Synthesis and antitumor activity of a library of sempervirine analogs. **X. Pan, T.D. Bannister**
- MEDI 152.** Synthesis and in vitro anticancer evaluation of spermatinamine analogs. **B. Moosa, S. Li, N.M. Khashab**
- MEDI 153.** Thalassomononic acids A-F: New anti-tyrosinase secondary metabolites from a marine *Thalassomonas* sp. **R. Deering, J. Chen, H. Ma, J. Dubert, S. Prado, N.P. Seeram, D.C. Rowley**

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- MEDI 154.** Discovery of novel small molecules for renal diseases. **E.C. Grimley**, C. Liao, E.J. Ranghini, Z. Nikolovska-Coleska, G. Dressler
- MEDI 155.** Investigation of nitroxyl (NO) reactions with the selenoprotein thioredoxin reductase. **B. Brosnan**, T. Zawahreh, **S. Mitroka**
- MEDI 156.** Discovery of novel autotaxin inhibitors. A. Ohhata, Y. Iwaki, S. Nakatani, K. Hisaichi, R. Miwa, Y. Okabe, A. Hiramatsu, T. Watanabe, S. Yamamoto, T. Nishiyama, J. Kobayashi, Y. Hirooka, N. Matsumura, T. Maeda, M. Kato, H. Saga, T. Sugiyama, A. Imagawa, H. Habashita
- MEDI 157.** New monocyclic, bicyclic, and tricyclic ethynylcyanodienones as activators of the Keap1/Nrf2/ARE pathway and inhibitors of inducible nitric oxide synthase. **W. Li**, S. Zheng, M. Higgins, R.P. Morra, A. Mendis, C. Chien, I. Ojima, D. Mierke, A. Dinkova-Kostova, T. Honda
- MEDI 158.** Differential loss of cell viability after exposure of breast cancer and normal cells to chloro-derivatives of S-nitroso-aryl-amides. **M. Fugimoto**, E.D. Castro, H.P. Monteiro, **A.C. Reis**
- MEDI 159.** Single diastereomer of a macrolactam core binds specifically to myeloid cell leukemia 1 (MCL1). **C. Fang**, B. D'Souza, C. Thompson, M. Clifton, J. Fairman, B. Fulroth, A. Lead, P. McCarren, L. Wang, Y. Wang, C. Feau, V. Kaushik, M. Palmer, G. Wei, T. Golub, B. Hubbard, M.H. Serrano-Wu
- MEDI 160.** Targeting novel protein complexes and interrogating small molecule inhibitors of the anticancer target HSP70. **L. Evans**, K. Jones, M.D. Cheeseman
- MEDI 161.** Withdrawn.
- MEDI 162.** Novel strategies for targeted therapies of cancer: Solid-phase-based synthesis of CCK-2-Receptor-targeting ligands and their Tubulysin conjugates. **G.L. Parham**, M. Nelson, M. Vetzal, C.M. Taylor, J.A. Reddy, C.P. Leamon, I.R. Vlahov
- MEDI 163.** Anticancer lycorine-glucose conjugates for CNS delivery. **K.N. Middleton**, R. Dasari, A.V. Kornienko
- MEDI 164.** Design, synthesis, and biological evaluations of novel PAMAM dendrimer-based tumor-targeting taxoid conjugates. **L. Wei**, T. Wang, S. Bahl, Y.G. Teng, I. Ojima
- MEDI 165.** Synthesis, cytotoxic evaluation and docking studies of novel 5-substituted 9-anilinothiazolo[5,4-b]quinoline derivatives. **A.K. Lopez-Rodriguez**, J. Solano-Becerra, A. Lira
- MEDI 166.** Synthesis, in vitro cytotoxic activity and docking studies of 2-dimethylaminoalkylamino-9-anilinothiazolo[5,4-b]quinoline derivatives. **B. Vega-Alanis**, **A. Lira**, J. Solano-Becerra
- MEDI 167.** Synthesis of two pure diastereomers of a newly identified anticancer lead agent and determination of their cytotoxicity in breast cancer cells. **R. Stenken**, K.M. Borland, A.P. Bercz, E.J. Merino, V.A. Litosh
- MEDI 168.** Probing ligand receptor interaction through molecular docking of synthesized library of coumarin-triazolothiadiazine hybrids against Gp63, HSP90 and ALP. **F. Jabeen**, A. Saeed, A. Ibrar, S. Zaib, J. Iqbal
- MEDI 169.** Synergistic combination of next-generation taxoid with CMC2.24, EGCG and MMP inhibitors. **X. Wang**, I. Ojima
- MEDI 170.** Design, synthesis, and biological evaluation of novel C-terminal hsp90 inhibitors. **L.K. Buckton**, H. Wahyudi, S.R. McAlpine
- MEDI 171.** Development of isoform selective compounds for Grp94 inhibition. **S. Mishra**
- MEDI 172.** New approach to inhibit HGF/MET oncogenic signaling: Inhibition of HGF activation. **R.A. Galemmon**, N. Bansal, B. Owusu, P. Venukadasula, L. Ross, J. Hobrath, T. Messick, L. Klampfer
- MEDI 173.** Identification of inhibitors of HIF2a as modulators of the hypoxia response for the treatment of cancer. **S. Johnstone**, **J. Albert**, M. Coupal, S. Lee
- MEDI 174.** Chemical modification of yeast cell wall beta glucans to enhance stimulation of innate immune cells directed toward cancer immunotherapy. **M.E. Danielson**, K.S. Michel, N. Bose, X. Qiu, N.C. Ottoson, P.M. Will, A.G. Rollings, T.M. Phelon, L.R. Wurst, R.B. Fulton, S.M. Leonardo, K.B. Gorden, Y. Yokoyama, A.S. Magee
- MEDI 175.** Conformationally-controlled late-stage modification to facilitate SAR studies of ipomoeassin F. **L.H. Whisenhunt**
- MEDI 176.** Total synthesis and SAR study of ipomoeassin F. **G. Zong**, H. Aljewari, M. Govindarajan, E. Barber, L.H. Whisenhunt, W. Shi
- MEDI 177.** Non-absorbable iron chelators as bowel cancer therapeutic and preventative agents. **J.S. Fossey**, R. Byravan, C. Tselepis
- MEDI 178.** Fragment-based discovery of 6-arylindazole JAK inhibitors. **A. Ritzen**, M. Sorensen, K. Dack, D. Greve
- MEDI 179.** Structure-based design of 2,4,6-trisubstituted pyridines as AKT-2 inhibitors. **E. Sanabria-Chanaga**, A. Hernandez Campos, R. Castillo-Bocanegra
- MEDI 180.** Optimization of furanopyrimidine-based kinase inhibitors: Identification of a BTK kinase inhibitor for the treatment of B cell lymphoma. **W. Wang**, Y. Chang Hsu, H. Shiao, H. Hung, C. Kuo, J. Lee, T.J. Hsu, H. Hsieh
- MEDI 181.** Design, synthesis, and biological evaluation of bioisosteric analogs of dasatinib as Src, Abl and Abl T3151 protein tyrosine kinase inhibitors. **J. Patel**, Z. Chen, V.L. Korlipara
- MEDI 182.** Discovery of 2,4-diaminopyrimidines bearing a unique pharmacophore as anaplastic lymphoma kinase inhibitors. **H. Shiao**, W. Wang, Y. Chang Hsu, Y. Ke, T.J. Hsu, H. Hsieh
- MEDI 183.** Structure-based design of potent and selective DLG-out RIPK1 inhibitors. **C. Suebsuwong**, M. Najjar, S.S. Ray, R.J. Thapa, J.L. Maki, S. Nogusa, S. Shah, D. Saleh, P.J. Gough, J. Bertin, J. Yuan, S. Balachandran, G.D. Cuny, A. Degterev
- MEDI 184.** Analog synthesis of the α -tubulin-binding natural product pironetin as an ovarian cancer chemotherapeutic agent. **D.S. Huang**, S.K. Coullup, H.L. Wong, G.I. Georg
- MEDI 185.** Benzothiofenyl flavones as new classes of mitotic inhibitors. **Y. Taniguchi**, H. Tsurimoto, Y. Saito, E. Hamel, M. Goto, K. Goto
- MEDI 186.** Synthesis of pteridine diones as potential monocarboxylate transporter 1 (MCT1) inhibitors. **H. Wang**, C. Wang, T.D. Bannister, C. Yang, J. Cleveland
- MEDI 187.** Synthesis of chromone derivatives as anticancer agents. **H. Wang**, C. Wang, T.D. Bannister, C. Yang, J. Cleveland
- MEDI 188.** Design, synthesis, and the biological evaluation of the novel HDAC and G9a dual inhibitors. **L. Zang**
- MEDI 189.** Nanocatalysis for sustainable synthesis of heterocyclic pharmacophores for anticancer activity. **U. Rajesh**
- MEDI 190.** Michael acceptor in Gambogic acid – its role and application for potent antitumor agents. **H. He**, W. Shen, Z. Jiang, **W. Jing**, W. Xiao, Z. Wang, Q. Guo, J. Li, S. Chen
- MEDI 191.** Overcoming CYP 3A5 selective metabolism in the design of oral pan-Notch inhibitors. **D.P. O'Malley**, A.V. Gavai, G.V. De Lucca, Y. Zhao, D. Norris, B.E. Fink, C.A. Quesnelle, W. Han, P. Gill, W. Vaccaro, T. Huynh, V. Ahuja, M. Saulnier, D.B. Frennesson, S. Kim, L. Chen, A. Tebben, R. Rampulla, D. Wu, C. Wang, Y. Zhang, A. Mathur, H. Wang, R. Moore, Z. Yang, A. Ranasinghe, C. Tye, C. Su, G. Everlof, Q. Ruan, M. Yarde, K. Menard, M. Wen, J.T. Hunt, G. Vite, R. Westhouse, F. Lee
- MEDI 192.** Possible genotoxic effect exerted by thio-sugars in cancer cells via the oxidative induction of DNA. **A. Czubatka**, A. Maciejka, J. Sarnik, T. Poplawski, **Z.J. Witczak**
- MEDI 193.** Indolo-pyrindo-isoquinolin based alkaloid inhibits growth of breast cancer cells. **S.V. Malhotra**, J.E. Tomaszewski, M. Difiilippantonio, P.A. Risboud, N. Arumugam, D.B. Avtanski, D. Sharma
- MEDI 194.** Inhibition of geranylgeranyl diphosphate synthase mediates selective apoptosis through a RhoA/ERK pathway. **S. Su**, C.C. Hsiao, J. Li, A.J. Wiemer
- MEDI 195.** Phthalocyanine bioconjugates and their applications in photodynamic therapy. **E. Carrion**, S.D. Kozuch, H. Patel, M. Patel, P. Patel, E.E. Borland
- MEDI 196.** Discovery of potent PIM1 inhibitors with different profiles by targeting an acidic site. **H. Nakano**, T. Hasegawa, Y. Tada, N. Saito, M. Abe, H. Kojima, T. Okabe, T. Nagano
- MEDI 197.** Optimization of polo-like kinase 1 (Plk1) polo-box domain-binding inhibitors using oxime-based post solid-phase fragment screening. **X. Zhao**, D. Hymel, T.R. Burke
- MEDI 198.** Synthesis and structure-activity optimization of 2-substituted imidazo[1,2-a]pyridin-8-carboxamides as poly(ADP-ribose)polymerase-1 inhibitors. **B. Patel**, O. Oyem, J.F. Vilachá, T.T. Talele
- MEDI 199.** Withdrawn.
- MEDI 200.** Identification of anticancer drug targets using cysteine reactive probes and shotgun proteomics. **J.C. Widen**, A.M. Kempema, J.K. Hexum, D.A. Harki
- MEDI 201.** Structure-guided design of potent, selective, and orally bioavailable Tankyrase inhibitors. **H.B. Bregman**, E. DiMauro, N. Chakka, A. Guzman-Perez, Z. Hua, H. Huang, M.W. Martin, J.L. Buchanan, H. Gunaydin, X. Huang, L. Huang, C. Wilson
- MEDI 202.** Synthesis and SAR study of third-generation taxoids. **C. Wang**, X. Wang, B. Lichtenhal, S. Lee, I. Ojima
- MEDI 203.** Boc-Lys(Ac)-GABA-taxoids as novel tumor targeted anticancer agents. **S. Lee**, C. Wang, I. Ojima
- MEDI 204.** Synthesis and DNA binding of novel Pd(II) curcuminoids. **K. Flynn**, M. Easop, S. Bellinger-Buckley, **J.J. Rochford**, **M. Lamberto**
- MEDI 205.** Design and regio-selective synthesis of folate-thapsigargin conjugates for cancer therapy. **H. You**, S. Kwak, Y. Jung, T. Kim, B. Son, J. Park, S. Choi, L. Sun-mi, P. Jeong, H. Ko, Y. Kim
- MEDI 207.** Withdrawn.
- MEDI 208.** Establishment of a strategy, "choice based change", in mode of inhibition: Development of imidazo[1,2-a]pyridines/pyrazines as novel topoisomerase II α catalytic inhibitors. **S.M. Amrutkar**, S.K. Guchhait, U.C. Banerjee
- MEDI 209.** Synthesis and biochemical evaluation of fluorinated 9-amino acridone derivatives on human type II topoisomerase. **C.O. Okoro**
- MEDI 210.** Design and development of quinazolinone natural products based novel dual topoisomerase inhibitors. **S. Rasapalli**, V. Sammeta, E. Tsogterel
- MEDI 211.** Efforts toward chiral non-nucleoside reverse transcriptase inhibitors (NNRTIs): Asymmetric synthesis and biological evaluation. **X. Han**
- MEDI 212.** Small molecule inhibitors of the transcription factor LSF. **J. Biagi**, U. Hansen, S. Schaus
- MEDI 213.** Triphenylmethanol conjugates of triptorelin as anti-lipid peroxidation agents. **S. Alhamed**, **Y. Ahmadibeni**, W. Boadi
- MEDI 214.** Triphenylmethanol conjugates of triptorelin as anticancer prodrugs. **J. Alnakhlil**, W. Boadi, K. Parang, A. Shirazi, **Y. Ahmadibeni**
- MEDI 215.** Alpha-substituted topolones induce leukemia apoptosis. **J. Li**, E.R. Falcone, A.C. Anderson, D.L. Wright, A.J. Wiemer
- MEDI 216.** Development of photoaffinity probes for non-covalent activation of Nrf2. **B.G. Richardson**, A.D. Jain, T.W. Moore
- MEDI 217.** Kinetic studies of organoruthenium complex as self-regenerative antioxidant. **Y. Htet**, A.G. Tennyson
- MEDI 218.** Withdrawn.
- MEDI 219.** Development of a PET radioligand targeting the VEGFR₂ receptor to image angiogenesis. **K. Brocklesby**, J. Waby, G. Smith
- MEDI 220.** Design and synthesis of novel positron emission tomography imaging agents for dopamine transporter. **Z. Huang**, L. Chang, Y. Huang, C. Shue, K. Tzen, L. Hsin
- MEDI 221.** Synthesis of fluoroalkyl-substituted 1,4-bis[(2-aminoethyl)amino]anthraquinones as potential PET imaging agents for P-glycoprotein function. **Y. Cheng**, H. Liu, Y. Huang, P. Kao, C. Shue, K. Tzen, L. Hsin
- MEDI 222.** Electric field of physiological strength induced monomerization of fully metalated ALS-linked SHD1. **Y. Shi**, M.J. Acerson, E. Huntley, B.F. Shaw
- MEDI 223.** Integrated microphysiological model for drug screening for ototoxicity and nephrotoxicity. **E.M. Frohlich**, A.J. Spencer, B.C. Isenberg, J.R. Coppeta, M.J. Mescher, A.S. Edge, J.T. Borenstein, **E.E. Pararas**

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MEDI 224. Fluorine scan at the active sites of rhodesein and human cathepsin L: Enhanced binding affinity by stacking of fluorinated phenyl rings on flat dipeptide fragments. **M. Giroud**, M. Harder, B. Kuhn, W. Haap, T. Schirmeister, F.N. Diederich

MEDI 225. Pharmacophore discovery using extended Huckel Theory. **A. Deschenes**

MEDI 226. Acetylation of lysine residues in Cu,Zn WT and ALS-mutant superoxide dismutase (SOD1) with aspirin inhibits its aggregation and promotes its amyloid destabilization. **A. Abdolvahabi**, Y. Shi, B.F. Shaw

MEDI 227. Investigating the selectivity of metalloprotein inhibitors (MPI) in the presence of competing metalloproteins. **Y. Chen**, S. Cohen

MEDI 228. Antifluorine and anticancer drugs targeting the proton motive force. **W. Zhu**, X. Feng, L.A. Schurig-Briccio, S. Lindert, J. Li, Y. Wang, N. Baig, J.A. McCammon, R.B. Gennis, E. Oldfield

MEDI 229. Potent small agonists of protease activated receptor 2. **M. Yau**, J.Y. Suen, W. Xu, J. Lim, L. Liu, M. Adams, Y. He, J. Hooper, R. Reid, D.P. Fairlie

MEDI 230. Fate of fluoroquinolones in drinking water treatment plants in China. **Y. Xu**, S. Liu, Y. Wang, H. Tao, F. Cui

MEDI 231. De novo designed metalloprotein captures and stabilizes radicals. **G. Ulas**, Y. Wu, T. Lemmin, W.F. Degradó

MEDI 232. Using automated reagent management to dramatically improve efficiency in library synthesis and drug discovery. **D. Miyao**

MEDI 233. Improved synthesis of *trans/cis*-4-(*boc*-amino)-4-methyl cyclohexanol. **S. Zhang**, L. Chen, Y. Chen, H. Li, X. Wu, M. Yang

MEDI 234. Design of hepatitis C virus NS3/4A protease inhibitors with improved activity against drug resistant variants. **A. Ali**, D. Soumana, K. Prachanonarong, A. Ozen, A. Matthew, L.N. Ruser, N. Kurt-Yilmaz, C. Schiffer

MEDI 235. Ligand-induced binding pocket in anthrax Lethal Factor: Renewed opportunities for drug design. **K.M. Maize**, E.K. Kurbanov, E.A. Amin, B. Finzel

MEDI 236. Targeting onchocerciasis: Development of a ligand-based pharmacophoric model and subsequent optimization of OvCHT1 inhibitors based on the 1,2,3-triazole ring. **A. Ducime**, S. Mensa, P. Kobauri, M. Gooyit, K.D. Janda, D. Boschi, M.L. Lollí

MEDI 237. Tether modifications of a potent series of triazine macrocycles for the inhibition of the hepatitis C virus (HCV) entry pathway. **E. Mull**, L. Sun, Q. Zhao, G. Li, A. Pendra, Z. Zhang, Z. Yin, T. Wang, E.P. Gillis, Y. Wang, H. Fang, B. Eggers, K. Pokornowski, G. Zhai, D. Tenney, S. Mason, C. Baldick, N.A. Meanwell, P.M. Scola

MEDI 238. Hydroxamic acids as new anti-HCV agents. **T. Ai**, Y. Xu, L. Qiu, R. Geraghty, **L. Chen**

MEDI 239. Synthesis and SAR of a series of functionalized macrocycles as potent, pan-genotypic HCV NS3 protease inhibitors. **L. Sun**, E. Mull, Q. Zhao, E.P. Gillis, M.S. Bowsher, K. Sarkunam, P. Nagalakshmi, S. D'Andrea, Z. Zheng, X.A. Wang, Y. Wang, H. Fang, P. Falk, F. Yu, D. Hernandez, A. Sheaffer, S. Jenkins, M. Kramer, N.A. Meanwell, F. McPhee, P.M. Scola

MEDI 240. 2nd Generation HCV protease inhibitors: Part 2, optimization of P₂*. **E.P. Gillis**, M.S. Bowsher, F. McPhee, S. Jenkins, Y. Wang, P.M. Scola, N.A. Meanwell

MEDI 241. 2nd Generation HCV protease inhibitors: Part 1, optimization of the P1'-P3 tether. **M.S. Bowsher**, E.P. Gillis, Z. Zheng, Y. Wang, F. McPhee, S. Jenkins, P.M. Scola, N.A. Meanwell

MEDI 242. Discovery of 5-(3-((1, 3-difluoro-2-(fluoromethyl)propan-2-yl)carbamoyl)phenyl)-6-(N-(2-fluoroethyl)methylsulfonamido)-2-(4-fluorophenyl)-N-methylbenzofuran-3-carboxamide, the first orally bioavailable pan-genotype coverage HCV NS5B inhibitor with sulfonamide moiety at C-6 of benzofuran core. **Z. Yin**, Z. Zhang, T. Wang, K.E. Parcella, K.J. Eastman, K. Grant-Young, K. Yeung, Y. Wang, H. Fang, J. Lemm, X. Zhuo, M. Liu, K. Masure, R. Krause, S. Roberts, M. Soars, J.F. Kadow

MEDI 243. Advanced Hepatitis C virus NS5B polymerase primer grip inhibitors. **K.E. Parcella**, K.J. Eastman, K. Yeung, K. Grant-Young, J. Zhu, T. Wang, Z. Zhang, Z. Yin, D.M. Parker, K. Masure, B.R. Beno, H. Fang, Y. Wang, J. Lemm, X. Zhuo, U. Hanumegowda, B.M. Johnson, R. Haskell, R. Krause, M. Liu, C. Poronsky, K. Rigat, S. Sheriff, M. Donoso, M. Tuttle, X. Huang, N.A. Meanwell, M. Soars, S. Roberts, J.F. Kadow

MEDI 244. Synthesis of 2'-C-methyl pseudouridines for the inhibition of HCV RNA polymerase. **I.K. Sappy**, J. Nunnari, **A.C. Bryant-Friedrich**

MEDI 245. Identification of active metabolites of lithocholic acid in respect to VDR binding. **K.A. Teske**, J.W. Bogart, L. Sanchez, A. Arnold

MEDI 246. Novel inhibitors and new chemical probes to study the protein arginine deiminases (PADs). **V. Subramanian**

MEDI 247. Discovery of novel 18 kDa tranlocator (TSPO) ligands for the treatment of Alzheimer's disease. **T. Kim**, B. Park, M.M. Neaz, S. Jung, J. Lee, A. Pae

MEDI 248. 1H-Pyrrolo[2,3-b]pyridine-6-carboxamide derivatives as 5-HT₄ partial agonists. **A. Mohammed**, A. Shinde, N. Madineni, R. Subramanian, G. Bhyrapuneni, V. Benade, N. Muddana, P. Jayarajan, R. Nirogi

MEDI 249. Identification of tetrahydroisoquinolines as potential anti-psychotics. **E. Ofori**, J.R. Etukala, B. Bricker, X.Y. Zhu, T. Jackson, X. Huang, B.L. Roth, S.Y. Ablordepppey

MEDI 250. Insights into lead optimization of protein kinase RNA-like endoplasmic reticulum kinase (PERK) inhibitors. **M.A. Nael**, S. Slater, D.J. Doerksen

MEDI 251. Design of a decapeptide for the inhibition of β -Amyloid aggregation and disaggregation of the mature fibrils. **Y. Zhi**, Q. Zhang, W. Wang, J. Liu

MEDI 252. Studying amyloid fibril formation and remodeling using fluorescently-labeled α -synuclein. **C. Haney**, R.F. Wissner, C. Cleveland, E. Petersson

MEDI 253. Research supporting platform for academic drug discovery in Japan. **H. Kojima**, T. Okabe, H. Ichijo, T. Nagano

MEDI 254. Dissolution behavior of amorphous formulations and its effects on f2 sensitivity. **C. Bottone**

MONDAY MORNING

Section A
Boston Convention & Exhibition Center Room 210B

Emerging Antibody Drug Conjugates: Applications of Medicinal Chemistry
V. A. Verma, Organizer, Presiding

9:00 Introductory Remarks.

9:05 MEDI 255. Antibody drug conjugates: History and emerging technologies. **B.A. Teicher**

9:35 MEDI 256. Advances in drug-linker design to improve the stability, homogeneity, and pharmacokinetics of antibody-drug conjugates. **R. Lyon**

10:05 MEDI 257. Delivery of potent cytotoxins as ADC payloads. **V.A. Verma**

10:35 MEDI 258. Design, synthesis, and evaluation of a novel class of potent DNA-alkylating agents for use in antibody-drug conjugates (ADCs). **M.L. Miller**

11:05 MEDI 259. Discovery of novel linkers, payloads, and antibody-drug conjugates for the treatment of cancer. **C.J. O'Donnell**

Section B
Boston Convention & Exhibition Center Room 210A

Advances in Predictive Toxicology: In Silico & In Vitro Approaches
D. F. Ortwine, J. Reilly, B. Wei, Organizers, Presiding

8:40 Introductory Remarks.

8:45 MEDI 260. Integrating physical property indices into drug design. **N.A. Meanwell**

9:15 MEDI 261. Integrated use of chemical and biological descriptors improves the accuracy and interpretability of toxicity prediction models. **A. Tropsha**

9:45 MEDI 262. Multiparameter in vitro approaches in assessing potential risk for drug induced liver injury in candidate drugs. **R.A. Thompson**

10:15 Intermission.

10:30 MEDI 263. Phosphatidylcholine affinity chromatography and link to compound promiscuity, non-specific binding, and phospholipidosis assessment. **J. Reilly**

11:00 MEDI 264. Lipidomic fingerprints for toxic endpoint prediction. **G. Cruciani**

11:30 MEDI 265. Chromatographic approaches for in-vitro early screening of drug-induced phospholipidosis risk. **Z. Jiang**, J. Reilly

Section C
Boston Convention & Exhibition Center Room 210C

Ophthalmic Drug Discovery
C. M. Adams, N. C. Goodwin, Organizers, Presiding

9:00 Introductory Remarks.

9:05 MEDI 266. Unique challenges in ophthalmic drug discovery. **C.M. Adams**

9:40 MEDI 267. Overcoming side-effects of Rho kinase inhibitors. **O. Defert**

10:15 MEDI 268. KAL-821, a novel and potent inhibitor of VEGFR2. **W. Ong**, P. Nowak, E. Enlow, L. Schopf, J. Bourassa, H. Chen

10:50 MEDI 269. Discovery of small molecule VEGFR-2 inhibitors with preferential ocular distribution and retention following oral dosing. **E.L. Meredith**, N. Mainolfi, S. Poor, Y. Qiu, K. Miranda, J.J. Powers, D. Liu, F. Ma, C. Solovay, C. Rao, L.L. Johnson, N. Ji, G. Artman, L. Hardegger, S. Hanks, S. Shen, A. Woolfenden, E. Fassbender, J. Sivak, Y. Zhang, D. Long, R. Cepeda, V.P. Hosagrahara, W. Lee, P. Tarsa, F. Liu, K. Anderson, R. Newton, P. End, J.M. Elliott, B. Jaffee

11:25 MEDI 270. Can deuterated vitamin A be used to prevent blindness? The case of ALK-001. **L. Saad**, I. Washington

Radiochemistry
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Innovation in Health and Medicine
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New Strategies and Applications of Aminoglycosides
Sponsored by CARB, Cosponsored by MEDI

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits
Sponsored by CHED, Cosponsored by BMGT, CEI, ENVR, I&EC, MEDI, PROF, SCHB and YCC

MONDAY AFTERNOON

Section A
Boston Convention & Exhibition Center Room 210B

Cancer Immunotherapy: The Next Big Thing for Small Molecules
A. Northrup, Z. Pei, Organizers, Presiding

2:00 MEDI 271. Arming the immune system to fight cancer. **J. Grogan**

2:30 MEDI 272. Structure, mechanism, and inhibition of arginase, a binuclear manganese metalloenzyme implicated in immune evasion. **D.W. Christianson**

3:00 MEDI 273. Crystal structures, identification and structure-activity relationships of imidazothiazole derivatives as indoleamine 2,3-dioxygenase 1 inhibitors. **S. Tojo**

3:30 MEDI 274. Reversal of tumoral immune resistance by inhibition of tryptophan 2,3-dioxygenase. **R. Frédéric**

4:00 MEDI 275. Insights and strategies in utilizing toll-like receptor agonists as immunotherapeutic agents. **S.A. David**

Section B
Boston Convention & Exhibition Center Room 210A

Advances in Predictive Toxicology: Case Studies in Drug Development
A. J. Peat, A. F. Stepan, J. Sutton, Organizers, Presiding

1:45 MEDI 276. Assessment and prediction of molecular toxicity: Lessons from acidic series of Na_v1.7 inhibitors. **R.I. Storer**

2:15 MEDI 277. Novel strategy to overcome genotoxicity liabilities for the RIP2K program. **P. Eidam**

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2:45 MEDI 278. Elevation of serum toxicity biomarkers by reduced protein clearance in the absence of organ injury. **A. Wolf, Y. Timist, F. Pognan**

3:15 MEDI 279. Bromodomain and extraterminal (BET) domain inhibitors induce a loss of intestinal stem cells and villous atrophy. **M. Wagener**

3:45 MEDI 280. Opportunities for integrated safety assessment – early and often. **S. Thohan**

4:15 MEDI 281. Rational derisking of covalent enzyme inhibitors. **A.M. Gilbert**

Section C

Boston Convention & Exhibition Center Room 210C

Strategies in the Design and Characterization of Allosteric Inhibitors

N. A. Meanwell, P. M. Scola, *Organizers, Presiding*

2:00 MEDI 282. Allosteric inhibitors of caspase-6. **J.A. Flygare**

2:35 MEDI 283. Allosteric ligands: New twists on old ensembles. **H. Carlson**

3:10 MEDI 284. Structure based design of allosteric inhibitors of hypoxia inducible factor. **U.K. Tambar**

3:45 MEDI 285. Discovery and pharmacological properties of ABL001, a novel potent and specific BCR-ABL allosteric inhibitor. **J. Schoepfer, G. Berellini, H. Cai, G. Caravatti, S. Dodd, P. Furet, G. Gangal, R.M. Grotzfeld, A. Hassan, T. Hood, S. Cowan-Jacob, W. Jahnke, A. Loo, P. Manley, X. Pellé, B. Salem, S. Sharma, W. Zhu, A. Marzinzik, T. Gabriel, N. Keen, L. Petruzzelli, G. Vanasse, W.R. Sellers, A. Wylie**

4:20 MEDI 286. Multimerization selective inhibitors of HIV-1 integrase. **M. Kvaratskhelia**

New Strategies and Applications of Aminoglycosides

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Radiochemistry

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Undergraduate Research Posters

Medicinal Chemistry

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MONDAY EVENING

Section A

Boston Convention & Exhibition Center Hall C

Sci-Mix

S. Plumlee, W. B. Young, *Organizers*

8:00 - 10:00

69, 79-80, 86, 106, 115, 133, 139-140, 159, 184, 187, 201, 239. See previous listings.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

409, 451, 454, 476, 491, 522.

See subsequent listings.

Chemical Innovation and Design (CID) Talks: The Future of Innovation Now

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TUESDAY MORNING

Section A

Boston Convention & Exhibition Center Room 210B

Medicinal Chemistry Toolbox: Understanding the Roles of Inducible Pockets, Water & Small Structural Changes

B. R. Beno, A. Regueiro-Ren, K. Yeung, *Organizers*

N. A. Meanwell, P. M. Scola, *Presiding*

9:00 MEDI 287. Coloring outside the lines: Exploiting induced binding pockets. **D.F. Ortwine**

9:30 MEDI 288. Making it fit: Inducible pockets in drug target proteins. **B.R. Beno**

10:00 MEDI 289. High end GPCR design: Experimental and computational insights into the key role of waters and water network energetics for potency, selectivity, and kinetics. **J.S. Mason, A. Bortolato, D.R. Weiss, B. Tehan, F. Deflorian**

10:30 MEDI 290. Conserved water-mediated hydrogen bond network defines bosutinib's kinase selectivity. **N.M. Levinson**

11:00 MEDI 291. Multiparameter optimization of pharmaceuticals: What big data can tell us about small groups that make a big difference? **A. Dossetter**

11:30 MEDI 292. Subtle structural changes (Molecular Switches) that modulate subtype selectivity and mode of pharmacology within GPCR allosteric modulators. **C.W. Lindsley**

Section B

Boston Convention & Exhibition Center Room 210A

MEDI Award Symposia

Financially supported by Portola Pharmaceuticals
W. B. Young, *Organizer*

J. E. Macor, *Presiding*

9:00 MEDI 293. 2015 Robert M. Scarborough Award for Excellence in Medicinal Chemistry: Lessons learned at the interface of medicinal chemistry and translational biology. **P.J. Coleman**

9:45 MEDI 294. 2015 Philip S. Portuguese Medicinal Chemistry Lectureship: Curing hepatitis C virus infection with direct-acting antiviral agents: The arc of a medicinal chemistry triumph

10:30 MEDI 295. Chemical probes for the lysine methyltransferases G9a and EZH2. **K.D. Konze, A. Ma, S.G. Pattenden, J. Jin**

10:50 MEDI 296. Probing the mode of action of ribosomally synthesized and posttranslationally modified peptide natural products. **P.M. Blair, D. Mitchell**

11:10 MEDI 297. Development of irreversible tethering and its use to discover inhibitors of HECT E3 Nedd4-1 processivity. **S.G. Kathman, I. Span, A.T. Smith, Z. Xu, J. Zhan, A.C. Rosenzweig, A. Statsyuk**

11:30 MEDI 298. Integrated chemical and metagenomic approach for the discovery of a novel class of anti-HIV lanthipeptides, the divamides. **T.E. Smith, J. Kwan, C. Pond, L. Barrows, C. Ireland, E.W. Schmidt**

11:50 MEDI 299. Design, synthesis, and evaluation of inhibitors targeting the iron-regulated heme oxygenase of *Pseudomonas aeruginosa*. **G.A. Heinzl, B.J. Giardina, K. Hom, A. Wilks, F. Xue**

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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Glycolipid Immunostimulants

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Herman Skolnik Award Symposium

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Radiochemistry

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Transforming University-Industry Partnerships for an Innovative Future

Envisioning, Enabling and Executing

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TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center Room 210B

Case Studies of Successful Drugs

J. J. Chen, *Organizer, Presiding*

2:00 MEDI 300. Drug discovery in academia: A successful case study. **M.E. Jung**

2:35 MEDI 301. Discovery and development of carfilzomib (CFZ) for multiple myeloma (MM). **Z. Wang**

3:10 MEDI 302. Discovery and early development of AZD9291: Learnings and reflections from the Mereside. **R. Finlay, M. Anderton, S. Ashton, P. Ballard, P. Bethel, M. Box, R.H. Bradbury, S.J. Brown, S. Butterworth, A.D. Campbell, C. Chorley, N. Colclough, D. Cross, G. Currie, M. Grist, L. Hassall, G.B. Hill, D. James, M. James, P. Kemmitt, T. Klinowska, G. Lamont, S. Lamont, N. Martin, H.L. McFarland, M.J. Mellor, J.P. Orme, D. Perkins, P. Perkins, G. Richmond, P. Smith, R.A. Ward, M.J. Waring, D. Whittaker, S. Wells, G. Wrigley**

3:45 MEDI 303. Development of trastuzumab emtansine (Kadcyla®) for the treatment of HER2-positive breast cancer. **G.D. Phillips**

4:20 MEDI 304. Sofosbuvir (Sovaldi®): A breakthrough therapy for the treatment of HCV. **M.J. Sofia**

Section B

Boston Convention & Exhibition Center Room 210A

Deuterated Drugs

L. Marcin, *Organizer, Presiding*

2:30 MEDI 305. Incorporation of deuterium into the corporate mindset. **T. Gant**

3:00 MEDI 306. Deuterated drugs: Challenges and opportunities for pharmacokinetic and toxicological enhancement of medicines. **A. Vaz**

3:30 MEDI 307. Deuterated drugs: An analysis of recent trends in intellectual property. **G. Timmins**

4:00 MEDI 308. Using deuterium-enabled chiral switching (DECS) to stabilize and differentiate enantiomers of thalidomide analogs. **S.H. Dewitt, A.W. Czarnik, V. Jacques, T. Judge, L. Van der Ploeg**

4:30 MEDI 309. Discovery of a second generation, pan genotype NS3/4A protease inhibitor (BMS-986144) for the treatment of hepatitis C. **P.M. Scola, L. Sun, E.P. Gillis, M.S. Bowsher, J. Chen, X.A. Wang, S. Sit, Y. Chen, Z. Zheng, S. D'Andrea, N. Sin, B. Venables, E. Mull, Q. Chen, S. Kandhasamy, N. Pulicharla, S. Vishwakrishnan, S. Reddy, R. Trivedi, S. Sinha, S. Sivaprasad, A. Rao, S. Desai, K. Ghosh, R. Rajamani, J. Friberg, S. Levine, C. Chen, P. Falk, S. Jenkins, M. Kramer, R. Haskel, K. Johnson, J. Loy, P. Levesque, J. Zhu, M. Cockett, N.A. Meanwell, F. McPhee**

5:00 MEDI 310. Deuterium-modified drugs: Discovery and development. **S.L. Harbeson**

Section C

Boston Convention & Exhibition Center Room 210C

General Orals

W. B. Young, *Organizer*

A. S. Ripka, *Presiding*

1:30 MEDI 311. Discovery of selective inhibitors for lysine methyltransferases EZH2/EZH1 and SETD8. **A. Ma, B. Xu, D.M. On, W. Yu, K.D. Konze, K.V. Butler, F. Li, M. Vedadi, P.J. Brown, G.G. Wang, J. Jin**

1:55 MEDI 312. Identification of PIM447, a potent and selective proviral insertion site of Moloney murine leukemia (PIM) 1, 2 and 3 kinase inhibitor in clinical trials for cancer. **M.T. Burger, G.A. Nishiguchi, W. Han, J. Lan, R. Simmons, G.B. Atallah, V. Tamez, Y. Zhang, Y. Ding, M. Mathur, K. Muller, C. Bellamacina, M. Lindvall, R. Zang, K. Huh, Y. Dai, E. Ginn, A. Aycinena, J. Langowski, A. Lambert, C. Fritsch, A. Kauffmann, E. Pfister, P. Garcia**

2:20 MEDI 313. Discovery of indazoles and indoles as potent and selective PIM inhibitors. **B. Wu, H. Wang, R.P. Wurz, V. Cee, F. Chavez, B. Berberich, C. Jackson, B.A. Lanman, T. Nixey, L.H. Pettus, A.B. Reed, J. Laszlo, P. Wang, C. Sastr, N. Guerrero, J. Winston, J.R. Lipford, M.R. Lee, C. Mohr, K. Andrews, Y. Xu, Y. Zhou, D.L. Reid, A.S. Tasker**

2:45 MEDI 314. Discovery of potent, orally bioavailable protease-activated receptor 4 antagonists. **A. Marinier, J. Banville, E. Bird, M. Callejo, D.H. Deon, L. Dubé, M. Gagnon, M.R. Giancarli, J. Guy, T. Harper, P.Y. Lam, J. Lavallée, M.R. Lawrence, A. Martel, M.M. Miller, H.R. O'Grady, S.L. Posy, S.E. Priestley, R. Rémillard, E. Ruediger, F. Tremblay, C.A. Watson, P.C. Wong, J. Yang, M. Bouvier, D. Seiffert, R.R. Wexler**

3:10 MEDI 315. Perturbation of the c-Myc/Max coiled-coil protein-protein interaction with synthetic α -helix mimetics. **K. Jung, H. Wang, P. Teriete, N.D. Cosford, E. Prochownik, S. Fletcher**

3:35 MEDI 316. Trifluoromethyl oxazines as highly potent and selective beta-secretase inhibitors that are efficacious in vivo. **Y. Cheng, M. Xue, T. Judd, P. Lopez, J. Low, A. Minatti, W. Qian, Q. Liu, N. Chen, W. Zhong, L. Liu, A.K. Amegadzie, S. Rumpfelt, R.M. Rzasza, M.D. Bartberger, K. Chen, D. Hickman, A. Nanez, H. Tan, L. Volak, P. Wen, D. Whittington, S. Wood, J.R. Allen**

- 4:00 MEDI 317.** Discovery of brigatinib (AP26113), a phosphine oxide-based, potent, orally active inhibitor of anaplastic lymphoma kinase and clinically relevant mutants. **W. Huang,** F. Li, L. Cai, Y. Xu, S. Zhang, S. Wardwell, Y. Ning, A. Kohlmann, T. Zhou, Y. Ye, X. Zhu, N. Narasimhan, T. Clackson, V. Rivera, D.C. Dalgarno, W.C. Shakespeare
- 4:25 MEDI 318.** Discovery of URAT1 inhibitors for the treatment of gout. **R.M. Owen**
- 4:50 MEDI 319.** Impact of historical synthetic methodologies on medicinal chemistry: Where have all the new reactions gone? **D.G. Brown,** J. Boström

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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Glycolipid Immunostimulants

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Herman Skolnik Award Symposium

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WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center Room 210B

Recent Advances in Heart Failure

W. R. Ewing, D. Pinto, *Organizers, Presiding*

- 8:45 MEDI 320.** GPCRs in heart failure. **P. Insel**
- 9:30 MEDI 321.** Targeting the angiotensin II type I receptor with a β -arrestin biased ligand: A novel therapeutic approach to the treatment of acute heart failure. **M. Lark**
- 10:00 MEDI 322.** Human iPSCs for cardiac drug discovery. **J.C. Wu**
- 10:30 MEDI 323.** Discovery and SAR evolution of ROMK inhibitor sub-classes toward identification of our clinical development compound. **A. Pasternak,** H. Tang, R. De Jesus, S. Walsh, A. Shahripour, Y. Zhu, N. Teumelsan, L. Yang, E. Parmee, B. Priest, J. Felix, B. Thomas-Fowkes, S. Andrew, G.J. Kaczorowski, M. Garcia, A. Weinglass, M. Alonso-Galicia, X. Zhou, L. Pai, C. Hampton, J. Kunkel, O. Price, M. Hernandez, C. Gill, M. Dajee, K. Shah, J. Metzger, M. Forrest, J. Ormes, M. Hu, K. Owens, K. Samuel, R. Miller, V. Tong, T. Bateman, S. Roy, K. Sullivan
- 11:00 MEDI 324.** Soluble guanylate cyclase (sGC) stimulator vericiguat as a potential treatment for heart failure. **M. Follmann**
- 11:30 MEDI 325.** *Omeacantiv mecarbii* the first, selective, small molecule activator of cardiac myosin. **B.P. Morgan**

Section B

Boston Convention & Exhibition Center Room 210A

General Orals

- W. B. Young, *Organizer*
J. E. Macor, *Presiding*
- 8:30 MEDI 326.** Discovery of a TARP gamma-8 dependent AMPA receptor antagonist (TDAA) for the treatment of epilepsy. **K.M. Gardinier,** D. Gernert, W.J. Porter, J. Reel, P.L. Ornstein, K. Burris, C. Ding, S. Gleason, P. Desai, S. Swanson, J. Witkin
- 8:55 MEDI 327.** Discovery of triazole aldosterone synthase inhibitors with in vivo activity in Rhesus monkeys. **S.B. Hoyt,** W. Petrilli, C. London, J. Tata, Q. Hu, L. Yin, C. van Koppen, R.W. Hartmann, M. Struthers, T. Wisniewski, N. Ren, C. Bopp, A. Sok, T. Cai, S. Stribling, L. Pai, X. Ma, J. Metzger, A. Verras, D.R. Mc Masters, Q. Chen, E. Tung, W. Tang, G. Salituro, N. Buist, J. Clemas, G. Zhou, J. Gibson, C.A. Maxwell, M. Lassman, T. McLaughlin, J. Castro-Perez, D. Szeto, G. Forrest, R. Hajdu, M. Rosenbach, Y. Xiong
- 9:20 MEDI 328.** Fragment-based drug discovery of potent and selective CYP121 inhibitors for tuberculosis. **M. Kavanagh,** A.G. Coyne, G.G. James, K. McLean, S.A. Hudson, L. Pedro de Carvalho, A.W. Munro, C. Abell
- 9:45 MEDI 329.** Disruption of the HCV NS5A replication complex through a novel synergy mechanism. **M. Belema,** P. Hewawasam, Y. Tu, N. Xu, O.D. Lopez, X.A. Wang, J.F. Kadow, A.K. Gupta, I. Kumar, S. Punugupati, F. Moulin, M. Nophsker, M. Kramer, B.M. Johnson, Y. Wang, J. Sun, D. O'Boyle, R. Fridell, C. Wang, S. Roberts, M. Liu, K. Rigat, P. Nower, J. Lemm, M. Cockett, N.A. Meanwell, M. Gao
- 10:10 MEDI 330.** Discovery of soluble epoxide hydrolase inhibitors through DNA-encoded library technology (ELT). **Y. Ding,** S.L. Belyanskaya, J.L. DeLorey, D. Israel, J.A. Messer, B.A. Morgan, S. Skinner, M.A. Clark, J.W. Cuzzo
- 10:35 MEDI 331.** Discovery of 6-((3H-imidazo[4,5-b]pyridin-2-yl)methyl)-3-(2,4,6-trifluorobenzoyl)-1H-pyrrolo[2,3-c]pyridin-7(6H)-one (MK2684): A potent inhibitor of MAP/MAPK2 (MK2) for the treatment of asthma. **K.D. Dykstra,** M. Chen, G. Yang, H. Koyama, D. Miller, S. Sahoo, P.T. Meinke, S.J. O'keefe, P. Gray, S. Chiu, G. Porter, J. DeMartino, D. Zaller, C. Tan, D. Slipetz, E. Corley, T. Nelson, H. Yu, B. Farrer, M. Madeira, B. Karram, K. Owens, K. Mitra, G. Miller, R.P. Nargund
- 11:00 MEDI 332.** Highly selective non-covalent inhibitors of EGFR T790M resistance mutants: HTS hits to candidate-quality molecules. **E.J. Hanan,** M.C. Bryan, D. Burdick, B. Chan, E. Chan, Y. Chen, C. Eigenbrot, R. Elliott, R. Heald, T.P. Heffron, P. Jackson, J. Knight, H. La, M. Lanchbury, S. Malek, S. Mann, H.E. Purkey, G. Schaefer, S. Schmidt, E. Seward, S. Sideris, L. Shao, S. Wang, S. Yeap, I. Yen, C. Yu
- 11:25 MEDI 333.** Strategies for the discovery of novel nonsteroidal mineralocorticoid receptor antagonists. **A. Casimiro-Garcia,** D.W. Piotrowski, K. Futatsugi, K. Song, S. Robinson, C.M. Ambler, G.B. Arhancet, T. Banks, M.E. Banker, C. Boustany-Kari, C. Cai, X. Chen, R. Eudy, D. Hepworth, C. Hulford, S.M. Jennings, P. Loria, M.J. Meyers, D.N. Petersen, N. Raheja, M. Sammons, N.J. Schmidt, L. She, D. Vrieze, L. Wei

- 11:50 MEDI 334.** Discovery of brain penetrant adaptor associated kinase (AAK1) inhibitors as a potential novel treatment for neuropathic pain. **R.A. Hartz,** V. Ahuja, C.D. Dzierba, W. Kostich, S. Nara, V. CM, A. Easton, C. Bourin, L. Bristow, J. Brown, L. Hunihan, M. Gulianello, R. Westphal, R. Rajamani, S. Kiefer, D. Camac, J. Muckelbauer, M. Pokross, K. Ghosh, R. Brown, N. Surti, J. Lippy, R. Padmanabha, K. Esposito, J. Grace, D. Parker, K.A. Lentz, B. Hamman, J. Allen, K. Baker, G. Ye, L. Lanthorn, K. Savelieva, B. Zambrowicz, S. Pattipati, M. Dokania, S. Elavazhagan, K. Dandapani, J.J. Bronson, J.E. Macor

Section C

Boston Convention & Exhibition Center Room 210C

Targeted Covalent Inhibitors

S. E. Conner, Z. Pei, *Organizers, Presiding*

- 9:00 MEDI 335.** Targeted covalent inhibitors vs. reactive drug metabolites: A risk-benefit perspective. **T.A. Baillie**
- 9:30 MEDI 336.** Exploring the kinome with selective and promiscuous chemical probes. **J.W. Taunton**
- 10:00 MEDI 337.** Discovery of rocletinib (CO-1686), a mutant-selective covalent inhibitor of EGFR. **D. Niu**
- 10:30 MEDI 338.** Covalent inhibition of Mcl-1 through modification of a non-catalytic lysine side chain. **G. Akçay,** N. Grimster, M.L. Lamb, A. Hird, Q. Su, B.M. Aquila
- 11:00 MEDI 339.** Discovery and development of CC-292, a covalent inhibitor of BTK. **R.C. Petter**
- 11:30 MEDI 340.** Reducing proteome reactivity of irreversible inhibitors of EGFR T790M. **J.C. Kath**

Innovation in Chemical Synthesis

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Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

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WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center Room 210B

First Time Disclosures

L. A. Thompson, *Organizer, Presiding*

- 1:30 MEDI 341.** Discovery of CFG920, a dual CYP17/CYP11B2 inhibitor, for the treatment of castration resistant prostate cancer. **C. Gaul,** P. Mistry, H. Moebitz, M. Perrone, B. Gruenenfelder, N. Guerreiro, W. Hackl, P. Wessels, E. Berger, M.G. Bock, S. Sengupta, V. Rao, M. Ramachandra, T. Antony, K. Narayanan, S. Dodheri, A. Basavaraju, S. Chelur
- 2:05 MEDI 342.** Inventing INCB24360 (epacadostat), an indoleamine-2,3-dioxygenase-1 (IDO1) inhibitor for immuno-oncology. **A.P. Combs**
- 2:40 MEDI 343.** Discovery of AG-221: A first-in-class inhibitor of IDH2 mutant enzymes for the treatment of acute myelogenous leukemia. **J.M. Travinis,** J. Saunders, F.G. Salituro, J.V. Popovici-Muller, K. Yen, K. Straley, E. Hansen, F. Wang, S. Gross, L. Dang, H. Yang, L. Utley, Y. Chen, L. Silverman, S. Agresta, M. Su, S.A. Biller

- 3:15 MEDI 344.** Discovery of AMG 337, a potent and selective inhibitor of c-Met with high unbound exposure and robust, extended in vivo antitumor activity. **A. Boezio,** B.K. Albrecht, D. Bauer, S.F. Bellon, C.M. Boezio, M.A. Broome, D.M. Choquette, K.W. Copeland, I. Dussault, S. Hirai, R.T. Lewis, M. Lin, J. Lohman, J. Liu, E.A. Peterson, M. Potashman, K. Rex, R. Shimanovich, Y. Teffera, D. Whittington, K. Romero, J. Hzmange
- 3:50 MEDI 345.** Tissue selective androgen receptor modulators (SARMs): A path to a clinical candidate. **E.L. Chekler**
- 4:25 MEDI 346.** Discovery of IKur inhibitor BMS-919373 and selection as a clinical candidate. **H. Finlay,** P. Gunaga, J.A. Johnson, J. Lloyd, J. Jiang, J. Neels, A. Kumar, N. Dhondi, A. Banerjee, S. Johnson, A. Chimalakonda, S. Mandekar, S. Putlur, A. Saxena, H. Sale, D. Xing, R. Smith, J. Hennis, P. Levesque, R.R. Wexler

Section B

Boston Convention & Exhibition Center Room 210A

General Orals

W. B. Young, *Organizer*

J. J. Bronson, *Presiding*

- 1:30 MEDI 347.** Wnt pathway inhibitors – indazoles. **K. Schiemann,** A. Mallingier, D. Wienke, C. Esdar, O. Poeschke, M. Busch, F. Rohdich, S.A. Eccles, R. Schneider, F. Raynaud, P. Czodrowski, D. Musil, D. Schwarz, J. Blagg
- 1:50 MEDI 348.** Discovery and modulation of carbonyl interactions in bioactive small molecules. **R.W. Newberry,** R.T. Raines
- 2:10 MEDI 349.** Rapid elaboration of fragment hits as inhibitors of DsbA, a novel antibacterial target. **J.S. Simpson,** B. Plumb, A. Kany, L.A. Adams, B.C. Doak, M. Vazirani, M. Mulcair, O. Ilychova, K. Rimmer, M.J. Scanlon
- 2:30 MEDI 350.** Discovery and optimization of potent, selective, and in vivo efficacious BCATm inhibitors. **H. Deng,** J. Zhou, F. Sundersingh, J. Messer, D. Somers, A. Beljean, S.L. Belyanskaya, R. Bingham, E. Blazensky, E. Boursier, J. Chai, P. Carter, C. Chung, A. Daugan, Y. Ding, E.N. Humphries, C. Kollmann, S.E. Smith, N. Dodic, N. Ancellin
- 2:50 MEDI 351.** Modifications to the A- and C-rings of EGCG for improved Hsp90 inhibition. **A. Khandelwal,** B. Blagg
- 3:10 MEDI 352.** Small molecule inhibitors of the CaaX protease Fce1 disrupt Ras localization. **I. Mohammed,** S. Hampton, L. Ashall, E.R. Hildebrandt, R. Kuttik, S.P. Manandhar, B.J. Floyd, J.K. Dozier, M.D. Distefano, W. Schmidt, **T.M. Dore**

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- 3:30 MEDI 353.** Antimalarial drug discovery: Lapatinib re-optimization as a case study of expedited drug discovery using target repurposing. **N. Mehta, P.J. Lee, S.E. Leed, R.J. Sciotti, M.P. Pollastr**
- 3:50 MEDI 354.** Design and synthesis of a novel series of γ -secretase modulators: Cyanoindoles, moving toward a better drug-like space? **A.I. Velter, F. Bischoff, M. De Cleyen, H. Gijzen, G. Macdonald, A. Dehrlrich, F. Rombouts, M. Surkyn, S. Van Brandt, C. Zavattaro, N. Austin, M. Mercken**
- 4:10 MEDI 355.** Discovery and synthesis of substituted amino-pyrimidines as inhibitors of 5-lipoxygenase-activating protein (FLAP) for the treatment of inflammatory disease. **W.K. Eccles, J. Blevitt, L. Chang, K. Coe, S. Crawford, A. De Leon-Tabaldo, D. DiSepio, J.P. Edwards, A. Everson, M. Feinstein, M.D. Hack, N. Hawrylyuk, K. Herman, W. Jones, J.M. Keith, S. Kim, T. Koudriakova, P. Krawczuk, A.D. Lebsack, J. Liu, R. Luna-Roman, N.S. Mani, K. McClure, P. McGovern, S.P. Meduna, M. Milla, N. Rao, M. Rizzolio, M. Rosen, B. Scott, K. Sepassi, J. Skaptason, M. Tootoonchi, X. Xue, J. Zhu**
- 4:30 MEDI 356.** Design and development of palladium-labile bioorthogonal prodrugs. **A. Unciti-Broceta**
- 4:50 MEDI 357.** Pharmacophore-based design of novel oxadiazoles as selective sphingosine-1-phosphate (S1P) receptor agonists with in vivo efficacy. **A. Quattropani, W. Sauer, S. Crosignani, J. Dorbais, P. Gerber, J. Gonzalez, D. Marin, M. Muzerelle, F. Beltran, A. Nichols, K. Georgi, M. Schneider, P. Vitte, V. Eligert, L. Novo-Perez, J. Hantson, S. Nock, S. Carboni, A.L. Soares de Souza, J. Arrighi, U. Boschert, A. Bombrun**

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by CINF, Cosponsored by AGRO, COMP, ENVR and MEDI

WEDNESDAY EVENING

Section A

Boston Convention & Exhibition Center Ballroom

General Posters

W. B. Young, Organizer

7:00 - 9:00

- MEDI 358.** Synthesis, in vitro and in vivo evaluation of tetrahydroquinolines featuring a diverse set of polar substituents at the 6 position as mixed efficacy mu opioid receptor/delta opioid receptor ligands. **A. Bender, N.W. Griggs, J.P. Anand, E.M. Jutkiewicz, J.R. Traynor, H.I. Mosberg**

- MEDI 359.** Structure activity relationships of various *N*-substitutions on mixed-efficacy μ -opioid receptor (MOR) agonist/ δ -opioid receptor (DOR) antagonist peptidomimetics. **A. Harland, A. Bender, N.W. Griggs, J.P. Anand, E.M. Jutkiewicz, J.R. Traynor, H.I. Mosberg**
- MEDI 360.** Discovery of potent and efficacious aminopyridines as inhibitors of phosphodiesterase 10A. **P.E. Harrington, K. Sham, S. Rumpfelt, N. Chen, J. Falsey, R.M. Rzasas, M.R. Kaller, E.H. Hu, K. Andrews, S. Chmait, X. Zhao, C. Davis, J. Ma, J. Shi, D. Lester-Zeiner, J. Danao, J. Able, C. Biorn, M. Cuevas, S. Talreja, T. Kornecook, H. Chen, A. Porter, R. Hungate, J. Treanor, J.R. Allen**
- MEDI 361.** Modifying native and fibrillar SOD1 by small anhydrides inhibits fibrillization and destabilizes its amyloid forms. **S. Rasouli, A. Abdolvahabi, Y. Shi, B.F. Shaw**
- MEDI 362.** Novel asymmetric total synthesis of (+)-tetrabenazine and (+)- α -dihydrotetrabenazine. **H. Hsieh, L. Chang, Y. Liu, L. Hsin**
- MEDI 363.** TAAR1 agonists as anti-diabetic agents: Discovery and characterization of (S)-4-[[ethyl-phenyl-amino-methyl]-4,5-dihydro-oxazol-2-ylamine (RO5166017). **R.D. Norcross, G. Galley, K. Groebke Zbinden, D. Türk, S. Mohr, M.C. Hoener, S. Raab, S. Sewing**
- MEDI 364.** Structural identification of the metabolites of a potent OXE receptor antagonist. **S. Chourey, Q. Ye, H.W. Alhamza, C.N. Reddy, R. Wang, S. Gravel, C. Cossette, I. Slobodchikova, D. Vuckovic, W.S. Powell, J. Rokach**
- MEDI 365.** Orai inhibitors: Novel pyrazoles with improved lipophilic efficiency vs. potent 7-azaindole series. **B. Vidal, C. Esteve, S. Gual, L. Vidal, S. Sentellas, I. Jover, R. Horrillo, J. De Alba, M. Miralpeix, G. Tarrason, J. Gonzalez**
- MEDI 366.** Fragment-based discovery of the first known inhibitors of PHGDH. **N.O. Fuller**
- MEDI 367.** Novel acylureidoinolin-2-one derivatives as dual Aurora B/FLT3 inhibitors for treatment of acute myeloid leukemia. **K. Wu, J. Liu, S. Fung, Y. Ho, K. Wang, G. Chen, A. Jagtap, J. Chern**
- MEDI 368.** Potential prodrugs of the tetrahydrofuran containing annonaceous acetogenins for tumor targeting. **P. Gonzalez, A. Ramdular, D.R. Mootoo**
- MEDI 369.** Synthesis and biological evaluation of novel 6-substituted pyrrolo[2,3-d]pyrimidines as targeted antifolates. **A. Gangjee, L. Golani, A. Wallace, C. O'Connor, L.H. Matherly**
- MEDI 370.** Discovery of novel amide bridged pyrrolo[2,3-d]pyrimidine classical antifolates with selective uptake by FR and PCFT over RFC: A practical way to aminomethylate pyrrolo[2,3-d]pyrimidines through the Mannich reaction. **A. Gangjee, W. Xiang, A. Wallace, C. O'Connor, L.H. Matherly**
- MEDI 371.** Design of hydrogen bond induced conformational constriction for improved selectivity and activity in classical antifolates. **A. Gangjee, M.P. Ravindra, L.H. Matherly**
- MEDI 372.** Identification and preliminary structure-activity relationships of novel pyrrolidinyl pyrimidine inhibitors of the Bcl-2 family of antiapoptotic proteins. **S. Breining, A. Shirokov, R. Jimenez-Moreno, O. Roberts, A. Rzepiela, V. Kochubey**
- MEDI 373.** Electrophilic modification of Hsp70 by sesquiterpene lactones. **A.S. McGowan, M. Shin, R.E. Connor**

- MEDI 374.** Solution stability of quaternary ammonium salts as prodrugs. **T.A. Zeidan, C. Sanrame, J.F. Remenar**
- MEDI 375.** Withdrawn.
- MEDI 376.** Exploiting bioorthogonal chemistry to refill drug delivery devices. **Y. Brudno, R. Desai, B. Kwee, N.S. Joshi, M. Aizenberg, D.J. Mooney**
- MEDI 377.** Gemcitabine pro-drugs as a self-assembling, intra-tumoural drug delivery platform for the treatment of gastric and pancreatic cancers. **K. Skilling, B. Kellam, M. Ashford, T.D. Bradshaw, M. Marlow**
- MEDI 378.** Formulation of insulin for oral dosing. **J. Catalano, J.F. McArthur, J. Hughes, L. Mielnicki, M.P. McCourt**
- MEDI 379.** Increasing the bioavailability of parthenolide derivatives for the treatment of chronic lymphocytic leukaemia. **D.T. Payne, X. Li, L. Male, A. Agathangelou, J.S. Fossey**
- MEDI 380.** Development of peptidomic assays for profiling, discovery, and testing of structure-activity relationship for endogenous peptides from the synovial fluid as novel modulators for the T cell-mediated immunity. **C.C. Clement, A. Becerra, H. Moncrieffe, L. Stern, L. Santambrogio**
- MEDI 381.** Simplified Brasilicardin A analog does not inhibit T-cell proliferation. **B.T. Chamberlain, K. Niazi, M.E. Jung**
- MEDI 382.** Synthesis and SAR studies of benzyl ether derivatives as potent orally active S1P₁ agonists. **T. Tsuji**
- MEDI 383.** Design and synthesis of heterocyclic S1P receptor modulators. **F. Li, H. Cho, C. Lim, J. Choi, S. Kim**
- MEDI 384.** Synthesis and biological activity of hydroxymethylbutenyl diphosphate mimics for T-cell activation. **R.R. Shippy, R.J. Barney, A.M. Kilcollins, J. Li, C.C. Hsiao, A.J. Wiemer, D.F. Wiemer**
- MEDI 385.** c-Met inhibitors from hit to lead: Discovery and optimization of a series of pyridazin-4(1H)-ones. **K. Lipford, M. Altman, M.H. Daniels, D. Falcone, Y.I. Garcia, D.J. Guerin, S.E. Hill, G. Marshall, E. Osimboni, L. Surdi, C. White, K.J. Wilson, J.R. Young**
- MEDI 386.** Novel class of hsp90 inhibitors that are designed to be soluble and synthetically accessible. **Y. Koay**
- MEDI 387.** Binding mode studies of lenvatinib to VEGFR2 and FGFR1. **M. Ikemori-Kawada, K. Okamoto, A. Jestel, K.V. Konig, Y. Funahashi, A. Tsuruoka, A. Inoue, J. Matsui**
- MEDI 388.** Structurally defined multivalent α MHC-II nanobody-drug conjugate: Synthesis and in vivo activity against A20 murine lymphoma model. **T. Fang, H. Floegh**
- MEDI 389.** Second-generation synthetic α -helix mimetics based on a 2,6,9-tri-substituted purine potentially disrupts the Mcl-1-Bim protein-protein interaction. **M.E. Lanning, S. Fletcher**
- MEDI 390.** Discovery, validation, and SAR of a novel series of diamino-pyridines as Mcl-1 antagonists. **A. Hird, S. Kazmirski, M. Belmonte, K. Embrey, A.D. Ferguson, E. Gangl, D. Hargreaves, M. Packer, T.W. Pontz, P. Rawlins, P. Secrist, N. Su, X. Zheng**
- MEDI 391.** Progress towards more potent and cell-active Mcl-1 inhibitors: Pro-drug and bioisosteric optimization of first-generation salicylates. **L. Chen, S. Fletcher**

- MEDI 392.** Design and synthesis of dual inhibitors of the MDM2-p53 and MDMX-p53 protein-protein interactions. **S. Adhikari, C. Cano, B.T. Golding, I.R. Hardcastle, S.J. Hamor, C. Jennings, J. Lunec, S.M. Myers, D.R. Newell, J. Reeks, A. Shouksmith, S. Tudhope, S.R. Wedge, E. Willmore, A. Wittner, Y. Zhao, R.J. Griffin**
- MEDI 393.** Design and synthesis of metabolically stabilized pironetin analogs for drug-resistant ovarian cancers. **S.K. Coulop, D.S. Huang, H.L. Wong, N.Y. Tretyakova, G.I. Georg**
- MEDI 394.** Heparin based glycomics research using SPR biosensors. **F. Zhang, R.J. Linhardt**
- MEDI 395.** Structure-activity relationship in the evaluation the antioxidant capacity of diaryl hydrazones. **W. Horton, R. Tulsan, N. Kugyela, B. Torok, M. Torok**
- MEDI 396.** Systematic study of the influence of small substituents on lipophilicity, membrane permeability, and metabolic stability: A matched molecular pairs analysis of four drugs. **J. Peiró, M. Clausen, M. Jorgenson**
- MEDI 397.** Synthesis and evaluation of 2,3-dihydrobenzofuran-3(2H)-one-7-carboxamide derivatives as poly(ADP-ribose)polymerase-1 inhibitors. **U. Velagapudi, A. Bhatt, T.T. Talele**
- MEDI 398.** Identification and optimization of 2,3-dihydrobenzo[b][1,4]dioxine-5-carboxamide as PARP-1 inhibitors. **X. Shao, S. Pak, B. Patel, U. Velagapudi, T.T. Talele**
- MEDI 399.** Process development of 6-amino-2,2-dimethyl-2H,3H,4H-pyrrolo[3,2-b][1,4]oxazin-3-one. **A. Xia, H. Li, X. Wu, M. Yang**
- MEDI 400.** Design, synthesis, and development of small-molecule modulators of paxillin that inhibit proliferation of ARPE-19 cells exposed to growth factors. **B.A. Alawi, J.J. Toutouanchian, C.R. Yates, D.D. Miller**
- MEDI 401.** Can strong solvents like DMSO and NMP be used as injection solvents in reversed-phase flash chromatography? **J.R. Bickler**
- MEDI 402.** Organic amine flash purification using a novel stationary phase. **J.R. Bickler**
- MEDI 403.** Synthesis and biological evaluation of 1H-benzimidazole-5-carbohydrazides derivatives, as oxidative stress promoters. **M. Melchor-Doncel de la Torre, M. Santiago-Martinez, E. Lira-Silvia, R. Jasso-Chavez, C. Vazquez, Z. Gonzalez-Chavez, E. Saavedra, R. Nieto, L. Yépez-Mulia, C. Mendoza-Martinez, F. Hernández-Luis**
- MEDI 404.** Protein and monoclonal antibody functionalization utilizing continuous flow microreactor technology. **M.M. Sebeika, N.G. Gedeon, S.E. Sadler, G.B. Jones**
- MEDI 405.** Facilitating antibody drug conjugate linker synthesis using solid phase synthetic techniques. **J.R. McCombs**
- MEDI 406.** Bridge and click conjugation strategies: A new paradigm in the synthesis of porphyrin antibody-drug conjugates. **F. Bryden, A. Maruani, H. Savoie, M. Smith, S. Caddick, V. Chudasama, R.W. Boyle**
- MEDI 407.** Amino acid efflux as a surrogate measure of the inhibition of plasmidial hemoglobin endocytosis by mefloquine and related antimalarials. **M. Ghavami, C. Dapper, S. Dalal, P.M. Krai, M. Klemba, P.R. Carlier**

Technical program information known at press time. The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

- MEDI 408.** In vitro evaluation of imidazo[4,5-c]quinolin-2-ones as gametocytocidal antimalarial agents. **M. Kim, W. Sun, X. Huang, T. Tanaka, W. Kimberley, W. Zheng, W. Huang, P.R. Patel**
- MEDI 409.** Identification of 2-amino-methylphenol antimalarials with potent in vitro and in vivo activity against *Plasmodium* blood stages. **G.D. Heffernan, D.P. Jacobus, P. Krasucki, K.W. Saionz, G. Schiehsler, H. Shieh, W. Zhao, A. Ager, M. Chavchich, G. Birrell, D. Shanks, M. Edstein**
- MEDI 410.** Trypanosoma brucei growth inhibitors: High-throughput screening hit exploration. **L. Silva, R. Diaz, C. Cordon-Obras, D. Rojas-Barros, M. Navarro, M.P. Pollastrí**
- MEDI 411.** Synthesis and tripanocidal activity of novel substituted *N*-(1*H*-benzimidazole-2-yl)-1*H*-benzimidazole carboxamides. **A. Hernandez Campos, P.J. Trejo, L. Yépez-Mulia, A. Téllez-Valencia, R. Nieto-Meneses, R. Castillo-Bocanegra**
- MEDI 412.** Targeting methionyl tRNA synthetase from *Trypanosoma brucei* for the discovery of orally and CNS available therapeutics to treat Sleeping Sickness. **Z. Zhang, C. Koh, S. Shibata, R.M. Ranade, J.R. Gillespie, S.A. Creason, C.L. Verlinde, W.G. Hol, F.S. Buckner, E. Fan**
- MEDI 413.** Assay for ligand binding to helix 69 tRNA. **H. Seo, C.S. Chow**
- MEDI 414.** 6-Substituted pyrido[3,2-*d*]pyrimidines as dihydrofolate reductase inhibitors and potential anti-opportunistic agents. **A. Gangjee, K.S. Shah, V. Cody**
- MEDI 415.** Synthesis and in vitro trichomonocidal and anti-*Candida* activity of some phenyl-2*H*-indazole derivatives. **J. Pérez-Villanueva, T. Sainz-Espuñes, L. Yépez-Mulia, O. Soría-Arteche, R. Gutiérrez-Lucas, M. Cortés-Gines, G.I. Pineda-Liceaga, D.B. Estrada-Castro**
- MEDI 416.** Synthesis, antiprotozoal activity, and structure-activity relationships of novel 1-methyl-2-(methylthio)-1*H*-benzimidazole-5-carboxamide derivatives: Identification of new selectivity compounds. **P. Flores Carrillo, R. Aguayo-Ortiz, R. Castillo-Bocanegra, P.J. Trejo, L. Yépez-Mulia, A. Hernandez Campos**
- MEDI 417.** New triple action drugs for ESKAPE pathogens. **D. Utic, E. Turos, D. Shaw, R. Fleeman**
- MEDI 418.** Structure-activity relationship studies of SB-443342 (NEU-1053), a potent inhibitor of *Trypanosoma brucei* proliferation. **W.G. Devine, D. Rojas-Barros, C. Cordon-Obras, M. Navarro, M.P. Pollastrí**
- MEDI 419.** Development of small molecule *C. jejuni* PglD inhibitors: New tools to investigate the roles of protein glycosylation in bacterial virulence. **J. De Schutter, C.Y. Zamora, B. Imperiali**
- MEDI 420.** Copper-binding sequence in the antimicrobial peptide ixosin is essential for its bactericidal and oxidative activity. **M. Libardo, A.M. Angeles Boza**
- MEDI 421.** Microwave-assisted one-pot synthesis of novel fluorinated octahydroquinazolinone derivatives as antibacterial agents. **C.O. Okoro**
- MEDI 422.** Investigation of the mechanism of action of oxazolidinones. **B. Koleva, J.B. Aggen, P.J. Beuning**
- MEDI 423.** Exploration of structure-activity relationship of oxadiazole antibiotics. **D. Ding, E. Spink, Z. Peng, M. Boudreau, M. Suckow, M.F. Chang, S. Mobashery**
- MEDI 424.** Structure-activity and metabolomics insights into a thiophene family of *M. tuberculosis* Pks13 inhibitors. **D. Awasthi, M.J. Szymoniaka, P. Kumar, K.Y. Rhee, D. Alland, J.S. Freundlich**
- MEDI 425.** Ldt_{ms} inhibitors for the potential treatment of tuberculosis. **J. Franco**
- MEDI 426.** Structure-activity relationships of 1,6-diazabicyclo[3.2.1]octane analogs as β -lactamase inhibitors. **S. Yang, J. Pan, Y. Root, E. Smith, J. Su, X. Linghu, V.M. Sprague, G. Scapin, L. Xiao, A. Villafania, P. Dayananth, R. Zhang, A. Mirza, D.E. Demong, M.W. Miller, A. Therien**
- MEDI 427.** Is there a role for the amino terminal copper and nickel binding motif in antimicrobial peptides? **A.M. Angeles Boza**
- MEDI 428.** Non-racemic antifolates stereo-selectively recruit alternate cofactors and overcome resistance in *S. aureus*. **S.K. Keshipeddy, S. Reeve, A.C. Anderson, D.L. Wright**
- MEDI 429.** Design and synthesis of a series of novel heteroaryl benzenesulfonamides as carbonic anhydrase II inhibitors. **V. Cochran, A. Dao, L. Gullett, J. Hoballah, E. Narro, M. Reeves, R. Saganty, G. Siddall, Z. Zinsli, A. Scharf, R. Spoering, R.R. Ranatunge**
- MEDI 430.** Optimization of a series of PDE10A inhibitors: Introduction of structural complexity leads to improved selectivity. **M. Ochse, H. Geneste, S.C. Turner, J. Dinges, K. Jantos, K. Drescher, B. Behl, L. Laplanche, A. Relo, C. Jakob**
- MEDI 431.** D-473, a novel triple dopamine, serotonin and norepinephrine transporters blocker as new generation orally active antidepressants: Characterization in in vitro and in vivo pharmacological and behavioral assays. **A.K. Dutta, S. Santra, O. Mabrouk, T. Antonio, M. Reith**
- MEDI 432.** Metabolic studies of drug candidates for neurological disorders and asthma based on GABA_A receptor subtype selective ligands using mass spectrometry. **R. Kodali, M.L. Guthrie, M.M. Poe, M. Stephen, R. Jahan, C.W. Emala, J.M. Cook, D. Stafford, A. Arnold**
- MEDI 433.** Design and regioselective synthesis of 3-substituted β -carbolines as a GABA_A subtype selective agents for the treatment of alcohol abuse. **V. Tiruveedula, K.T. Warnock, H.L. June, X. Simeone, M. Ernst, M. Gondre-Lewis, J.M. Cook**
- MEDI 434.** Alkoxy substituted bicyclic pyrimidine modulators of gamma secretase. **Y. Zhang, K. Xie, S.E. Mercer, A. Lin, J. Toyn, M. Ahljanian, K.A. Lentz, J.E. Macor, L.A. Thompson, R.E. Olson, K.M. Boy**
- MEDI 435.** Synthesis, SAR and biological evaluations of novel bicyclic pyrimidines as Gamma-secretase modulators. **L. Xu, D.S. Zuev, K.M. Boy, L.A. Thompson, J. Guernon, Y. Zhang, Y. Wu, J. Shi, J. Toyn, J.E. Meredith, C. Burton, C. Albright, K.A. Lentz, J. Grace, R. Denton, J. Morrison, R.E. Olson, J.E. Macor**
- MEDI 436.** Reaction optimization affords scalable synthesis of a fluorinated pyridopyrazine gamma secretase modulator. **J.M. Humphrey, C. am Ende, T.W. Butler, M.S. Lall, C.M. Stiff, M. Pettersson, E. Yang**
- MEDI 437.** Accelerating the transition from drug discovery to FIH studies: Case examples in medicinal chemistry reaction and route optimization. **E. Yang, J.M. Humphrey**
- MEDI 438.** Synthetic optimization of MDW941 enables the development of a high content glucocerebrosidase assay. **C. am Ende, P. Loos, P. Buckett, M. Beyna, S. Hasson, L. Rose, S. Hallowell, D. Gebhard, R. Doyonnas, M. Calabrese, J. Schwartz, A.F. Stepan, Z. Berger, C. Oborski, W. Hirst**
- MEDI 439.** Acrylamide compounds as potent and selective histamine H₃ receptor ligands. **R. Nirogi, A. Shinde, A. Mohammed, L. Kota, V. Tiriveedhi, S. Saraf, R. Subramanian, G. Bhyrapuneni, V. Benade, N. Muddana, P. Jayraján**
- MEDI 440.** Discovery of biaryl acyl sulfonamides as selective and highly efficient Nav1.7 inhibitors. **E. DiMauro**
- MEDI 441.** Synthesis and medicinal chemistry of cyathane diterpenoid inspired scaffolds. **A.L. Courtney, R. Rosen, A.B. Beeler**
- MEDI 442.** mGluR3 PAM: A novel approach to neuroprotection in Parkinson's disease, from HTL to in vivo proof of concept. **I. Dorange**
- MEDI 443.** Design, synthesis, and evaluation of CDK5 inhibitors with improved solubilities. **Y. Sonawane, S. Rana, G. Hollis, M. Taylor, J. Contreras, A. Natarajan**
- MEDI 444.** Frequent hitters revisited. **R. Schneider**
- MEDI 445.** Encoded library technology (ELT): An emerging platform for target validation and hit identification. **C.P. Davie, G. Evindar, C.C. Arico-Muendel, S.L. Belyanskaya, K.E. Lind, J. Messer, C.B. Phelps, C.P. Donahue**
- MEDI 446.** Discovery of novel selective ER subtype ligands by multimodeling and in silico screening. **W. Huang, W. Wei, Y. Yang, T. Zhang, W. Du, Z. Shen**
- MEDI 447.** Using a combined cheminformatic and bioinformatic approach to address proteolytic stability challenges in peptide-based drug discovery. **A.S. Bayden, J. Audie, D.J. Diller**
- MEDI 448.** Targeting specific interactions to improve binding properties of EGFR-kinase ligands. **A. Ajamian**
- MEDI 449.** Distributed drug discovery: Collaborative target repurposing accelerates identification of new leads for neglected tropical diseases. **M.P. Pollastrí**
- MEDI 450.** In silico methods in fragment-based drug design — a Protein Kinase B case study. **C. Detering**
- MEDI 451.** Discovery of phenylalanine derived diamide inhibitors of FX1a. **L.M. Smith, M.J. Orwat, Z.D. Hu, W. Han, C. Wang, K. Rossi, K.B. Pabbisetty, J. Luetting, J. Bozarth, S. Sheriff, J. Myers, P. Morin, M.L. Quan, R.R. Wexler, D. Pinto**
- MEDI 452.** Lead optimization studies on PAR-1 antagonist F16618. **W. Tan, L. Wang, L. Gao, Y. Feng, H. Cui, J. Shi, Y. Tang, L. Jiang, Y. Xia**
- MEDI 453.** Synthetic cardiolipin based nanoparticles to manage excess cholesterol and its metabolism for coronary heart diseases. **R. Wen, S. Dhar**
- MEDI 454.** Discovery of the hydan-toin based MMP-12 inhibitor drug candidate AZD3342 for the treatment of COPD. **M. Munck af Rosenschold**
- MEDI 455.** Benserazide, the first allosteric inhibitor of Coxsackievirus B3 3C protease. **B. Kim, S. Kwak, Y. Jung, T. Kim, B. Son, J. Park, S. Choi, J. Kim, J. Cho, P. Jeong, Y. Kim**
- MEDI 456.** Engineering natural side-chains from leucine and isoleucine into "stapling" amino acids to inhibit the estrogen receptor/coactivator interaction. **T.W. Moore, T. Spletz**
- MEDI 457.** Optimization of tetrahydronaphthalene inhibitors of Raf with selectivity over hERG. **S. Huang, S. Adhikari, R. Afroze, K. Brewer, E.F. Calderwood, J. Chouitar, D.B. England, C. Fisher, K.M. Galvin, J. Gaulin, P.D. Greenspan, S.J. Harrison, M. Kim, S.P. Langston, L. Ma, S. Menon, H. Mizutani, M. Rezaei, M.D. Smith, D. Zhang, A.E. Gould**
- MEDI 458.** Design, synthesis, and SAR of 2-acetamido-3-pyrrolidinepropanamide derivatives as uterensin-II receptor antagonists. **A. Soni, A. Agarwal, S. Saha, M. Das, K.R. Shripati, S. Aeron, B. Das, I. Cliffe, R. Tandon, R.K. Singh, R. Sodhi, S.G. Dastidar, S.K. Singh, S. Sinha, R.K. Shriummalla, V.P. Semwal, S. Murumoto, T. Nagayama**
- MEDI 459.** CYP3A4-specific inhibitors: Rational design of simpler analogs. **P. Kaur**
- MEDI 460.** 4-Dibenzocyclooctynol as a fluorescent probe for sodium azide detection. **K. Wang, F.J. Friscourt, C. Dai, L. Wang, Y. Zheng, G. Boons, S. Wang, B. Wang**
- MEDI 461.** New agonists of the Keap1 – Nrf2 pathway: A potential solution for oxidative stress related diseases. **L. Deny, G. Belanger, E. Marsault, M.V. Richter, H. Traboulsi**
- MEDI 462.** Discovery of novel LPA1 antagonist: Design synthesis and SAR studies. **M. Terakado, K. Hashimura, M. Tanaka, M. Asada, H. Ueda, N. Matsunaga, K. Hirai, M. Ikura, H. Kohno, H. Suzuki, H. Saga, S. Nakade, H. Kurata, M. Toru, Y. Takaoka, T. Seko, H. Habashita**
- MEDI 463.** Withdrawn.
- MEDI 464.** Development of 8-phenylisoquinolines as potential therapeutic agent for inflammatory bowel disease. **Y. Chen, Z. Huang, C. Yang, Y. Huang, C. Shiue, K. Tzen, L. Hsin**
- MEDI 465.** Design and synthesis of selective 5-HT₂ receptor antagonists for the treatment of inflammatory bowel disease. **K. Blattner, D.J. Canney, R. Gao, J.C. Gordon, B.E. Blass, M. Abou-Gharbia, M. Ramanjulu, G.C. Morton**
- MEDI 466.** Study of the structure-activity relationship of the 5-OXE receptor antagonists leading to an improved potency. **Q. Ye, S. Chourey, N. Chintam, H.W. Alhamza, R. Wang, S. Gravel, C. Cossette, W.S. Powell, J. Rokach**
- MEDI 467.** Structure-based design, synthesis, and crystallographic studies of novel HIV-1 protease inhibitors with enhanced backbone interactions. **H.L. Osswald, C. Martyr, A.K. Ghosh, J. Agniswamy, Y. Wang, M. Amamo, I. Weber, H. Mitsuya**
- MEDI 468.** Boronic acid analogs of anti-HIV therapies: Synthesis and biological evaluation. **S.J. Burke, J.M. Gamrat, J.W. Tomsho**

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- MEDI 469.** Isolation and characterization of an immune complex of Imprime PGG₂, a cancer immunotherapeutic agent. **K.S. Michel**, M.E. Danielson, N. Bose, L.R. Wurst, A.B. Jonas, A.S. Chan, D.E. McMurray, B.C. Harrison, K.E. Ertelt, R.M. Walsh, B.T. Rathmann, S.M. Leonardo, P.M. Will, A.S. Magee
- MEDI 470.** RNA-based immuno-stimulatory liposomal spherical nucleic acids for antigen presenting cell activation. **C. Guan**, N. Chernyak, C.A. Mirkin
- MEDI 471.** Design, synthesis, and SAR of a novel series of heterocyclic phenylpropanoic acids as GPR120 agonists. **X. Zhang**, C. Cai, M.P. Winters, Z. Sui, Y. Wang, W. Yan, C. Jenkinson, J. Gunnet, J. Leonard, W.V. Murray
- MEDI 472.** Discovery of isothiazole- and thiophene-containing phenylpropanoic acids as potent and orally efficacious GPR120 agonists for the treatment of type 2 diabetes. **X. Zhang**, C. Cai, Z. Sui, M.J. Macielag, Y. Wang, W. Yan, A. Suckow, H. Hua, A. Bell, P. Haug, W. Clapper, C. Jenkinson, J. Gunnet, J. Leonard, W.V. Murray
- MEDI 473.** Identification of novel insulin-regulated aminopeptidase (IRAP) inhibitors by high throughput screening. **K. Engen**, T. Lundbäck, F. Svensson, U. Rosenström, C. Sköld, M. Hallberg, A. Jenmalm-Jensen, M. Larhed
- MEDI 474.** Search for novel PTP 1B inhibitors: Targeting both catalytic and allosteric sites via integrated approaches. **Z. Xiao**, Y. Tang, Y. Yang, J. Tian, F. Ye
- MEDI 475.** Novel 1,2,3-triazole analogs as DPP4 inhibitors. **H. Park**, T. Pham
- MEDI 476.** Discovery of novel cyclic peptides which exhibit glucagon-like peptide-1 (GLP-1) receptor agonism. **C. Limberakis**, G.E. Aspnes, D.R. Darksen, D.J. Edmonds, H. Eng, D.P. Fairlie, G.H. Goetz, A. Gopalsamy, D.A. Griffith, T.A. Hill, H.N. Hoang, A.S. Kalutkar, W.M. Kok, S. Liras, V. Mascitti, A.M. Mathiowitz, J.M. Mitchell, D.W. Piotrowski, D. Price, C.J. Rotter, R.B. Ruggeri, K. Song, R.V. Stanton, J.Y. Suen, J.M. Withka
- MEDI 477.** Design and synthesis of novel bicyclic GPR119 agonists as drug target for the treatment of type 2 diabetes. **G. Poissonnet**, O. Russo, F.M. Perron-Sierra, I. Theret, O. Della-Zuana, M. Brun, E. Harley, A. Ktorza
- MEDI 478.** Discovery and SAR of pyrrole derivatives as agonists of GPR120 for the treatment of type II diabetes. **M.P. Winters**, J. Lanter, M.J. Wall, Z. Sui, J. Leonard, J. Gunnet, Y. Wang, H. Hua, W. Yan, A. Suckow, C. Jenkinson, P. Haug, A. Bell, W. Clapper, N. Huebert, W.V. Murray
- MEDI 479.** Parallel synthesis of novel peptides containing N-terminal heterocyclic triazoles. **S.B. Coffey**, G.E. Aspnes, A.T. Londregan, D.W. Piotrowski
- MEDI 480.** Syntheses of spiro 7-azaindolones. **G. Pan**, J. Mao, H. Wang, H. Li, X. Wu, M. Yang
- MEDI 481.** Strategies for the identification and characterization of atropisomers. **J. Davoren**
- MEDI 482.** Late-stage functionalization platform for lead optimization and diversification: Generation of high value compounds directly for biological testing. **R.S. Buzdygon**, M. Cushner, F. Feru, M.J. Bazin
- MEDI 483.** Syntheses of 5-halo-1*H*-pyrazoles. **S. Yu**, H. Li, X. Wu, M. Yang
- MEDI 484.** Bromo-alkaloids from the Turkish marine sponge *Ircinia variabilis*. **J. Zhao**
- MEDI 485.** Property-based optimization of NOP receptor antagonists based on a potent thienospiro-piperidine scaffold. **M.A. Martinez-Grau**, C. Pedregal, M.A. Toledo, N. Diaz, C. Lafuente, A. Jimenez, A.B. Benito, J. Witkin, M.A. Starnick, D.L. McKinzie, L. Rorick-Kehn, V. Barth, S. Kahl, D.R. Mudra
- MEDI 486.** Biased multicomponent reactions to develop novel bromodomain inhibitors. **S. Liu**, M. McKeown, H. Fu, D. Buckley, J. Qi, J. Bradner, W. Zhang
- MEDI 487.** Withdrawn.
- MEDI 488.** Detecting intratumoral heterogeneity of EGFR activity by liposome-based in vivo transfection of a fluorescent biosensor. **R. Bofinger**, N. Mitchell, M. Lythgoe, Z. Wright, S. Ameer-Beg, T. Kalber, B. Vojnovic, A. Cheung, R. Evans, G. Fruhwirth, M. Keppler, P. Barber, W. Wulaningsih, H. Hailes, A.B. Tabor, T. Ng
- MEDI 489.** Synthesis and biological studies of porphyrinoid-based cancer imaging and photo dynamic therapy (PDT) agents. **N. Bhupathiraju**, C.M. Drain
- MEDI 490.** Optimization of quinazolinone-based kinase inhibitors: Identification of a dual FLT3/AURKA kinase inhibitor for the treatment of acute myeloid leukemia. **H. Hsieh**, Y. Chang Hsu, Y. Ke, H. Shiao, C. Chang, W. Lin, T.J. Hsu, T. Yeh, C. Chen
- MEDI 491.** Discovery of selective potent TBK1 and IKKε dual kinase inhibitors. **L. Gingipalli**, C. Chuagui, S. Cowen, **J.W. Jeffrey**, E. Devereaux, A. Molina, T. Wang, D. Whitstonb, X. Wu, H. Zhang, M. Zinda
- MEDI 492.** Small molecule regulation of bromodomains. **D. Buckley**, J. Roberts, G. Winter, J. Bradner
- MEDI 493.** Lysis of cancer cells by Vγ9Vδ2 T cells requires phosphoantigen interaction with BTN3A1. **A.M. Kilcollins**, J. Li, C.C. Hsiao, A.J. Wiemer
- MEDI 494.** One pot protection free synthesis of N-(1-(9-alkyl-6-(heteroarylamino)-9*H*-purin-2-yl)pyrrolidin-3-yl)acrylamides; next generation irreversible EGFR T790M inhibitors. **S. Cho-Schultz**, S.K. Nair, D. Behenna, K. Tran, R. Zhou, J. Matthews, N. Sach, M.A. Pairish, H. Shen, J.G. Deal, S.T. Orr
- MEDI 495.** Synthesis of 2-aminoaryl-4-alkoxy-5-heteroaryl-7*H*-pyrrolo[2,3-*d*]pyrimidines; Next generation irreversible EGFR T790M inhibitors. **R. Zhou**, D. Behenna, S. Cho-Schultz, J.C. Kath, S. Kephart, K.K. Liu, J. Matthews, S.K. Nair, M.A. Ornelas, S.T. Orr, M.A. Pairish, D.T. Richter, N. Sach, H. Shen, S.C. Sutton, Y. Tao, K.N. Tran
- MEDI 496.** Development of biotinylated derivatives for pull-down analysis of compounds inducing a mesenchymal to epithelial transition. **A.J. Motta**, P.T. Flaherty, T. Wright, J. Cavanaugh, M. Burrow, V. Hoang, S. Elliot
- MEDI 497.** Chemistry of folate-everolimus and folate-rapamycin conjugates: Avoiding side reactions and improving their physical properties. **I.R. Vlahov**, L. Qi, H.K. Santhapuram, S.J. Hahn, P.J. Kleindl, F. You, K.Y. Wang, J.F. Vaughn, C.P. Leamon
- MEDI 498.** Cancer associated protein FXR5 (dysadherin) may promote tumorigenicity by stimulating the secretion of the chemokine CCL2 (MCP-1). **C. Asher**, I. Lubarski, H. Garty
- MEDI 499.** Novel strategies for targeted therapies of cancer: GARFTase inhibitors and additional chemotherapeutic payloads to cancer cells. **I.R. Vlahov**, F. You, H.F. Klein, P.J. Kleindl, M. Nelson, M. Vetzal, J.A. Reddy, C.P. Leamon, L.H. Matherly, A. Gangjee
- MEDI 500.** Hydroxamic acid based HDAC inhibitors containing macrolide antibiotic as enzyme surface recognition group. **S. Tapadar**, J.R. Kornacki, I. Raji, S. Fathi, M. Mrksich, A.K. Oyelere
- MEDI 501.** Azithromycin based HDAC inhibitors. **S. Fathi**
- MEDI 502.** Exploration of internal H-bond mimics as MEK5/ERK5 inhibitors. **M. Gupta**, P.T. Flaherty, T. Wright, J. Cavanaugh
- MEDI 503.** Structure-activity relationship and in vitro evaluation of pyrrolo[2,3-*d*]pyrimidines as microtubule disrupting agents. **A. Gangjee**, **R. Mohan**, S. Mooberry
- MEDI 504.** Design, synthesis, and biological evaluation of thieno[3,2-*d*]pyrimidines as potent antimetabolic and antitumor agents. **A. Gangjee**, **T.M. Quadery**, K.S. Shah, W. Xiang, X. Zhou, A. Perez, S. Mooberry
- MEDI 505.** Substituted thieno[2,3-*d*]pyrimidines: Design, synthesis, and biological evaluation as tubulin targeting antitumor agents. **A. Gangjee**, **F. Islam**, W. Xiang, S. Mooberry
- MEDI 506.** Monocyclic pyrimidine analogs as novel colchicine site binding antitubulin agents. **A. Gangjee**, **S. Choudhary**, A. Perez, S. Mooberry, E. Hamel
- MEDI 507.** Chemical probes for PIM1 and CLK4. **M. Beltran Molina**, N. Tomkinson
- MEDI 508.** Withdrawn.
- MEDI 509.** Application of a multicomponent reaction in the discovery and optimization of inhibitors of human polynucleotide kinase/phosphatase for use as tumor radiosensitizing agents. **T. Verdelet**, R. Ward, D. Shire, R. Mani, S. Bernard, V. Lamontagne, G.F. Freschauf, F. Karimi-Busheri, M. Weinfeld, D.G. Hall
- MEDI 510.** Discovery of a potent, selective inhibitor of RET kinase including the V804L/V804M gate-keeper mutants. **H. Yoon**, Y. Kwak, S. Choi, N. Kim, K. Cho, T. Sim
- MEDI 511.** Synthesis and evaluation of chemically modified dangling end units for optimization of RNA interference. **Y. Kitamura**, S. Ogawa, R. Nakashima, M. Kandeel, Y. Kitade
- MEDI 512.** Structure-activity relationships of silybin derivatives as anticancer agents. **B. Vue**, S. Zhang, K. Parisi, Q. Chen
- MEDI 513.** Discovery and synthesis of substrate competitive SMYD2 inhibitors. **S. Throner**, S. Cowen, D.J. Russell, L. Dakin, H. Chen, N.A. Larsen, R.E. Godin, X. Zheng, A. Molina, J. Wu, T. Cheung, T. Howard, R. Garcia-Arenas, N. Keen, A.D. Ferguson
- MEDI 514.** Spiroisobenzofuranone derivatives as potential anticancer agents. **C. Yin**, P. Chen, Z. Chen, R. Stephani, V.L. Korlipara
- MEDI 515.** Evaluation of trehalose derivatives as radiotracers specific for tuberculosis in animal models of disease. **G.A. Marriner**, D.O. Kiesewetter, S.S. Lee, F. D'Hooge, O. Boutoureira, R. Raj, N. Khan, L.E. Via, B.G. Davis, C.E. Barry
- MEDI 516.** Design and synthesis of novel tubulysin analogs. **I.R. Vlahov**, F. You, P.J. Kleindl, M. Vetzal, J.A. Reddy, C.P. Leamon
- MEDI 517.** Reducing off-target activity of folate-tubulysin conjugates by introducing unnatural amino acids and by increasing steric bulk within the peptidic spacer. **P.J. Kleindl**, H.K. Santhapuram, F. You, J.F. Vaughn, K.Y. Wang, S.J. Hahn, N. Parker, M. Vetzal, M.R. Pugh, C.P. Leamon, I.R. Vlahov
- MEDI 518.** Design, synthesis, and evaluation of 2,5-dioximidazolidine based conformationally constrained analogs of KN62 as novel P2X₂ receptor antagonists. **J. Park**, S. Kwak, Y. Jung, T. Kim, B. Son, J. Park, S. Choi, H. Ko, Y. Kim
- MEDI 519.** Scaffold replacement and 3D ligand optimization applied to the discovery of tyrosine kinase inhibitors. **R. Alvarez**
- MEDI 520.** Targeting the sweet spot of cancer: Multivalent glycopolymer as potential cancer vaccines. **Q. Qin**
- MEDI 521.** Design, synthesis, and preliminary biological evaluation of vitamin D₂ glycoside analogs. **Y. Liu**, **Z. Fang**
- MEDI 522.** Discovery of potent small molecule inhibitors of Wnt signaling. **A. Mallinger**, K. Schiemann, C. Rink, F. Stieber, S. Crumpler, D. Waalboer, M. Calderini, M. Stubbs, O. Adeniji-Popoola, M. Ortiz-Ruiz, R. Schneider, P. Workman, T. Dale, D. Wienen, C. Esdar, P.A. Clarke, F. Raynaud, F. Rohdich, S.A. Eccles, J. Blagg
- MEDI 523.** Discovery of G protein biased EP2 receptor agonists. **S. Ogawa**, T. Watanabe, A. Watanabe, A. Kinoshita, K. Tsuboi, I. Sugimoto, K. Moriyuki, Y. Goto, S. Yamane, K. Tani, M. Toru
- MEDI 524.** Applications of thioamides in protease studies: Fluorescent probes and peptide stabilization. **X. Chen**, J.M. Goldberg, E.K. Keenan, N. Meinhardt, D. Greenbaum, E. Petersson
- MEDI 525.** Chemical modifications of 4,6-bisphenyl-2-(3-alkoxyanilino)pyrimidine focusing on the activity-sensitive aminoalkoxy moiety for a therapeutically useful inhibitor of receptor for advanced glycation end products (RAGE). **T. Kim**, J. Hur, K. Kim, H. An, Y. Suh
- MEDI 526.** Discovery and structure-activity relationships of pyrazolodiazepine derivatives as the first small molecule agonists of the *Drosophila* sex peptide receptor. **J. Kim**, P. Jeong, S. Kwak, Y. Jung, T. Kim, B. Son, J. Park, S. Choi, H. Ko, Y. Kim
- MEDI 527.** Structure-activity-relationship studies investigating the substitution pattern around the indole ring of sphingosine kinase 2 selective inhibitors. **M. Congdon**, Y. Kharel, K.R. Lynch, W.L. Santos
- MEDI 528.** Structure-activity relationship studies of guanidine-based aminothiazole inhibitors of sphingosine kinase. **E. Childress**, Y. Kharel, K.R. Lynch, W. Santos
- MEDI 529.** Revisiting the development of active site directed protein kinase inhibitor probes for in vivo studies: An isoform selective case study from the integrated use of structural biology and pharmacoinformatics. **S.M. Roy**, D. Wattersson, G. Minasov, W.F. Anderson, V. Tokars
- MEDI 530.** Facile conjugation of biotargeting motifs to a chlorin platform for biomedical applications. **J. Gonzales**, C.M. Drain

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MEDI 531. Impact of anomeric linkage between GalNAc sugar moiety and siRNA on biological activity. **P. Kandasamy**, S. Matsuda, J. Nair, K. Charisse, J. Willoughby, N. Taneja, J. O'Shea, K. Yucius, A. Borodovsky, T. Nguyen, S. Milstein, S. Shulga-Morskaya, J. Liu, R. Hutabarat, M.A. Maier, K.R. Rajeev, M. Manoharan

MEDI 532. Development of a new generation of photodynamic chemotherapeutic dyes for post-operative wound care. **H. Faki**, A. Jones, G. Morton, R. Smith

MEDI 533. Zinc-metallochaperone complexes that restore wildtype structure and function of mutant p53 in cancer. **D.J. Augeri**, S.D. Kimball, X. Yu, J.A. Gilleran, A.R. Blanden, S.N. Loh, D.R. Carpizo

MEDI 534. MCC22 targets putative spinal MOR-CCR₂ heteromers in a mouse model of inflammatory pain. **E. Akgun**, M.I. Javed, M. Lunzer, M.D. Powers, Y.Y. Sham, P.S. Portoghesse

NUCL

Division of Nuclear Chemistry and Technology

J. Terry and D. Hobart, Program Chairs

SUNDAY AFTERNOON

Section A

Seaport World Trade Center
Waterfront 2

Analytical Chemistry in Nuclear Technology

R. Lascola, Z. Wang, Organizers

S. A. Bryan, Organizer, Presiding

1:00 Introductory Remarks.

1:10 NUCL 1. Plenary:

Spectroelectrochemical sensors for measurements on complex samples in harsh environments.

W.R. Heineman, S.D. Branch, S.A. Bryan

1:40 NUCL 2. Thin-film spectroelectrochemical sensor for technetium. **S.D. Branch**, J. Bello, S.A. Bryan, W.R. Heineman

2:00 NUCL 3. Formation and subsequent spectroelectrochemical sensing of Ru and Eu species in both solution and ion selective films. **A. Lines**, S.D. Branch, W.R. Heineman, S.B. Clark, S.A. Bryan

2:20 NUCL 4. On-line process monitoring for plutonium oxide production. **L.T. Sexton**, S. Branney, P. O'Rourke, W.C. Hardy, J. Wilson, M. Jones, M.K. Holland, N. McIntosh

2:40 Intermission.

2:55 NUCL 5. Batch, column, and timed-resolved U(VI) luminescence study on the effect of phosphate on U(VI) sorption and retardation in subsurface sediments. **Z. Wang**, Z. Pan, L. Taylor, D. Giammar, J.G. Catalano

3:15 NUCL 6. Development of a dual excitation fiber optic Raman microscope for the identification of mineralogical samples. **J. Bello**, C. Gasbarro

3:35 NUCL 7. Methods for Pu valence determination in nuclear material processing solutions. **R. Lascola**, P. O'Rourke, C. Johnson, E.A. Kyser

3:55 NUCL 8. Spectroscopic online monitoring for process control and safeguarding of radiochemical streams. **S.A. Bryan**, A.J. Casella, L.R. Ahlers, N. Navindra, F.D. Heller, T.G. Levitskaia, G.J. Lumetta

MONDAY MORNING

Section A

Seaport World Trade Center
Waterfront 2

Analytical Chemistry in Nuclear Technology

H. Cho, D. P. Diprete, Organizers

D. S. Peterson, Organizer, Presiding

8:00 Introductory Remarks.

8:05 NUCL 9. Single droplet analysis of metal-ligand solutions by electrospray ionization mass spectrometry using an induction-based fluidics source. **K.M. Roscioli**, C.A. Zarzana, A.D. Sauter, G.S. Groenewold

8:25 NUCL 10. Innovation in XRF: Determination of plutonium in spent fuel. **K.G. McIntosh**, G.J. Havrilla, R. Gilmore, D. Missimer, M.K. Holland

8:45 NUCL 11. Where is the plutonium? Detection and location of plutonium-containing particles in Tank 18 waste at Savannah River site (SRS) using scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), wavelength dispersive spectroscopy (WDS), and X-ray diffraction (XRD). **H. Ajo**, M. Hay, D. Missimer, P. O'Rourke

9:05 NUCL 12. Characterization of synthetic urban nuclear melt glass. **A. Giminaro**

9:25 Intermission.

9:40 NUCL 13. High resolution solid-state NMR on nuclear materials. **L. Martel**, C. Selfslag, J. Somers

10:00 NUCL 14. Computational studies of magnetic properties of f-element complexes. **J. Autschbach**

10:20 NUCL 15. Spectroscopic investigation for the structure of actinides sorption on the solid/liquid inter-surface. **W. Wu**

10:40 NUCL 16. Analytical methods in support of waste processing operations at the Savannah River site. **T.B. Peters**, K.M. Taylor-Pashow, T. White, F.F. Fondeur, A.L. Washington, D.P. Diprete, **D.T. Hobbs**

11:00 NUCL 17. ²²⁶Ra analyses on Savannah River site radioactive waste matrices. **D.P. Diprete**, C.C. DiPrete, C.J. Coleman, M. Hay, S.H. Reboul, T.J. Aucott

MONDAY AFTERNOON

Section A

Seaport World Trade Center
Waterfront 2

Analytical Chemistry in Nuclear Technology

J. D. Auxier, J. Giaquinto, C. R. Hexel, Organizers

D. P. Diprete, Presiding

1:00 Introductory Remarks.

1:05 NUCL 18. Development of the Field Alpha Spectrometry Tool (FaST). **D.S. Peterson**, R. Jung, C. Armenta

1:25 NUCL 19. High precision trace element determination for standard material production. **C.R. Hexel**, J. Giaquinto

1:45 NUCL 20. Investigation for source term for the incident in WIPP'S Panel 7 Room 7EHE. **J. Giaquinto**, S. Croft, S. Myers, D.K. Veirs

2:05 NUCL 21. Validation of Neptune Plus MCICPMS for high precision isotope ratio analysis of environmental U and Pu samples. **B.W. Ticknor**, C.R. Hexel, D.A. Bostick, E.H. Mccay, J. Giaquinto

2:25 Intermission.

2:40 NUCL 22. Retardation and release of uranium on phlogopite mica at the absence and presence of humic acid: A batch and TRLFS study. **D. Pan**, Z. Wang, W. Wu

3:00 NUCL 23. Scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) applied to Waste Isolation Pilot Plant (WIPP) samples. **H. Ajo**, J. Young, C. Gregory

3:20 NUCL 24. Results of an international interlaboratory comparison of NBL CRM 124-3 material. **L.P. Colletti**, L. Tandon

3:40 NUCL 25. Sharing the experience of changing gamma detector systems in a production laboratory. **T. Whiteside**, C. Diprete

4:00 NUCL 26. Radionuclide analyses supporting waste acceptance criteria for low level waste at the Savannah River site. **C.L. Crawford**

TUESDAY AFTERNOON

Section A

Seaport World Trade Center
Waterfront 2

Transformation & Transport of Radionuclides in the Environment

Cosponsored by GEOC

M. Boyanov, Organizer

K. M. Kemner, E. J. O'Loughlin, Organizers, Presiding

1:00 NUCL 27. Speciation of U(IV) in sediment microcosms and model biogeochemical systems under reducing conditions. **M. Boyanov**, E.J. O'Loughlin, D. Latta, B. Mishra, T. Flynn, D. Antonopoulos, **K.M. Kemner**

1:20 NUCL 28. Predicting plutonium behavior in the environment: Linking mechanistic behavior to field processes. **A. Kersting**

1:50 NUCL 29. Using flow-cell desorption experiments to understand colloid-facilitated Pu transport. **J. Begg**, M. Zavarin, S.J. Tumeay, A. Kersting

2:10 NUCL 30. Microbial iodine cycling: Effects on fate and transport in the Hanford subsurface. **B. Lee**, J. Ellis, E. Eisenhauer, S. Saurey, D. Saunders, M. Lee

2:30 NUCL 31. Determination of the spatial distribution and chemical state of Cs in model environmental samples. **J.I. Pacold**, S.G. Minasian, T. Tyliczszak, A.B. Altman, S. Suzuki, D.K. Shuh, T. Yaita

2:50 Intermission.

3:10 NUCL 32. Interactions of uranium and co-occurring elements in abandoned mine wastes. **J.M. Cerrato**, S. Avasarala, J. Blake, A. Ali, A. Brearley, K. Artyushkova, J. Lezama-Pacheco

3:40 NUCL 33. Alkali technetium oxides as model compounds for Tc-99 incorporation in glass. **J.L. Weaver**, J. McCloy, N. Wall, C. Soderquist

4:00 NUCL 34. Effect of uranium toxicity on the immobilization of uranium by subsurface microorganisms. **M. Taillefer**, K. Belli, K. Salome

WEDNESDAY MORNING

Section A

Seaport World Trade Center
Waterfront 2

General Topics in Nuclear & Radiochemistry

J. Braley, T. A. Bredeweg, Organizers

W. Loveland, Organizer, Presiding

1:00 NUCL 35. Structure and dynamics of mixtures of molten salts for the pyroprocessing of nuclear waste. **D. Corradini**, M. Levesque, P. Madden, M. Salanne

1:25 NUCL 36. Development of block copolymer materials for f-element separations. **L. Mitchell**, T.T. Nguyen, **B.J. Holliday**

1:50 Intermission.

2:05 NUCL 37. Study of chemical behaviour of Tl and in as light homologues of element 113. **E. Tereshatov**, M. Boltoeva, C.M. Folden

2:30 NUCL 38. Production of heavy and superheavy elements using projectiles with $Z \geq 20$. **C.M. Folden**

2:55 NUCL 39. Deposit thickness effects on nuclear recoil attenuation and emission. **A. Roman**, R.S. Rundberg

3:20 NUCL 40. Update on the observation of gamma rays from the nuclear isomer of ²²⁹Th. **R.S. Rundberg**

WEDNESDAY AFTERNOON

Section A

Seaport World Trade Center
Waterfront 2

General Topics in Nuclear & Radiochemistry

T. A. Bredeweg, W. Loveland, Organizers

J. Braley, Organizer, Presiding

8:00 NUCL 41. Interpreting radioactive microspheres released in Fukushima Daiichi Nuclear Plant accident in view of XANES and thermodynamic database. **T. Ogawa**, T. Do, S. Sujatanond, T. Ogitsu, H. Shiwaku, M. Nakada, M. Akabori

8:25 NUCL 42. Advanced tritium storage bed development at the Savannah River site. **K.J. Heroux**

8:50 NUCL 43. Assessment of down-hole membrane-diffused hydrogen for stimulating uranium reduction and immobilization. **L. Haynes**, L.W. Clapp, W. Yang

9:15 Intermission.

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9:30 NUCL 44. Particle induced gamma-ray emission spectroscopy as a probe for perfluoroalkyl substances. **G.F. Peaslee**, D. Lunderberg, N. Hubley, M. Dickinson, P. DeYoung, J.A. Field, A. Robley, B. Allred

9:55 NUCL 45. Extraction comparison of light and heavy fission elements nuclear forensics analysis. **J.D. Auxier**, S. Stratz, J.A. Jordan, A.V. Jones, H.L. Hall

10:20 NUCL 46. Destructive assay of nuclear melt glass for rapid forensic analysis. **J. Gill**, J.D. Auxier, A.V. Giminaro, H.L. Hall

10:45 NUCL 47. Polynuclear technetium iodides cluster compounds. **W.M. Kerlin**, C. Malliakas, P. Forster, K. Czerwinski, A.P. Sattelberge

ORGN

Division of Organic Chemistry

M. McIntosh and R. Broene, Program Chairs

OTHER SYMPOSIA OF INTEREST:

Innovation in Metabolism, Bioavailability and Formulations Research Leading to the Discovery of Agrochemicals: Symposium Honoring Dr. Keith D. Wing, AGRO International Award for Research in Agrochemicals (see AGRO, Monday)

International Entrepreneurship: How to Start a Business and Thrive in the Global Marketplace (see IAC, Tuesday)

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials (see ENVR, Tuesday, Wednesday, Thursday)

Formulation Technologies for Improved Crop Protection (see AGRO, Wednesday)

Using Passive Sampling Techniques to Detect Organic Contaminants (see ENVR, Wednesday)

SOCIAL EVENTS:

Social Hour, 8:30 PM: Wednesday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 203

Peptides, Proteins, and Amino Acids

M. C. McIntosh, *Organizer*

J. M. Holub, *Presiding*

8:00 ORGN 1. Bioactive peptide nanofibers for bone regeneration. **G. Tansik**, E. Ergul, A. Tekinay, M.O. Guler

8:20 ORGN 2. Targeting anti-apoptotic Bcl2 proteins with synthetic biologics. **J.M. Holub**, Z. Coon, M. Harris, B. Swords

8:40 ORGN 3. Synthesis and conformational studies of pseudopeptidic macrocycles [$\omega\alpha$ -Nⁿ-hydrazino] towards nanotubular structures in solid and gel state. **E. Romero**, B. Jamarat-Gregoire

9:00 ORGN 4. Structure, function, and inhibition of the filovirus fusion protein GP2. **J.R. Lai**

9:20 ORGN 5. Designed self-assembling antimicrobial peptides: Probing supramolecular structure-dependent antimicrobial activity and biocompatibility. **D. Xu**, L. Jiang, H. Dong

9:40 ORGN 6. Study of charge transport across oligoglycines using EGaIn junctions. **M. Baghbanzadeh**, C.M. Bowers, D. Rappoport, Z. Zaba, M. Gonidec, M.H. Al Sayah, P. Cyganik, A. Aspuru-Guzik, G.M. Whitesides

10:00 ORGN 7. Solid phase synthesis of constrained 13-membered peptide macrocycles employing Fukuyama-Mitsunobu alkylations. **S. Broussy**, L. Wang, W. Liu, M. Vidal

10:20 ORGN 8. Fluorescent labeling of peptides through photoacylation. **A. Ornelas**, E.A. Iniguez, J.E. Rincon, R. Roacho, R.A. Maldonado, T. Boland, E. Pena-Cabrera, K.H. Pannell, K. Michael

10:40 ORGN 9. NMR characterization of noncanonical isopeptidic bonds in K48 dimers of ubiquitin. **K. Herrera**

11:00 ORGN 10. Withdrawn.

11:20 ORGN 11. Development of one- and two-photon activatable thiol containing peptides using nitrobenzofuran and 3-methyl bromohydroxy coumarin as efficient photoremovable protecting groups. **M. Mahmoodi**

Section B

Boston Convention & Exhibition Center
Room 204A

Nanomaterials

M. C. McIntosh, *Organizer*

A. Greer, *Presiding*

8:00 ORGN 12. Synthesis and characterization of fluorescent rosette nanotubes from guanine-cytosine (GAC) motif. **B. Legesse**, J. Cho, R.L. Beingsneser, T. Yamazaki, H. Fenniri

8:20 ORGN 13. CNT filament wound prepreg for composite overwrap pressure vessels. **T. Williams**, J.C. Thesken, P. Heimann, D. Gorican, A. Ring, J. McCrone, L. McCorkle, C. Ramirez, J. Baker, B. Lerch, P. Abel, A. Biaggi-Labiosa

8:40 ORGN 14. Alkaline phosphatase mimicking peptide nanofibers for osteogenic differentiation. **G. Gulseren**, C.I. Yasa, A. Tekinay, M.O. Guler

9:00 ORGN 15. Tuning the physical properties of MoS₂ membranes through organophosphonate interfacial chemistry. **R. Cszik**, E. Parzinger, J. Schwartz, M. Stutzmann, U. Wurstbauer, A. Cattani-Scholz

9:20 ORGN 16. Use of atomic pair distribution function (PDF) for the structural characterization of amorphous and nanocrystalline organic compounds. **A. Adibhatla**, D. Beckers, M. Gateshki

9:40 ORGN 17. Tuning the properties of nanoparticle stabilized capsules from the inside-out. **B. Duncan**, R. Landis, X. Li, H.A. Jerri, V. Normand, L. Wang, A. Gupta, S. Kim, D. Benczedi, L. Ouali, R. Ramanathan, R. Tang, J.A. Boerth, V.M. Rotello

10:00 ORGN 18. Bioinspired and programmable nanotheranostics and their use in the development of nanophotosensitizers. **J. Bhaumik**, N.S. Thakur, S. Kirar, J. Laha, U.C. Banerjee

10:20 ORGN 19. Synthesis of phthalocyanine derivative with near IR absorption for materials and biomedical applications. **W. Rizvi**, C.M. Drain

10:40 ORGN 20. Regeneration of cartilage tissue and chondrogenesis in 3D microenvironment by supramolecular glycopeptide nanofibers. **E. Arslan**, M. Sardan, A. Tekinay, M.O. Guler

11:00 ORGN 21. Teflon nanocomposite as a new sensitizer drug photorelease medium. **G. Ghosh**, M. Minnis, A.A. Ghogare, I. Abramova, K. Cengel, T. Busch, A. Greer

11:20 ORGN 22. Self-assembled supramolecular chiral peptide amphiphile nanostructures. **M. Hatip**, M. Khalily, M. Guler

11:40 ORGN 23. Preparation of triptycene-derived imine-linked polymers-encapsulated Pd nanoparticles and catalytic application in Suzuki-Miyaura coupling reaction. **X. Zhang**, X. Liu, Y. Zhang, Z. Zhao, J. Liu, G. Du, Y. Lu, S. Yan

Section C

Boston Convention & Exhibition Center
Room 204B

New Reactions and Methodology

M. C. McIntosh, *Organizer*

T. K. Shah, *Presiding*

8:00 ORGN 24. Synthesis of di-, tri-, and tetrasubstituted pyridines from (phenylthio)acetic carboxylic acids and 2-[aryl(tosylimino)methyl]acrylates. **D.G. Stark**, A.D. Smith

8:20 ORGN 25. Harnessing complex mixtures for catalyst discovery. **J. Moran**

8:40 ORGN 26. Transition metal catalyzed carbon-carbon bond activation. **P. Chen**, G. Dong

9:00 ORGN 27. Steric-controlled C-H activation strategy for primary amino alcohols. **T. Gorman**, J. Calleja-Priede, D. Pla, V. Domingo, B. Haffemayer, M. Gaunt

9:20 ORGN 28. Hetarynes as building blocks for natural products and unique heterocycles. **T.K. Shah**, N.K. Garg

9:40 ORGN 29. General platform for the C-H activation of aliphatic secondary amines. **D. Willcox**, B. Chappell, K. Hogg, M. Gaunt

10:00 ORGN 30. Nickel in the high speed ball mill: A new concept for metal mediated cycloaddition reactions. **R. Haley**, A. Zellner, J. Mack, H. Guan

10:20 ORGN 31. First one-step aqueous Barton decarboxylation: A green avenue for maleimide derivatives. **C. Len**, F. Mangin, E. Leonard

10:40 ORGN 32. First pinacol coupling under micellar conditions: Key role of surfactant and impact of alternative activation technologies. **C. Len**, M. Billamboz

11:00 ORGN 33. Development of regioselective alkyne functionalization methodology. **Y. Xing**

11:20 ORGN 34. Mechanosynthesis as a powerful tool for reaction discovery: New mechanochemical copper catalyzed C-N coupling reactions for the synthesis of pharmaceutically attractive compounds. **D. Tan**, T. Friscio

11:40 ORGN 35. Aromatic H-D exchange using CF₃COOD and an NHC-amidate-palladium catalyst. **K. LaCroix**, R. Narain, R.A. Giles

Section D

Boston Convention & Exhibition Center
Room 206A

Asymmetric Reactions and Syntheses

M. C. McIntosh, *Organizer*

T. Benkovic, *Presiding*

8:00 ORGN 36. Stereoselective synthesis of a nucleoside reverse transcriptase inhibitor via organocatalytic dynamic kinetic resolution. **T. Benkovic**

8:20 ORGN 37. Kinetic resolution of vinyl sulfoxides by Rh-mediated asymmetric hydrogenation: A new efficient methodology for the preparation of enantiopure sulfoxides. **J. Lao Mulinari**, H. Fernandez-Perez, A. Vidal-Ferran

8:40 ORGN 38. Enantioselective radical olefin aziridination via Co(II)-based metalloradical catalysis. **L. Jin**, X. Cui, P.X. Zhang

9:00 ORGN 39. Bridged D₂-symmetric chiral amidoporphyrins for Co(II)-based metalloradical catalysis: Highly enantio-switchable, intramolecular C(sp³)-H radical amination controlled by bridge-regulated cavities. **K. Lang**, P.X. Zhang

9:20 ORGN 40. Development of manufacturing route to Elbasvir. **J. Yin**, H. Li, K.M. Belyk, A.M. Hyde, Q. Chen, Y. Ji Chen, L.C. Campeau, K.R. Campos

9:40 ORGN 41. Origins of stereoselectivities in asymmetric Nazarov reactions catalyzed by bifunctional primary amine-thioureas. **Y. Lam**, A.H. Asari, K.N. Houk

10:00 ORGN 42. Metal-free metathesis reaction of C-chiral allylic sulfilimines with aryl isocyanates: Construction of chiral nonracemic allylic isocyanates. **R. Grange**, P. Evans

10:20 ORGN 43. Palladium-catalyzed asymmetric allylic alkylation of nitrogen nucleophiles with cycloalkene carbonates. **N.K. Zaware**, D. Kastrinsky, G. Narla, M. Ohlmeyer

10:40 ORGN 44. Paraldehyde as an acetaldehyde precursor: Site isolation of incompatible catalysts and use in asymmetric organocatalysis. **C. Rodriguez-Esrich**, X. Fan, S. Wang, S. Sayalero, M.A. Pericas

11:00 ORGN 45. Development of a catalytic enantioselective Mannich reaction. **J. Shikora**, S.R. Chemler

11:20 ORGN 46. Cu-catalyzed asymmetric allylic arylation with aryl lithium reagents. **S. Guduguntla**

11:40 ORGN 47. Stereocontrolled synthesis of adjacent acyclic quaternary-tertiary motifs and its application to a concise total synthesis of (-)-filiformin. **D.J. Blair**, C.J. Fletcher, K. Wheelhouse, V.K. Aggarwal

Section E

Boston Convention & Exhibition Center
Room 206B

Molecular Recognition and Self-Assembly

M. C. McIntosh, *Organizer*

S. Wezenberg, *Presiding*

8:00 ORGN 48. Use of electroactive phenylenediamine ureas to manipulate binding strength in linear H-bond arrays. **D.K. Smith**, L.A. Clare, R. He

8:20 ORGN 49. Bowl-shaped molecular probe for xenon-129 magnetic resonance imaging. **B.L. DeBoef**

8:40 ORGN 50. Multistate regulation of anion binding affinity by light and heat. **S. Wezenberg**, M. Vlatkovic, J. Kistemaker, B. Feringa

9:00 ORGN 51. Construction of chiral materials using supramolecular atropisomers. **Q.R. Chu**

9:20 ORGN 52. Conformationally rigid pseudo-bicyclic guanidinium-based oxanion receptors. **C. Seipp**, N.J. Williams, V. Bryantsev, R. Custelcean, B.A. Moyer

9:40 ORGN 53. Supramolecular imidazolium frameworks: Node-and-linker charge-inverted analogs of metal azolate frameworks. **C. Mottillo**, T. Friscio

10:00 ORGN 54. Acceleration of wound healing with GAG mimetic peptide nanofiber gel in diabetic rats. **B. Senturk, M.O. Guler, A.B. Tekinay**

10:20 ORGN 55. Protein binding self-assembled peptide nanofibers for controlled cell fate. **M.O. Guler**

10:40 ORGN 56. Complex nanoscale shapes created with chirality-assisted synthesis. **S.T. Schneebeli, X. Liu, K.E. Murphy, J.P. Campbell, Z.J. Weinert**

Advances in Oligonucleotide Therapeutics

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SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center Ballroom East

JOC/OL Lectureship Symposium

C. D. Poulter, A. B. Smith, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 57. Free radical approaches to complex molecule synthesis. **C. Stephenson**

1:35 ORGN 58. Synthetic versatility of N-O bond rearrangements. **L.L. Anderson**

2:05 ORGN 59. Toward stereoselective cross-coupling with chiral alkyl nucleophiles. **M.K. Brown**

2:35 ORGN 60. New avenues in synthesis via organic photoredox catalysis. **D.A. Nicewicz**

3:05 *The Journal of Organic Chemistry* Award Presentation.

3:15 ORGN 61. Analog-oriented synthesis of bioactive natural products. **C.D. Vanderwal**

4:00 *Organic Letters* Award Presentation.

4:10 ORGN 62. New strategies and tactics for efficient and divergent synthesis of bioactive alkaloids and macrolides. **M. Dai**

Section B

Boston Convention & Exhibition Center Room 205B/C

Small Splash, Big Waves: Research at Primarily Undergraduate Institutions

S. M. Biros, *Organizer*

T. A. Davis, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 63. Toward a better understanding of liver alcohol dehydrogenase: Synthesis, characterization, and activity of zinc(II) model complexes based on bis-triazole and bis-imidazole precursors and water-soluble functionalities. **J.R. Miecznikowski, M.A. Lynn, W. Lo, J.P. Jasinski, S.S. Jain**

1:25 ORGN 64. Polyphenols for antioxidant delivery. **S.L. Goh, T.A. Brenner, D.M. Barber, L. Qiao**

1:45 ORGN 65. Form and function: Foldamers for catalysis and biochemical inquiry. **B.C. Gorske**

2:05 ORGN 66. Rationale modification of macromolecular scaffolds to mediate water purification. **A.M. Balija**

2:25 ORGN 67. Synthesis, switching, and supramolecular chemistry of a calixarene-capped azobenzene: A tale of undergraduate persistence. **P.A. Bonvallet**

2:45 Intermission.

3:05 ORGN 68. Calcium catalyzed addition reactions. **K.A. Nolin**

3:25 ORGN 69. Acetylene-activated S_NAr /intramolecular cascade sequence for the synthesis of indoles, benzofurans, and related heterocycles in water or DMSO. **R. Hudson, N. Bizier, K.N. Esdale, J.L. Katz**

3:45 ORGN 70. Direct, early stage guanidinylation as an enabling strategy for the total synthesis of bioactive marine natural products. **S. Chamberland**

4:05 ORGN 71. Adventures with the natural product montamine: Synthetic efforts and structural insights. **E.A. Colby Davie**

Section C

Boston Convention & Exhibition Center Room 203

Peptides, Proteins, and Amino Acids

M. C. McIntosh, *Organizer*

A. Kreutzer, *Presiding*

1:00 ORGN 72. Assessment of protein structure and stability at high cby a single platform combining Raman spectroscopy and dynamic light scattering. **W. Qi, S. Blake, S. Amin, N. Lewis**

1:20 ORGN 73. X-ray crystallographic structures of amyloid oligomers: A toxic crosslinked trimer of β -hairpins derived from $A\beta_{17-36}$. **A. Kreutzer, R.K. Spencer, J.S. Nowick**

1:40 ORGN 74. X-ray crystallographic structures of amyloid oligomers: A dodecamer of $A\beta_{17-36}$ that forms an annular pore. **A. Kreutzer, J.S. Nowick**

2:00 ORGN 75. Membrane anchored ligands for modulation of GPCR activity. **V.S. Raman, J. Doyle, B. Harwood, A. Kopin, K. Kumar**

2:20 ORGN 76. Synthesis of trimeric coiled coils presenting lactose as glycoclusters. **S. Sweeney, G.A. Bullen, M.R. Berwick, R.B. Gillis, A.J. Rowe, G.G. Adams, A.F. Peacock, P.V. Murphy**

2:40 ORGN 77. Discovery of D-peptide antibiotics using mirror-image phage display. **E. Adaligil, K. Kumar**

3:00 ORGN 78. Using peptide substrates and inhibitors to study the biological role of immunoglobulin-A1 proteases (IgA1Ps). **S.K. Choudary, F. LaGreca, E.Z. Eisenmesser, A.V. Kane, G.M. Knudsen, C.S. Craik, J. Kritzer**

3:20 ORGN 79. Expanding the substrate scope of sortase-catalyzed ligations using sortase homologs. **K. Nigkhalb, P.A. Filipov, T. Roark, J. Antos**

3:40 ORGN 80. Targeting bacteria via iminoboronate chemistry of amine-presenting lipids. **A. Bandyopadhyay**

4:00 ORGN 81. LoopFinder: A computational tool identifying loops at protein interfaces for the design of macrocyclic peptides that inhibit PPIs. **T. Siegert, M. Bird, B. Sheneman, J. Gavenonis, J. Kritzer**

4:20 ORGN 82. Single stereodynamic center modulates the rate of self-assembly in a biomolecular system. **Y. Zhang**

Section D

Boston Convention & Exhibition Center Room 204A

Nanomaterials

M. C. McIntosh, *Organizer*

R. N. Grass, *Presiding*

1:00 ORGN 83. Metal nanoparticles supported on carbon-coated magnetic nanobeads for catalysis. **F. Besostri, Q.M. Kainz, R. Linhardt, O. Reiser**

1:20 ORGN 84. Magnetic superbasic proton sponges are readily removed and permit direct product isolation. **E.M. Schneider, C. Hofer, M. Zeltner, R.N. Grass, W.J. Stark**

1:40 ORGN 85. Efficient large scale recycling of highly magnetic enzymes. **V. Zlateski, R. Fuhrer, F. Kohler, M. Zeltner, W.J. Stark, R.N. Grass**

2:00 ORGN 86. Biodiesel production using magnetic-lipase. **S. Fernandes, O. Reiser**

2:20 ORGN 87. Asymmetric transfer hydrogenation with chiral 1,2-diamines immobilized on magnetic nanoparticles. **C.M. Eichenseer, M.A. Pericas, R.N. Grass, O. Reiser**

2:40 ORGN 88. Investigation of PEI-coated magnetic nanoparticles and their potential in nanomagnetic transfection using dynamic magnetic systems. **K.K. Narayanasamy**

3:00 ORGN 89. Cyclic RGD peptidomimetics and magnetic nanoparticles conjugates as potential hyperthermia agents. **S. Panzeri, S. Fernandes, U. Piarulli, O. Reiser**

3:20 ORGN 90. Immobilization of MacMillan organocatalysts onto polymers and magnetic nanoparticles: Applications in Friedel-Craft alkylation. **S. Ranjbar, P. Riente, C. Rodriguez-Esrich, J. Yadav, M.A. Pericas**

3:40 ORGN 91. Hybrid magnetic materials (polysaccharide@Fe₃O₄ NPs) used for catalytic applications. **C. Mak, S. Ranjbar, P. Riente, C. Rodriguez-Esrich, M.A. Pericas**

4:00 ORGN 92. Microwave-assisted synthesis of magnetically recoverable silver-iron oxide supported on carboxymethyl cellulose (Ag-Fe₃O₄@CMC) nanoparticle catalysts for carbonyl compounds hydrogenation. **A. Li, M. Kaushik, A.H. Moores, C. Li**

Section E

Boston Convention & Exhibition Center Room 204B

New Reactions and Methodology

M. C. McIntosh, *Organizer*

J. A. Prieto, *Presiding*

1:00 ORGN 93. Oxidopyriliium cycloaddition/ring-opening strategy for the synthesis of 3,7-dihydroxytropolones. **D. Hirsch, R.P. Murelli**

1:20 ORGN 94. Systematic evaluation of the steric and electronic drivers governing the catalytic performance of aryl iodo catalysts for the α -oxytosylation of ketones and the oxidative lactonization of δ -keto-carboxylic acids. **D.C. Whitehead**

1:40 ORGN 95. Accessing molecularly complex azaborines: Transition-metal catalyzed reactions of 2,1-borazaronaphthalenes. **S.R. Wisniewski, J. Amani, K.M. Traister, E. Etemadi-Davan, G.A. Molander**

2:00 ORGN 96. Divergent synthesis of the acid and alcohol polypropionate subunits of dolabriferol from a common epoxide precursor. **J.A. Prieto, K. Morales**

2:20 ORGN 97. Synthesis of boryl arylene precursors via catalytic C-H activation and their orthogonal derivatization. **E. Demony, K. Devaraj, A. Orthaber, P. Gates, L.T. Pilarski**

2:40 ORGN 98. Hydridophosphoranes as intermediates in P(III)/P(V) redox catalysis. **N. Dunn, A.T. Radosevich**

3:00 ORGN 99. Amide and amine nucleophiles in polar radical crossover cycloadditions: Synthesis of γ -lactams and pyrrolidines. **N. Gesmundo, J. Grandjean, D.A. Nicewicz**

3:20 ORGN 100. Enantioselective rhodium-catalyzed allylic substitution with a nitrile anion: Construction of acyclic quaternary carbon stereogenic centers. **B.W. Turnbull, P. Evans**

3:40 ORGN 101. Ammonium-catalyzed alkyne additions: A unified method for the synthesis of isoxazolidines and pyrazolidines. **E. Nagy, S.D. Lepore**

4:00 ORGN 102. Reductive coupling of internal alkynes bearing arylacetamide: Stereoselective synthesis of functionalized E,E-dienes and total synthesis of NFAT-68. **B. Cai, R. Evans, J. Wu**

4:20 ORGN 103. Efficient access to conjugated bipyridinium containing macrocycles and oligomers using the Zincke reaction: Synthesis, spectroscopic, and electrochemical properties. **B. Greenland, L. Chen, H. Colquhoun**

4:40 ORGN 104. Metal-free Lewis acid mediated dehydrocoupling of phosphines and concurrent hydrogenation. **R. Dobrovetsky, K. Takeuchi, D.W. Stephan**

Section F

Boston Convention & Exhibition Center Room 206A

Asymmetric Reactions and Syntheses

M. C. McIntosh, *Organizer*

M. Eno, *Presiding*

1:00 ORGN 105. Organocatalytic asymmetric [2,3]-rearrangement of allylic ammonium ylides. **T. West, A.D. Smith, D.S. Daniels, D.M. Walden, P. Cheong, R.C. Johnston**

1:20 ORGN 106. Withdrawn.

1:40 ORGN 107. Synthesis and application of two novel BiFOX ligands and the Sml₂ mediated stereoselective cross-coupling and desulfonation reaction. **P. Janssens, T. Noël, J. Goeman, J. Van Der Eycken**

2:00 ORGN 108. Cinchona alkaloid-catalyzed formal [4+2] cycloaddition of allenates and α,β -unsaturated trifluoromethylketones. **K. Kasten, A.D. Smith**

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- 2:20 ORGN 109.** Asymmetric petasis alkylation catalyzed by chiral diols. **Y. Jiang, S. Schaus**
- 2:40 ORGN 110.** Enantioselective synthesis of spirocyclic ethers via copper (II)-catalyzed carboetherification of 1, 1-disubstituted alkenes. **S.D. Karyakarte, S.R. Chemler**
- 3:00 ORGN 111.** Dynamic kinetic resolutions of stereolabile carbonyl compounds. **G. Goodman**
- 3:20 ORGN 112.** Enantioselective synthesis of γ -amino acid derivatives via iridium catalyzed activation of sp^3 C-H bond. **Y. Tahara, M. Michino, M. Ito, T. Shibata**
- 3:40 ORGN 113.** Desymmetrization of cyclic sulfates via enantioselective Ni-catalyzed Kumada coupling. **M. Eno, A. Annis, J.P. Morken**
- 4:00 ORGN 114.** Recyclable organocatalysis for asymmetric synthesis of organofluorine compounds. **X. Huang**
- 4:20 ORGN 115.** Anionic phospho-Fries rearrangement: A new approach to 1,2-*P,O*-substituted ferrocenes. **M. Korb, H. Lang**
- 4:40 ORGN 116.** Total synthesis of δ -lactone of tetrahydroxyhexacos-2-enoic acid and its analogs: Diastereo-divergent asymmetric synthesis to *syn*-1,3-polyol. **J. Zheng, G.A. O'Doherty**

Section G

Boston Convention & Exhibition Center
Room 206B

Molecular Recognition and Self-Assembly

M. C. McIntosh, *Organizer*
S. Blake, *Presiding*

- 1:00 ORGN 117.** Structure activity studies on a 4-component assembly for HTS of chiral alcohol ee values. **C. Lin, E.V. Anslyn**
- 1:20 ORGN 118.** Supramolecular polymers as high performance binders for silicon anodes in lithium ion batteries. **A. Coskun**
- 1:40 ORGN 119.** Self-assembly of cationic multidomain peptide hydrogels: Supramolecular nanostructure and rheological property dictate antimicrobial activity. **L. Jiang, D. Xu, H. Dong**
- 2:00 ORGN 120.** Allosteric threading of polymer chains through macrocyclic complexes: Toward a molecular Turing machine. **J.A. Elemans, S. Cantekin, A. Deutman, K. Stout, A.E. Rowan, R. Nolte**
- 2:20 ORGN 121.** Revealing self-assembly processes that underlie fibrillation of b-lactoglobulin through dynamic light scattering, Raman spectroscopy, and optical microrheology. **S. Blake, S. Amin, N. Lewis, W. Qi, M. Majumdar**
- 2:40 ORGN 122.** Investigation of the driving forces for supramolecular interactions leading to ground state charge transfer in transient organic mixed-valence systems. **A.M. Bischof, B.J. Lear**

Technical program information known at press time. The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

- 3:00 ORGN 123.** Solid-state reactivity and new salt forms involving the conformationally flexible pharmaceutical ingredient cimetidine. **G. Ayoub, C. Mottillo, V. Štrukil, T. Friscic**
- 3:20 ORGN 124.** Organocatalytic functionalization of self-assembled monolayers on SiO₂. **R. Chisholm, J.D. Parkin, G. Haehner, A.D. Smith**
- 3:40 ORGN 125.** Assembly of amphiphilic baskets with singular and dual cavities. **S. Chen, Y. Ruan, M. Yamasaki, J.D. Badjić**
- 4:00 ORGN 126.** Click-fluors: Synthesis of fluorescent saccharide sensors via a copper-catalyzed azide-alkyne cycloaddition reaction. **W. Zhai, L. Male, J.S. Fossey**

Advances in Oligonucleotide Therapeutics

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SUNDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Asymmetric Reactions and Syntheses; Chemistry of Fullerenes, Carbon Nanotubes, and Graphene; Materials, Devices and Switches; Nanomaterials; Physical Organic

R. D. Broene, *Organizer*

8:00 - 10:00

- ORGN 127.** Recyclable, supported, and homogeneous Noyori-Ikariya catalyst for asymmetric transfer hydrogenation in water. **M. Dauphinais, A.B. Charette, J. Zimbron**
- ORGN 128.** Hydrogen bond mediated enantioselective organic transformations by bifunctional Werner complexes. **S.K. Ghosh, J.A. Gladysz**
- ORGN 129.** Asymmetric synthesis of α -heteroatom-substituted β -keto esters via S_N2 substitution of tertiary chlorides. **K. Shibatomi, M. Kotozaki, N. Sasaki, S. Iwasa**
- ORGN 130.** Organocatalyzed enantioselective conjugate addition of heteroaryl and aryl trifluoroborates: A synthetic strategy for discolorpore D. **J. Shih, T.S. Nguyen, J. May**
- ORGN 131.** Exploration of the catalysis of homoallylboration using chiral and achiral carboxylates and related structures. **A. Klein, S. Popov, G. Dugas, H. Lin, I.J. Krauss**
- ORGN 132.** Copper-catalyzed enantioselective addition of silicon nucleophiles to aldimines using new planar chiral [2.2]paracyclophane-based triazolium carbene precursors. **Y. Ma, Z. Chen, C. Song**
- ORGN 133.** Enantioselective β -boration of α,β -unsaturated esters by fluorine substituted [2.2]paracyclophane-based catalyst. **Y. Ma, J. Chen, C. Song**
- ORGN 134.** Synthesis of optically active β - or γ -alkyl substituted alcohols through copper-catalyzed asymmetric allylic alkylation with organolithium reagents. **S. Guduguntla**
- ORGN 135.** Enantioselectivity switch in the copper(I)-catalyzed boron additions. **H. Lee, J. Yun**
- ORGN 136.** One-pot synthesis of 3,5-disubstituted and polysubstituted phenols from acyclic precursors. **J. Qian, W. Yi, X. Huang, W. Zhang**
- ORGN 137.** Novel convergent total synthesis of biologically active sulfur-containing curvularin derivatives from the fungus *Penicillium sumatrense* MA-92. **L. Eliopoulos**
- ORGN 138.** Formation of acyclic quaternary carbon center by enantioselective α -allylation of branched aldehydes with allylic alcohols via dual boronic acid and chiral amine catalysis. **X. Mo, D.G. Hall**
- ORGN 139.** Novel iron catalysts for biomimetic asymmetric epoxidations. **D. Gaona, F.G. Gelalcha, C. Hahn**
- ORGN 140.** Molecular-motor-based switchable phosphorus ligand for Pd-catalyzed allylic substitution. **W. Chen, B. Feringa**
- ORGN 141.** Asymmetric catalysis: From traditional static ligand to dynamic smart ligand. **D. Zhao, B. Feringa**
- ORGN 142.** Trapping of Payne rearrangement intermediates with arylselenide anions. **D. Sun**
- ORGN 143.** Total synthesis of (+)-Negamycin. **R.W. Bates, N.R. Khanizeman**
- ORGN 144.** Concise synthesis of (-)-protoematinol. **J. Hur, T. Kim, H. Moon, H. An, J. Sim, K. Kim, Y. Suh**
- ORGN 145.** Synthesis of nonracemic β -azido and β -amino alcohols via a highly regio- and stereoselective ring opening of optically pure epoxides by sodium azide in hot water. **M. De Jesus, H. Wang, K. Huang, S. Espinosa-Diaz, R. Quinones, L.E. Pinero-Santiago, C. Garcia, M. Ortiz-Marciales**
- ORGN 146.** Continuous flow microfluidic chemistry: Synthesis of [F-18] fluoro analogues of aniracetam as brain imaging agents. **M.R. Akula, D. Blevins, G.W. Kabalka, D. Osborne**
- ORGN 147.** Withdrawn.
- ORGN 148.** Large scale and flow processes for the synthesis of *N*-mesyloxy carbamate: Application to the synthesis of trichloromethylcarbinols. **J. Bartholomeus, H. Piras, S. Blais, H. Lebel**
- ORGN 149.** Microwave heated flow synthesis of angiotensin II type 2 receptor (AT2R) ligands. **R. Isaksson, J. Wannberg, J. Sävmarker, M. Hallberg, M. Larhed**
- ORGN 150.** Fullerene-Starphene chemistry: Syntheses of tris[60] fullerene adducts of [4,4,4]tridecastarphenes. **H. Geng, G.P. Miller**
- ORGN 151.** Synthesis of a C₃ symmetric cyclooligo(3,3'-*para*-terphenylene ethynylene) as a precursor of a [9,9] armchair carbon nanobelt. **T.A. Dietsche, W.S. Jjaz, S.P. Singh, T.S. Hughes**
- ORGN 152.** Nano CuO/ZnO as a new catalyst for the one-pot, three component synthesis of heterocyclic α -amino-phosphonates. **S. Hosseini-Sarvari**
- ORGN 153.** Enzymatic transformation of phosphate decorated magnetic nanoparticles for selectively sorting and inhibiting cancer cells. **X. Du, J. Zhou, B. Xu**
- ORGN 154.** Nanoparticles for antimicrobial and antibiofilm applications. **A. Gupta, X. Li, T. Mizuhara, R. Das, G. Tonga**
- ORGN 155.** Direct functionalization of nanodiamonds with maleimide. **O. El Tall, Y. Hou, E. Abou-Hamad, I. U. Raja, M. N. Hedhili, W. Peng, R. Mahfouz, O. Bakr, P. Beaujuge**

- ORGN 156.** Nanoparticles at the interface of chemistry and biology, what chemists can do is not necessarily what biologists need, or how cross-discipline ignorance can hinder scientific progress in academic research: A biologist's view. **E.M. Luther**
- ORGN 157.** Nanofibrous hydrogel self-assembled from naphthalenediimide-peptide amphiphile as a potential imaging agent. **Z. Hu, J. Zhao, Z. Song**
- ORGN 158.** Spray sonocrystallization for preparation of nanoparticles of pharmaceutical agents. **H. Kim, J.R. Sander, B.W. Zeiger, K. Suslick**
- ORGN 159.** Supramolecular regulation of bioorthogonal catalysis in cells using nanoparticle-embedded transition metal catalysts. **R. Das, G. Tonga, Y. Jeong, B. Duncan, T. Mizuhara, R. Mout, S.T. Kim, Y. Yeh, B. Yan, S. Hou, V.M. Rotello**
- ORGN 160.** Combinatorial protein films fabricated via inkjet printing and nanoimprint lithography. **B. Duncan, L. Wang, R. Tang, B. Creran, J. Doble, M. Fessenden, V.M. Rotello**
- ORGN 161.** Fluororous liquid-soluble quantum-dots for the construction of solution-processed light emitting diode. **S. Jung, Y. Kim, J. Son, J. Lee**
- ORGN 162.** Preparation of cationic polymer-grafted magnetic nanoparticles and their applications. **M. Takafuji, Z. Xu, H. Ihara**
- ORGN 163.** Magnetic calcium phosphate nanoparticles for targeted gene delivery. **M. Puddu, N. Broguiere, D. Mohn, M. Zenobi-Wong, W.J. Stark, R.N. Grass**
- ORGN 164.** Programmed photodegradation of polymer/oligomer derived from sustainable resources: A mechanistic perspective. **R. Raghunathan, R. Krishnan, S. Rajendran, M.P. Sibi, D.C. Webster, S. Jayaraman**
- ORGN 165.** Excited state photochemistry of 2-(azidomethyl)benzophenone via enol intermediates. **K.R. Thenna Hewa, S. Muthukrishnan, A.D. Gudmundsdottir**
- ORGN 166.** Photochemical study of 1,4 substituted 1,2,3-triazole. **D.M. Sriyarthne, A.D. Gudmundsdottir**
- ORGN 167.** Computational investigation of lactam vs. lactone annulation of benzoxazoles and benzothiazoles: Origins of entantio- and regiocontrol and the dramatic effect of the S/O interaction on transition state structures. **D.M. Walden, E.R. Robinson, C. Fallon, A.D. Smith, P. Cheong**
- ORGN 168.** Synthetic and enzymatic oxidation of oxepins: An investigation into the mechanism of benzene metabolism. **H. Guevara, A. Greenberg**
- ORGN 169.** Study of triplet-excited state intramolecular proton transfer of aromatic Schiff bases using transient spectroscopy and DFT calculations. **G.K. Weragoda, A.D. Gudmundsdottir**
- ORGN 170.** Singlet oxygen generation on superhydrophobic surfaces: Effect of convection on trapping efficiency. **Y. Liu, Y. Zhao, Q. Xu, A. Greer, A. Lyons**
- ORGN 171.** Synthesis and antiproliferative activity of poly(ethylene glycol) and ceramide conjugated benzopolyulfanes that resemble tunicate-derived natural products. **A. Mahendran, A.A. Ghogare, E. Greer, Y. Gong, R. Bittman, G. Arthur, A. Greer**
- ORGN 172.** Cyclodextrin-mediated supramolecular catalysis of organic reactions under mild reaction conditions. **S. Chaudhuri**
- ORGN 173.** High resolution mass spectrometry CID study of thiophene octacyclol derivatives. **K.J. Kolonko, J. Hebert**

ORGN 174. Electronic structures of $\text{Ph(R}^1\text{)C=N-CH=C(X)}_2$ 2-azabuta-1,3-dienes ($\text{R}^1 = \text{Ph, CN; X = Cl, SR}$). **M.M. Kubicki, A. Khatyr, M. Knorr**

ORGN 175. Photoacoustic Z-scan studies of commercial dyes. **E. Ahmad, S. Bellinger-Buckley, M. Hatami, C. Yelleswarapu, J.J. Rochford**

ORGN 176. Understanding reactivity and selectivity in inverse electron demand Diels-Alder reactions of 1,2,3-triazine derivatives. **R. Maji, S.E. Wheeler**

ORGN 177. Where is the lone pair? Resonance in the sila-allyl anion. **E. Gulotty, W.R. Winchester**

ORGN 178. Mechanism of carbocycles formation by intramolecular conjugate displacement. **G. Jimenez-Oses, D.L. Olive, K.N. Houk**

ORGN 179. Mechanistic study of Rh and Pd catalyzed alkoxyacylation/alkoxyacyanation reactions. **M. Alghamdi, L. Cavallo**

ORGN 180. Probing the formose reaction with hydroxycarbenes as key intermediates. **M.M. Linden, P.R. Schreiner**

ORGN 181. Photophysical and electrochemical properties of asymmetric coumarin-1,3-diketonate curcuminoid dyes. **S. Bellinger Buckley, E. Ahmad, M. Lamberto, J.J. Rochford**

ORGN 182. Withdrawn.

ORGN 183. Theoretical studies on conformation of symmetric diesters. **S. Niwayama, M. Kato, Y. Yamaguchi, H. Cho**

ORGN 184. Solid and solution state characterization of lithium enolates of amides. **C. Liu, P.G. Williard**

ORGN 185. Approaches to new solid state reactions. **T. Harrison, A. Oakley, S. Thota, T. Carter, J. Xu, D.J. Sandman**

ORGN 186. Synthesis and electrochemical characterization of stable organic radicals derived from singlet carbenes. **C.L. Deardorff, T.W. Hudnall**

ORGN 187. Photophysical and electronic investigations of a donor-p-acceptor type 1,3-diketonate chromophore toward photoacoustic imaging applications. **Y.S. Bouyou**

ORGN 188. Mechanistic studies of a novel low-temperature cycloaromatization of o-benzoyl enediyne. **K.L. Gillespie, T.S. Hughes**

ORGN 189. Alkyl-functionalized dibenzophthalenes board-shaped thermotropic liquid crystals. **P. Repasky, S. Hartley**

ORGN 190. Origin of aggregation induced emission in BF_2 -hydrazones (BODIHYs) — a novel class of fluorescent molecular rotors. **H. Qian, E.H. Horak, A. Wakefield, M.D. Liptak, I. Aprahamian**

ORGN 191. Synthesis of cross-linked molecular rotors in pursuit of fast rotational dynamics in the solid state. **M. Howe, P. Commins, M.A. Garcia-Garibay**

ORGN 192. Near IR activated Azo- BF_2 switches. **C. Gill, I. Aprahamian**

ORGN 193. Self-assembly and aggregation behavior of discrete, hexagonal boronate ester macrocycles resembling COF-5. **A. Chavez, B.J. Smith, M. Smith, B.H. Northrop, W. Dichtel**

ORGN 194. Chiral vicinal di-amides fitted with photo-responsive azobenzene groups: A new family of light-regulated chiroptical switching elements. **G.D. Jaycox**

ORGN 195. Progress toward the total synthesis of psigualid B. **L.M. Chapman, S.E. Reisman**

ORGN 196. Cyclic L-tryptophan-based building blocks for the synthesis of medically relevant complex molecules. **J. Cubello, L. Sanchez, S. Scharmach**

ORGN 197. Progress toward an affordable synthetic route to aurantioclavine. **Z.D. Mariani, L. Sanchez**

ORGN 198. Total synthesis of biologically active diterpenoids. **P. Riehl, C. Schindler**

ORGN 199. BACE inhibitors: Construction of prime-side heterocycles from a late-stage aldehyde intermediate. **J. Dutra, J.C. Murray, L.A. Martinez-Alsina, K. Ogilvie, L.M. Buzon, K.E. Henegar, B.T. Oneill**

ORGN 200. BACE inhibitors: Thioamidinone core ring syntheses. **K. Ogilvie, J. Dutra, J.C. Murray, L.A. Martinez-Alsina, L.M. Buzon, M.W. Bundesmann, K.E. Henegar, D.B. Damon, B.T. Oneill**

ORGN 201. BACE inhibitors: Construction of prime-side heterocycles from a late-stage carboxylic acid intermediate. **P.J. Mikochik, L.M. Buzon, J. Dutra, L.A. Martinez-Alsina, J.C. Murray, K. Ogilvie, K.E. Henegar, B.T. Oneill**

ORGN 202. Progress toward total synthesis of albocycline. **V.K. Chatare, R.B. Andrade**

ORGN 203. Concise and efficient total synthesis of dehaloperophoramidate: A stereodivergent approach. **K. Popov, A. Hoang, P. Somfai**

ORGN 204. Syntheses of bioactive decalinoyl tetramic acids. **M. Winterer, K. Kempf, M. Ullmann, R. Schobert**

ORGN 205. Total synthesis and determination of absolute stereochemistry of hortonone C. **R. Tello-Aburto, D. Niroula, P. Trujillo**

ORGN 206. Studies toward the total synthesis of Trigonoinone B. **F. Damkaci, N. Boke Sarikahya**

ORGN 207. Enantioselective synthesis of anticancer natural product Actinopolymorphol B and analogs. **C.C. Kim, J. Lee, B. Catano, Y. Xing**

ORGN 208. Toward the rapid synthesis of brevenal core structure via diastereoselective oxacyclizations of linear polyenes. **J.A. Hurtak, K. Stoltz, X. Lu, F.E. McDonald**

ORGN 209. Concise and scalable strategy for the total synthesis of dictyodendrin B based on sequential C-H functionalization. **A.K. Pitts, F. O'Hara, R.H. Snell, M. Gaunt**

ORGN 210. Synthesis of alkaloids with the potential to inhibit NF- κ B via a reductive aldol methodology. **Y.C. DePorre, C. Schindler**

ORGN 211. Progress toward the total synthesis of (2S)-hydroxy-3,4-dehydronemajucin via titanium metallacycle-mediated annulation. **X. Cheng, G.C. Micalizio**

ORGN 212. Synthetic strategy to access potential modulators of the transcription factor NF- κ B. **A.M. Amaly, S. Bar, C. Schindler**

ORGN 213. Efficient synthesis of the EF-fragment of Spongistatin 1 and analogs thereof. **J. Infantine, K.S. Williamson, J.L. Leighton**

ORGN 214. Synthesis of common macrocyclic intermediate for the divergent synthesis of divergolides and hygrocin. **S. Rasapalli, U. Javed, G. Jarugumilli, A. Fantan**

ORGN 215. Synthesis of (-)-mandelalide A southern hemisphere employing anion relay chemistry tactic and analog development. **M. Imanishi, M.H. Nguyen, T. Kurogi, A.B. Smith**

ORGN 216. General synthetic strategy toward eight-membered heterocyclic natural products. **A.N. Golonka, C. Schindler**

ORGN 217. Selective alkylation of intermediates for preparation of Pawhuskin analogs. **K.D. Gardner, D.F. Wiemer**

ORGN 218. Sequential Sonagashira and Larock indole synthesis reactions in a general strategy to prepare biologically active β -carboline-containing alkaloids. **X. Pan, T.D. Bannister**

ORGN 219. Preclinical synthetic routes to the dual Bcl2/Bcl-x l inhibitor AZD4320 and related prodrugs and analogs. **J.G. Varnes, T.W. Gero, R.B. Diebold, S.C. Glossop, P. Grover, S. Huang, C. Ogoe, M. Su, S. Ioannidis**

ORGN 220. Total synthesis of sphingoid bases. **Y. Dai**

ORGN 221. Biogenetically inspired synthesis and skeletal diversification of indole alkaloids. **H. Mizoguchi, H. Oikawa, H. Oguri**

ORGN 222. Total synthesis of caduomycin. **Z. Ruan, Q. Xiao**

MONDAY MORNING

Section A

Boston Convention & Exhibition Center Ballroom East

Teva Pharmaceuticals Scholars Grant Symposium

N. Jensen, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 **ORGN 223.** Studies in terpene synthesis. **P.S. Baran**

9:10 Reception.

9:40 **ORGN 224.** Synthetic lectin (SL) arrays to target tumor associated carbohydrate antigens (TACAs) for the detection and management of cancer. **J.J. Lavigne, P.M. Thompson, K.M. O'Connell, E.E. Gatrone, A.A. Veldkamp**

10:40 **ORGN 225.** Explore new molecular entities for hydrogen sulfide research. **M. Xian**

11:40 Concluding Remarks.

Section B

Boston Convention & Exhibition Center Room 205B/C

Process Chemistry: New Developments in Pharmaceutical Process Development

A. F. Abdel-Magid, J. A. Pesti, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 **ORGN 226.** Application of crystallization induced dynamic resolution (CIDR) for the preparation of drug candidates for the treatment of HCV. **L. Anzalone, Y. Jung, C. Blich, T. Martinot, C. Harrison, M.E. Kubryk, S. Ibrahim, T. Curran**

9:10 **ORGN 227.** Chemistry of cyclosporins — the importance of crystalline intermediates. **F. Gallou**

9:50 **ORGN 228.** Process development of pyridine containing drug candidates. **J.R. Rizzo, T. Zhang**

10:30 **ORGN 229.** Pilot plant production of a P2Y $_{12}$ -antagonist containing (R)-3-phosphonoalanine. **S. Abele**

11:10 **ORGN 230.** Process development for the scale-up of a pre-clinical candidate. **S.J. Bader**

Section C

Boston Convention & Exhibition Center Room 203

Young Investigator Symposium

S. Dreher, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 **ORGN 231.** Total synthesis of 6-deoxypladienolide D and assessment of splicing inhibitory activity in a mutant SF3B1 cancer cell line. **K. Arai, S. Buonamici, B. Chan, L. Corson, A. Endo, B. Gerard, M. Hao, C. Karr, K. Kira, L. Lee, X. Liu, J.T. Lowe, T. Luo, L.A. Marcaurrelle, Y. Mizui, M. Nevalainen, M.W. O'Shea, E. Park, S. Perino, S. Prajapati, M. Shan, P.G. Smith, P. Tivitmahaisoon, Y. Wang, M. Warmuth, K. Wu, L. Yu, H. Zhang, G. Zheng, G. Kearney**

9:00 **ORGN 232.** Development and implementation of innovative high-throughput screening and analysis solutions to support discovery and development of active pharmaceutical ingredients in the pharmaceutical industry. **R.M. Helmy**

9:25 **ORGN 233.** Organic acid applications within the cosmetic industry "chemical peels". **P.M. Brieve**

9:50 **ORGN 234.** Structure-guided design and optimization of fluoroquinolone-substituted bacterial type IIA DNA topoisomerase inhibitors. **R.K. Thalji**

10:15 **ORGN 235.** Application of synthetic organic chemistry in the design of cationic initiators for next generation photoresists. **P.J. LaBeaume, J.F. Cameron, J.W. Thackeray, A.A. Rachford, S. Coley, J. Vipul, A. Kwok, D. Valeri, M. Wagner, O. Ongayi**

10:40 **ORGN 236.** Continuous processing: Chemical route development and GMP implementation. **K.P. Cole**

11:05 **ORGN 237.** DNA-programmed chemistry toward macrocycle libraries for drug discovery. **T.F. Briggs**

11:30 **ORGN 238.** Cobalt catalyzed reductive carbonylation of methanol. **A.J. Vetter, J. Penney, D.W. Norman**

Section D

Boston Convention & Exhibition Center Room 204A

Magnetically Recyclable Nanocatalysts

M. A. Pericas, O. Reiser, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **ORGN 239.** Development of magnetic-core @ catalytic - shell nanostructures. **D. Ma**

8:30 **ORGN 240.** Magnetically recoverable fibrous nanosilica (mKCC-1). **V. Polshettiwar, A. Raghavan, B. Singh**

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8:55 ORGN 241. Colloidal and immobilized iron oxide nanocrystals as efficient and selective catalysts for the reduction of nitroarenes in batch and continuous flow mode. D. Cantillo, M. Bagbanzadeh, C. Kappe

9:20 ORGN 242. Sustainable chemistry using magnetically retrievable nanocatalysts. R.S. Varma

9:45 ORGN 243. Magnetic zeolites: Does iron oxide matter? C.M. Leonard, J. Mann, Z. Shifrina, A.I. Sidorov, V.Y. Doluda, E.M. Sulman, E. Rebrow, L. Bronstein

10:10 ORGN 244. Size control in the synthesis of magnetic nanoparticle catalysts. D. Huber, G.C. Bleier, E.C. Vreeland, J. Watt

10:35 ORGN 245. Reduced iron nanoparticles as magnetically retrievable catalysts for alkenes hydrogenation and as galvanic reducers to access Cu and Ru-based catalysts for azide-alkyne condensation and transfer hydrogenation. A.H. Moore, R. Hudson, M. Masnadi, M. Bateman, C. Li

11:00 ORGN 246. Mag(net)ic catalysts: Synthesis and application. O. Reiser

11:25 Concluding Remarks.

Section E

Boston Convention & Exhibition Center
Room 204B

New Reactions and Methodology

M. C. McIntosh, *Organizer*

D. Bandyopadhyay, *Presiding*

8:00 ORGN 247. Condensation vs. hydroamination for one-step access to tetrasubstituted carbons bearing amines. C.H. Larsen, C. Pierce, M. Nguyen, Z. Palchak, H. Yoo, D. Lussier

8:20 ORGN 248. Solution structural and mechanistic studies of sodium diisopropylamide (NaDA): Selective elimination of alkyl bromides and epoxides, and sodiation of arenes and imines. Y. Ma, R.F. Algera, D.B. Collum

8:40 ORGN 249. Phosphatene-catalyzed regioselective reductive transposition of allylic bromides. K.D. Reichl, A.T. Radosevich

9:00 ORGN 250. Nitro compounds as organocatalysts: Rapid azidation of tertiary aliphatic alcohols. M. Dryzhakov, M. Hellal, E. Wolf, J. Moran

9:20 ORGN 251. Mild and atom-economic Friedel-Crafts benzylation of arenes by direct activation of benzylic alcohols using a ferrocenium boronic acid catalyst. D.G. Hall, X. Mo, J. Yakiwchuk, J. Dansereau, A. McCubbin

9:40 ORGN 252. Organocatalytic methods for aliphatic C–H oxidation. M.K. Hilinski, C. Pierce

10:00 ORGN 253. Design, synthesis, and anticancer assessment of 1,4-dia-ryl-3-(1*H*-pyrrol-1-yl)azetid-2-ones. J. Cruz, D. Bandyopadhyay, B.K. Banik

10:20 ORGN 254. Design, synthesis, and antitubercular evaluation of diversely substituted quinoxalines. O. Espino, F. Olazarán-Santibañez, S. Mukherjee, I. Balderas-Rentería, J. Luna-Herrera, J.M. Collin-Navarrete, R. Ruiz-Nicolás, G. Rivera, B.K. Banik, D. Bandyopadhyay

10:40 ORGN 255. New type of aza-MBH reaction and its application to highly diastereoselective one-pot syntheses of 2, 5-dihydropyrroles. M. Zhang, L. Kang, Y. Chai

11:00 ORGN 256. Nondirected, Pd catalyzed C–H aminations. M. Emmert

11:20 ORGN 257. Two novel syntheses of benzylidene hydantoin derivatives. R.M. Rajapaksha, G.B. Rowland, C.U. Pittman, T.E. Mlsna

11:40 ORGN 258. Unique reactions of the best oxygen transfer agent in organic chemistry - HOF/CH₃CN. S. Rozen

Section F

Boston Convention & Exhibition Center
Room 206A

Asymmetric Reactions and Syntheses

M. C. McIntosh, *Organizer*

A. Smith, *Presiding*

8:00 ORGN 259. Chiral DMAP derivatives utilising cation- π interactions as asymmetric nucleophilic catalysts. D.T. Payne, A.S. Deeming, L. Male, J.S. Fossey

8:20 ORGN 260. Kinetic resolution of terminal alkynes utilising triazole formations. W.D. Brittain, L. Male, B. Buckley, J.S. Fossey

8:40 ORGN 261. Origins of the stereoselectivities of type II intramolecular 5+2 cycloadditions of oxidopyridiniums. A. Patel, K.N. Houk

9:00 ORGN 262. Three-component catalytic asymmetric *trans*-aziridination. Y. Zhou

9:20 ORGN 263. Bronsted acid-catalyzed intramolecular nucleophilic substitution of the hydroxyl group in stereogenic alcohols with chirality transfer. A. Bunrit, C. Dahlstrand, S. Olsson, P. Srika, G. Huang, P. Sjöberg, S. Biswas, F. Himu, J.S. Samec

9:40 ORGN 264. Novel cyclopropanation organocatalyst and other tales: Hydrogen-bonding activation in action. A.A. Cobb

10:00 ORGN 265. Dual divergent/convergent asymmetric syntheses of γ -secretase modulator BMS-932481 featuring a *bis*-benzylic stereocenter in a cyclopentapyrimidine. J. Deeborg, O. Soltani, A. Parsons, N. Strotman, E. Simmons, Y. Fan, J. Janey, Y. Hsiao, J.R. Sawyer

10:20 ORGN 266. Development of a scalable dynamic kinetic resolution toward the synthesis of AMG 232. A. Smith, S. Caille

10:40 ORGN 267. New phosphine ligands for enantioselective hydrogenation of unfunctionalized alkenes. B. Qu

11:00 ORGN 268. Withdrawn.

11:20 ORGN 269. Preparation of enantiopure tropone derivatives by oranocatalysis. Y. Yuan

11:40 ORGN 270. Catalytic kinetic resolution of primary allylic amines via direct substitution of the amino group. S. Tian, Y. Wang

Section G

Boston Convention & Exhibition Center
Room 206B

Molecular Recognition and Self-Assembly

M. C. McIntosh, *Organizer*

S. Ganapati, *Presiding*

8:00 ORGN 271. Biofunctionalization and dynamics of supramolecular polymers. M.B. Baker, L. Albertazzi, C.M. Leenders, R.P. Gosens, I.K. Voets, G.M. Pavan, A. Palmans, E.W. Meijer

8:20 ORGN 272. Tunable morphologies of rationally designed coiled-coil based supramolecular polymers. N.A. Tavenor, K. Silva, M.J. Lawless, C.P. Parris, M.J. Murnin, S.K. Saxena, W.S. Horne

8:40 ORGN 273. Tunable solid-state fluorescent materials for supramolecular encryption. X. Hou, C. Ke, J.F. Stoddart

9:00 ORGN 274. In vitro selectivity of an acyclic cucurbit[n]uril molecular container toward neuromuscular blocking agents over some commonly used drugs. S. Ganapati, L.D. Isaacs

9:20 ORGN 275. Chiral compounds to assess substituent effects of π - π interaction. C. Yang, C. Chen, S.E. Snyder, J. Carey

9:40 ORGN 276. Aqueous assembly and ultrasensitive pH control of biomimetic supramolecular polymers and hydrogels. B. Cafferty, R. Avirah, M. Chen, I. Gállego, G.B. Schuster, N.V. Hud

10:00 ORGN 277. Self-sorting of dynamic imine libraries driven by three orthogonal stimuli. C. Hsu, O. Miljanić

10:20 ORGN 278. Photophysical properties of self-assembled supramolecular peptide nanofiber organic semiconductors. M. Khalily, H. Usta, M. Güler

10:40 ORGN 279. Weak non-covalent intermolecular interactions involving perfluoroalkyl substituents: Insights for rational design of molecular assemblies. H. Sun

Innovation in Metabolism, Bioavailability and Formulations Research Leading to the Discovery of Agrochemicals: Symposium Honoring Dr. Keith D. Wing, AGRO International Award for Research in Agrochemicals

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MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Ballroom East

Tetrahedron Prize for Creativity in Organic Chemistry Symposium

S. S. Hall, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 280. Enantioselective catalysis with cations and anions. D. Toste

2:00 ORGN 281. Alkylboron cross-coupling enabled by single electron transmetalation. G.A. Molander

2:55 ORGN 282. Hydrogen-mediated C–C bond formation: Discovery and development. M.J. Krische

3:50 Tetrahedron Prize Presentation.

4:00 ORGN 283. On the invention of Pd catalyzed allylic alkylations for enabling chemical synthesis. B.M. Trost

5:00 Concluding Remarks.

Section B

Boston Convention & Exhibition Center
Room 205B/C

Green Chemistry Makes a Difference: Pharmaceutical Industry/Academic Collaborations

Financially supported by ACS GCI Pharmaceutical Roundtable

M. E. Kopach, *Organizer, Presiding*

1:00 ORGN 284. Mechanistic approach to efficient organocatalysts. E.N. Jacobsen

1:40 ORGN 285. Green chemistry technology and culture at Amgen: Innovating for sustainability during pharmaceutical development. M. Faul, J. Tucker

2:20 Intermission.

2:40 ORGN 286. Base metal catalysis for organic synthesis. P.J. Chirik

3:20 ORGN 287. Synthetic evolution and chemical innovation: Developing an efficient synthesis of the potent JAK2 inhibitor, BMS-911543. M.D. Eastgate

4:00 ORGN 288. Synthetic fermentation of bioactive peptides in water without reagents or organisms. J.W. Bode

Section C

Boston Convention & Exhibition Center
Room 203

Young Investigator Symposium

S. Dreher, *Organizer, Presiding*

1:30 ORGN 289. Designed hybridization – acrylic-epoxy hybrid dispersions for industrial coating applications. A. Hejl

1:55 ORGN 290. Development of a commercial manufacturing process for Ibrance® (palbociclib). N.D. Ide

2:20 ORGN 291. Approaches to the heterocyclic core of Ilorasertib. J. Kallemeyn

2:45 ORGN 292. Carbonyl containing heterocycles as aromatic isosteres in 4-hydroxyphenylpyruvate dioxygenase (HPPD) herbicides. A.D. Satterfield, A. Taggi, B.T. Smith, K.A. Hughes, M. Tiscione, W. Patzoldt

3:10 ORGN 293. Discovery of adenosine analog inhibitors of S-adenosylhomocysteine hydrolyase. A. Converso, T.J. Hartingh, E. Brnardic, R. Garbaccio, M.E. Fraley

3:35 ORGN 294. Overcoming steric and electronic obstacles: Development of efficient syntheses of active pharmaceutical ingredients. K. Chen

4:00 ORGN 295. Near-IR uncaging chemistry: Discovery and applications. M.J. Schnermann, R. Nani, A.P. Gorka

4:25 ORGN 296. Chiral chemistry for API synthesis. S. Cui

4:50 Concluding Remarks.

Section D

Boston Convention & Exhibition Center
Room 204A

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*

T. W. Hudnall, *Presiding*

1:00 ORGN 297. Carbene-stabilized organic radicals with tunable electrochemical properties. T.W. Hudnall, C.L. Deardorff, R.E. Sikma, M.B. Gildner

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

- 1:20 ORGN 298.** Excited state expulsion of N₂ to achieve efficient release of alcohol by photolactonization. **K.R. Thenna Hewa, A.D. Gudmundsdottir, S. Muthukrishnan, D.L. Phillips**
- 1:40 ORGN 299.** Ionic liquid based on 6-amino-6-deoxy hexopyranose cation and BF₄⁻, PF₆⁻ and ClO₄⁻ as anion: A DFT study on the structure and electronic properties. **S. Kheirjou, A. Fattahi**
- 2:00 ORGN 300.** Synthesis of di- and tri-aryl pentanes as model for conducting organic polymers. **A. Agrahari**
- 2:20 ORGN 301.** Computational challenges in olefin metathesis. **A. Poater**
- 2:40 ORGN 302.** Fragmentation mechanisms of aryltrialkyl- Group 14 cation radicals. **A.M. Feinberg, J.P. Dinnocenzo**
- 3:00 ORGN 303.** Theoretical study of the metalla-Diels-Alder cyclizations: An examination of the effect of RH replacement of CH₂ and CH in ethylene and 1,3-butadiene via the isolobal analogy. **E. Votto, E. Greer**
- 3:20 ORGN 304.** Touring the sights and sounds of nonlinear effects in photoacoustic imaging: Excited-state absorption dramatically improves contrast for tailored BODIPY and curcuminoid chromophores. **M. Frenette, M. Hatamimoslehbabadi, S. Bellinger-Buckley, S. Laoui, J. La, Y.S. Bouyou, S. Bag, C. Yelleswarapu, J.J. Rochford**
- 3:40 ORGN 305.** Study of bridge effects on electronic coupling of donor-bridge-acceptor biradicals. **J. Zhang, D. Shultz, M.L. Kirk, D.E. Stasiw, B. Stein**
- 4:00 ORGN 306.** Computational studies of sulfur incorporation into poly(hexahydrotriazine) (PHT) rings. **G.O. Jones, R. Wojtecki, A.Y. Yuen, D. Boday, A. Nelson, J.M. Garcia, Y. Yang, J. Hedrick**
- 4:20 ORGN 307.** First principles group additivity scheme for organics in aqueous solution. **J. Kua**
- 4:40 ORGN 308.** Sunlight-driven hydrogen peroxide production from water and molecular oxygen by graphitic carbon nitride-based photocatalysts. **Y. Shiraishi, Y. Kofuji, T. Hirai**

- 2:40 ORGN 314.** Enabling turnover in catalytic dehydrative substitution of tertiary aliphatic alcohol. **M. Hellal, F.C. Falk, M. Dryzhakov, J. Moran**
- 3:00 ORGN 315.** Regio-, diastereo- and enantioselective C-H functionalization of hydrocarbons. **K. Liao, H.M. Davies**
- 3:20 ORGN 316.** Controlling regiochemistry in metal-catalyzed spiroketal synthesis from alkynols. **P. Paioti, J. Ketcham, A. Aponick**
- 3:40 ORGN 317.** Au(I)-catalyzed spiroketalizations: Problems and solutions, en route to spirastrellolide A. **B.B. Butler, J.N. Mandala, A. Aponick**
- 4:00 ORGN 318.** Catalytic formal [5+2] cycloaddition approach to azepino[1,2-a]indoles and cyclohepta[b]indoles. **M. Martin, R. Shenje, S.A. France**
- 4:20 ORGN 319.** Synthesis of vicinal diamines via rhodium mediated intermolecular hydroamination reaction. **A.K. Gupta, A.R. Ickes, S. Ensign, K.L. Hull**
- 4:40 ORGN 320.** General approach for catalytic β-selective glycosidation. **N. Kuhl, K. Harper, Y. Park, R.Y. Liu, E.N. Jacobsen**

Section F

Boston Convention & Exhibition Center Room 206A

Asymmetric Reactions and Syntheses

- M. C. McIntosh, *Organizer*
F. Gonzalez Bobes, *Presiding*
- 1:00 ORGN 321.** Virtual chemist: Development and application of a user-friendly tool for asymmetric catalyst design. **N. Moitessier, J. Pottel**
- 1:20 ORGN 322.** Catalytic asymmetric synthesis of indole-containing macrocycles. **P.A. Woods, M.J. Waring, T. Moss, D. Dixon**
- 1:40 ORGN 323.** Process research and development of BMS-955829, a positive allosteric modulator of the metabotropic glutamate receptor 5 (mGluR5). **F. Gonzalez Bobes, N. Strotman, H. Ronald, A. Goswami, Z. Guo**
- 2:00 ORGN 324.** Stereoselective synthesis of 5'-C-methyl pyrimidine nucleosides. **A.V. Kel'in, I. Zlatev, S. Matsuda, M. Jayaraman, K.R. Rajeev, M. Manoharan**
- 2:20 ORGN 325.** Investigation of tert-butylsulfanyl group as a chiral auxiliary for condensation between its arylalkene derivatives and aldehydes. **Z. Sun**
- 2:40 ORGN 326.** Industrial synthesis of pharmaceutical compounds using novel doubly-quaternized cinchona alkaloid-based phase transfer catalysts. **B. Xiang, T. Andreani, K.M. Belyk, S. Dalby, G.R. Humphrey, M. Luzung, R.A. Reamer, Z. Song, N. Yasuda**
- 3:00 ORGN 327.** Development of a diastereoselective phosphorylation of a complex nucleoside via a dynamic kinetic resolution. **K. Tran, G. Beutner, M. Schmidt, J. Janey, K. Chen, V.W. Rosso, M.D. Eastgate**
- 3:20 ORGN 328.** Synthesis and reactions of 3,8-dichloro-6-ethyl-1,2,5,7-tetramethyl-BODIPY. **N. Zhao, G. Vicente, F. Fronczek, K.M. Smith**
- 3:40 ORGN 329.** Enantioselective synthesis of a novel group of 3,4-dihydrocoumarin derivatives containing quaternary amino acid moiety. **J. Pieta, J. Hejmanowska, A. Albrecht, L. Albrecht**
- 4:00 ORGN 330.** Enantioselective biomimetic strategies in the synthesis of α-amino acids and their analogs. **L. Albrecht, D. Kowalczyk, J. Hejmanowska, M. Dziegielewska**

Section E

Boston Convention & Exhibition Center Room 204B

New Reactions and Methodology

- M. C. McIntosh, *Organizer*
N. Kuhl, *Presiding*
- 1:00 ORGN 309.** ArCF₃-forming reductive elimination from LPd(Ar)(CF₃) complexes based on bulky biaryl phosphine ligands. **Y. Yang, S.L. Buchwald**
- 1:20 ORGN 310.** Trifluoroacetic anhydride as a reagent for trifluoromethylation. **J.W. Beatty, J.J. Douglas, C. Stephenson**
- 1:40 ORGN 311.** Access to oxindoles, isatins, and isoxazolinones via multicomponent reactions and facile 6π electrocycloization. **S. Chuang, J. Deng**
- 2:00 ORGN 312.** α-/β-Functionalization of allylamines via a dual nickel/Bronsted acid catalyzed approach. **E. Richmond, J. Moran**
- 2:20 ORGN 313.** Simple salts of sustainable metals (Fe, Bi, Cu, and Ti) supported on Montmorillonite as efficient and recyclable catalysts for regioselective intramolecular and intermolecular hydroalkoxylation reactions of double bonds and tandem processes. **I. Notar Francesco, B. Cacciuttolo, M. Puchault, S. Antoniotti**

- 4:20 ORGN 331.** Theoretically-guided optimization of new ligand libraries for asymmetric hydrogenation of minimally functionalized olefins: Application to high value chiral intermediates. **M. Diéguez, O. Pamies**
- 4:40 ORGN 332.** Chiral Werner complexes as hydrogen bond donor catalysts for enantioselective organic synthesis. **A. Kumar, S.K. Ghosh, K.L. Lewis, J.A. Gladysz**

Section G

Boston Convention & Exhibition Center Room 206B

Molecular Recognition and Self-Assembly

- M. C. McIntosh, *Organizer*
M. Levine, *Presiding*
- 1:00 ORGN 333.** *ortho*-Phenylenes: Control of folding behavior and incorporation within complex architectures. **S. Hartley, M. Chu, G. Vemuri**
- 1:20 ORGN 334.** Self-assembly mechanism and stability of covalent organic frameworks. **B.J. Smith, A. Chavez, N. Hwang, W. Dichtel**
- 1:40 ORGN 335.** PHYSStructural modifications of cryptophanes: Towards new Xenon biosensors. **L. Chapellet, J. Cochrane, E. Mari, C. Boutin, P. Berthault, T. Brotin**
- 2:00 ORGN 336.** Cyclodextrin-promoted energy transfer as a tool for probing noncovalent interactions. **M. Levine**
- 2:20 ORGN 337.** Progress toward the synthesis of pyruvate-derived cyclic RNA precursors. **G.W. Ward, S.A. France, R. Krishnamurthy, N.V. Hud**
- 2:40 ORGN 338.** Equilibrium studies and sensing applications of *ortho*-iminomethylphenylboronic acids. **B.M. Chapin, P. Metola, W.D. Brittain, W. Zhai, J. Stanton, J.S. Fossey, E.V. Anslyn**
- 3:00 ORGN 339.** Simultaneous chirality sensing of multiple amines by ¹⁹F NMR. **Y. Zhao, T.M. Swager**

Innovation in Metabolism, Bioavailability and Formulations Research Leading to the Discovery of Agrochemicals: Symposium Honoring Dr. Keith D. Wing, AGRO International Award for Research in Agrochemicals

Sponsored by AGRO, Cosponsored by ORGN

MONDAY EVENING

Section A

Boston Convention & Exhibition Center Hall C

Sci-Mix

R. D. Broene, M. C. McIntosh, *Organizers*

8:00 - 10:00

127, 141, 160, 178, 188, 191, 195, 209-210, 221. See previous listings.

- ORGN 340.** NSF chemistry (CHE): Programmatic structure and funding opportunities. **D.B. Berkowitz, C.A. Bessel, K.J. Covert, C.A. Murillo, C.M. Jenkins**
- ORGN 341.** Initiatives/new directions in the chemistry (CHE) and chemical, bioengineering, environmental, and transport systems (CBET) divisions at NSF. **D.B. Berkowitz, J.S. Lighty, C.A. Bessel, T.E. Patten, T. Li, M.Y. Hawkins, R.W. McCabe, R. Mutharasan**

ORGN 342. Broader impacts/broadening participation/education and outreach in NSF-CHE. **D.B. Berkowitz, C.A. Bessel, C.R. Wilkerson, T.D. Mitchell, M. Bushey, G. Yancey**

482, 491, 505, 517, 550, 556-567, 695, 717, 722, 734, 744, 752, 765, 767, 770, 781. See subsequent listings.

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center Ballroom East

Cope Award Symposium

M. C. McIntosh, *Organizer*
P. E. Mahaney, *Presiding*

8:00 Introductory Remarks.

8:05 ORGN 343. Award Address (Arthur C. Cope Mid Career Scholars Award sponsored by the Arthur C. Cope Fund). Catalyst-enabling nanocarbon science and plant/animal biology. **K. Itami**

8:45 ORGN 344. Award Address (Arthur C. Cope Mid Career Scholars Award sponsored by the Arthur C. Cope Fund). Secret lives of crystals: Control of chemical reactivity and rotational dynamics for the design of molecular machines. **M.A. Garcia-Garibay**

9:25 ORGN 345. Award Address (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). From molecules to dynamic molecular systems. **B. Feringa**

10:05 ORGN 346. Award Address (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). Vanadium chemistry at the interface of organic and inorganic chemistry. **D.C. Crans**

10:45 ORGN 347. Award Address (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). Transition metals in service of organic synthesis. **K.M. Nicholas**

11:25 ORGN 330. Award Address (Arthur C. Cope Mid Career Scholars Award sponsored by the Arthur C. Cope Fund). Reversible DNA and RNA Methylation in Gene Expression Regulation. **C. He**

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Section B

Boston Convention & Exhibition Center
Room 205B/C

Young Academic Investigator Symposium

M. S. Sigman, *Organizer*

H. M. Davies, L. McElwee-White, *Organizers, Presiding*

8:00 **Introductory Remarks.**

8:05 **ORGN 348.** Design and application of biphlic organophosphorus catalysts. A.T. Radosevich

8:35 **ORGN 349.** No strain, no gain: Advances in the synthesis and use of cyclobutanes. M.K. Brown

9:05 **ORGN 350.** Structure and reactivity of gold (I) complexes relevant to catalysis. A.C. Jones

9:35 **ORGN 351.** Palladium and nickel catalyzed carbon-carbon bond formation. D. Kalyani

10:05 **ORGN 352.** Searching for new reactivity: Iron-catalyzed stereoselective olefin aminohydroxylation and aminofluorination reactions. H. Xu

10:35 **ORGN 353.** New amination strategies to access biologically important nitrogen-containing molecules. Q. Wang

11:05 **ORGN 354.** Leveraging process analytical technology to enable reaction discovery and optimization. J. Hein

11:35 **ORGN 355.** Generalized total synthesis of the sarpagine alkaloids. T. Gaich, S. Krüger

Section C

Boston Convention & Exhibition Center
Room 203

Materials, Devices and Switches

M. C. McIntosh, *Organizer*

Q. Li, *Presiding*

8:00 **ORGN 356.** Solid-state rotational dynamics of photoresponsive molecular rotors. A. Aytou, M.A. Garcia-Garibay

8:20 **ORGN 357.** Wireless detection of gases and vapors with a smartphone via radio frequency communication. J.M. Azzarelli, K.A. Mirica, J.B. Ravnsbæk, T.M. Swager

8:40 **ORGN 358.** Molecular design and synthesis of heliconical twist-bend nematic liquid crystals. Y. Wang, H. Bisoyi, Q. Li

9:00 **ORGN 359.** Stimuli directing self-organized 3D liquid crystalline nanostructures. Q. Li

9:20 **ORGN 360.** Enhanced fluorescence quenching sensitivity in metal organic frameworks. C. Thompson, G.T. McCandless, R.A. Smaldone

9:40 **ORGN 361.** Responsive surfactants for biosensing with dynamic complex emulsions. J.A. Kalow, L.D. Zarzar, X. He, T.M. Swager

10:00 **ORGN 362.** Photoswitchable phosphine ligands for Pd-catalyzed asymmetric reactions. D. Zhao, B. Feringa

10:20 **ORGN 363.** Fluorescent compounds from [5]helicene derivatives for organic electronics application. T. Sooksimuang, S. Sahasithiwat, L. Kangkaew, W. Panchan

10:40 **ORGN 364.** Fundamental photo-physics and the structural implications for a series of substituted phthalocyanine dyes. C. Farley, C.M. Drain

Section D

Boston Convention & Exhibition Center
Room 204A

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*

M. S. Oderinde, *Presiding*

8:00 **ORGN 433.** Surprising impact of the 2,2,6,6-tetramethylpiperidinyl group on the chemical shift and conformation of singly-masked 1,2-diols. S. Chatterjee, E. Fought, J.S. Chen, T.L. Windus

8:20 **ORGN 434.** Vinylnitrene formation from an isoxazole in solution and in solid state. R. Ranaweera, E.J. Kidd, N. Sajkovic, E. McCoy, J. Coffman, D. Chapman, F. Jasuthasan, J.A. Krause, B.S. Ault, A.D. Gudmundsdottir

8:40 **ORGN 435.** Understanding solvent-induced red-shifts for the proton stretch vibrational frequency in a hydrogen-bonded complex. P.M. Kiefer, D. Pines, E. Pines, J.T. Hynes

9:00 **ORGN 436.** Organic chemistry at the air/water interface: Regioselective synthesis of allylic hydroperoxides via singlet oxygenation of a trisubstituted alkene. B. Malek, A.A. Ghogare, R. Choudhury, A. Greer

9:20 **ORGN 437.** New photooxygen-atom exchange reaction of nitrosamines with molecular oxygen: Dependence on nitrosamine substituents. A.A. Ghogare, M.S. Oliveira, I. Abramova, E. Greer, F.M. Prado, P. Di Mascio, A. Greer

9:40 **ORGN 438.** Thermodynamic evaluation of aromatic CH/ π interactions and rotational entropy in a molecular rotor. S. Perez Estrada, B.V. Rodriguez-Molina, G. Jimenez-Oses, K.N. Houk, M.A. Garcia-Garibay

10:00 **ORGN 439.** Design, synthesis, and computational studies of novel rhodamine dyes for imaging applications. A.K. Muthusamy, J. Grimm, L.D. Lavis

10:20 **ORGN 440.** Hybrid functional approach to the investigation of the isosteric substitutions on Garratt-Braverman cyclization and its implications. K. Kwon, J. Marino Creto, E. Greer

10:40 **ORGN 441.** Measurement of substituent- π interactions. J. Hwang, K.D. Shimizu

11:00 **ORGN 442.** Effect of molecular oxygen on iridium-photoredox carbon-carbon bond-forming reactions: Synergistic catalysis. M.S. Oderinde, A. Varela-Alvarez, B.M. Aquila, D. Robbins, J.W. Johannes

11:20 **ORGN 443.** Synthesis of tetracene derivatives, study of their stability, and photooxidation with singlet oxygen. R.N. Baral, S.W. Thomas

11:40 **ORGN 444.** Anion-abstracting catalysis: Mechanistic studies and development of dimeric thiourea catalysts. D. Lehnher, D.D. Ford, N.S. Rajapaksa, E.N. Jacobsen

Section E

Boston Convention & Exhibition Center
Room 204B

New Reactions and Methodology

M. C. McIntosh, *Organizer*

G. G. Melikyan, *Presiding*

8:00 **ORGN 377.** Designing recyclable silylating reagents that double as purification handles. C. Chao, A. Leibham, D.E. Bergbreiter

8:20 **ORGN 378.** Diastereoselective carbenoid insertion into unsymmetrical diboron species. A. Cuenca, J. Cid, D. Garcia, J.J. Carbó, E. Fernández

8:40 **ORGN 379.** Design and synthesis of a chiral and conformationally constrained natural product-inspired oligomers. C. Aquino, G.C. Micalizio

9:00 **ORGN 380.** Studies towards ligand-enabled C(sp³)-H activation using Pd(0) and Pd(II) catalysts. J. He, J. Yu

9:20 **ORGN 381.** Polyolefin oligomers as solvents and tools for Ru(II)-catalyzed metathesis reactions. J. Suriboot, W. Guzman, D.E. Bergbreiter

9:40 **ORGN 382.** Cu(II)-catalyzed regio-, stereo-, and chemoselective β -boration of acetylenic esters in water. C. Peck, J. Calderone, W. Santos

10:00 **ORGN 383.** Withdrawn.

10:20 **ORGN 384.** Reductive amination of carbonyl compounds in water as solvent and hydrogen source. C. Schäfer, B. Nisanci, M. Bere, A. Dastan, B. Torok

10:40 **ORGN 385.** Withdrawn.

11:00 **ORGN 386.** Transition metal and phosphorous mediated transformations for C-C and C-N bond formations. A. Lepore, B.L. Ashfeld

11:20 **ORGN 387.** Nickel-catalyzed cross-electrophile coupling reactions of vinyl halides. K.A. Johnson, D.J. Weix

11:40 **ORGN 388.** Catalytic carbon-olefin metathesis. J.R. Ludwig, J.B. Gianino, C. Schindler

Section F

Boston Convention & Exhibition Center
Room 206A

Total Synthesis of Complex Molecules

M. C. McIntosh, *Organizer*

J. G. Pierce, *Presiding*

8:00 **ORGN 389.** Studies toward the synthesis of complex oxaphenalenone natural products. T. Purgett, J.A. Porco

8:20 **ORGN 390.** Modular synthetic approach to polycyclic xanthone natural products, hybrids and analogs. M. Himmelbauer, J.A. Porco

8:40 **ORGN 391.** Studies towards the total syntheses of the Swerilactones and related natural products. D. Hamann, J.A. Porco

9:00 **ORGN 392.** Studies toward the total syntheses of tetrahydroswertianolin and puniceaside B. G.-J. Kim, J.A. Porco

9:20 **ORGN 393.** Marine natural products synthesis: A platform for chemical and biological discovery. J.G. Pierce, N.V. Shymanska, G.A. Edwards

9:40 **ORGN 394.** Total synthesis of type B PPAps utilizing biomimetic and diastereoselective cyclization strategies. J.H. Boyce, J.A. Porco

10:00 **ORGN 395.** 1,5-Antiselective aldol reactions for the total synthesis of the brasilinoides. M. Housden, C. Cordier, P. Burton, F. Muehlthau, I. Paterson

10:20 **ORGN 396.** Studies toward the total syntheses of the Sanggenon C and related natural products. C. Qi, Y. Xiong, H. Cong, J.A. Porco

10:40 **ORGN 397.** Synthesis and Diels-Alder reactions of 1'-heterosubstituted 4-vinylimidazoles: A novel approach en route to the total synthesis of dimeric oroidin alkaloids. A. Ray, C.J. Lovely

11:00 **ORGN 398.** Bioinspired platform for the synthesis of lignan natural products. J. Lumb, A. Albertson

11:20 **ORGN 399.** Biomimetic approach to resveratrol-derived oligomeric natural products. M.H. Keylor, B.S. Matsuura, B. Li, D.A. Pratt, C. Stephenson

11:40 **ORGN 400.** Synthesis of breittfussin B by tunable site-selective bromination. A.H. Khan, J.S. Chen

Section G

Boston Convention & Exhibition Center
Room 206B

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*

K. H. Shaughnessy, *Presiding*

8:00 **ORGN 467.** Catalytic aerobic platform for the functionalization of phenols. J. Lumb, Z. Huang, K. Esqueria

8:20 **ORGN 468.** Iron catalyzed direct diazidation of a broad range of olefins. Y.A. Yuan, D. Lu, Y. Chen, H. Xu

8:40 **ORGN 469.** Selective C-H functionalization reaction. D. Maiti

9:00 **ORGN 470.** Stereocontrolled radical C-H alkylation via Co(II)-based metalloradical catalysis. X. Cui, X. Xu, L. Jin, L. Wojtas, P.X. Zhang

9:20 **ORGN 471.** Directing group strategies for the beta-functionalization of ketones via C-H activation. M. Young, G. Dong

9:40 **ORGN 472.** Multicatalytic reactions: Tandem catalysis to achieve hydrofunctionalization of olefins. J.C. Holder, J.F. Hartwig

10:00 **ORGN 473.** Off-cycle Pd(0)/Pd(II) intermediates and their implications on Pd-catalyzed C-N bond forming efficiency. P. Arrechea, S.L. Buchwald

10:20 **ORGN 474.** Control of reaction selectivity in palladium-catalyzed transformations through tuning of ligand structures. K.H. Shaughnessy

10:40 **ORGN 475.** Advances in palladium-catalyzed nucleophilic fluorination. A.C. Sather, H. Lee, S.L. Buchwald

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Electron and Energy Transfer: From Molecular to Device Engineering for Minimizing Environmental Impacts

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

Glycolipid Immunostimulants

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Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Ballroom East

Cope Award Symposium

M. C. McIntosh, *Organizer*

D. M. Huryn, *Presiding*

- 1:05 ORGN 411.** Award Address (Arthur C. Cope Early Career Scholars Award sponsored by the Arthur C. Cope Fund). Synthetic biology approaches to new fluorine chemistry. **M. Chang**
- 1:45 ORGN 412.** Award Address (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). Gold-catalyzed cycloisomerizations. **A.M. Echavarren**
- 2:25 ORGN 413.** Award Address (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). Recent forays in methods development and complex molecule synthesis. **N.K. Garg**
- 3:05 ORGN 414.** Award Address (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). Strategies and methods for chemical synthesis inspired by complex natural products. **R. Sarpong**
- 3:45** Introduction of Cope Awardee.
- 3:55 ORGN 415.** Award Address (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). Chemistry-medicine continuum: Computer-guided, synthesis-informed design of new therapeutic leads for HIV/AIDS eradication, Alzheimer's disease, and cancer. **P.A. Wender**

Section B

Boston Convention & Exhibition Center
Room 205B/C

Young Academic Investigator Symposium

M. S. Sigman, *Organizer*

H. M. Davies, L. McElwee-White, *Organizers*,
Presiding

1:00 Introductory Remarks.

- 1:05 ORGN 416.** Increasing the scope of organic reactions and tools for tailoring the biotic/abiotic interface. **A.B. Braunschweig**
- 1:35 ORGN 417.** Some hard lessons in biocojugation: When is what important, and why. **D.G. Gillingham**
- 2:05 ORGN 418.** Chemical tools for probing, manipulating, and imaging biological systems. **D.M. Chenoweth**
- 2:35 ORGN 419.** Natural products diversity inspires new reaction development and impacts insect biodiversity. **C. Jeffrey**
- 3:05 ORGN 420.** Chemical tools for investigating biological hydrogen sulfide. **M.D. Pluth**
- 3:35 ORGN 421.** Emerging view on hapalindole-type alkaloid biogenesis. **X. Liu**
- 4:05 ORGN 422.** Expanding the biorthogonal toolkit. **J.A. Prescher**
- 4:35 ORGN 423.** RNA-based fluorescent biosensors for visualizing enzyme reactions. **M.C. Hammond**

Section C

Boston Convention & Exhibition Center
Room 203

Materials, Devices and Switches

M. C. McIntosh, *Organizer*

D. Chiridon, *Presiding*

- 1:00 ORGN 424.** Increased carrier mobilities in end-functionalized oligosilanes. **S. Surampudi**, M.L. Yeh, J.M. Hardigree, T. Kasl, H.E. Katz, R.S. Klausen
- 1:20 ORGN 425.** Pyrene-based compounds in organic optoelectronic applications. **B.R. Kaafarani**
- 1:40 ORGN 426.** Noncovalent aromatic interactions that control the geometry and piezochromism of conjugated oligomers. **S.W. Thomas**
- 2:00 ORGN 427.** Withdrawn.
- 2:20 ORGN 428.** Benzodithiophene and benzothiadiazole donor-acceptor (D-A) small molecules for solution-processed small molecule organic solar cells. **J. Du**, P. Bulumulla, D. Barrera, J.W. Hsu, M.C. Biewer, M.C. Stefan
- 2:40 ORGN 429.** Development of electron accepting thiophene dioxides with applications in electrochromics and photocatalytic hydrogen generation. **D. Chiridon**, C. Tsai, H. Kagalwala, A. Maurer, A. Kaur, T. Pintauer, K.J. Noonan, S. Bernhard
- 3:00 ORGN 430.** Electrochemical molecular switching using thianthrene-containing cavitated. **W. Ong**, F. Bertani, T.M. Swager
- 3:20 ORGN 431.** Design and prototyping of biodegradable polymeric drug delivery device for inner ear disease treatment. **J. Wang**, A.M. Ayoob, J.T. Borenstein
- 3:40 ORGN 432.** More is different: Convergent and divergent synthesis of nanoscale molecular rotors and their rotational dynamics in the solid state. **X. Jiang**, Z.J. O'Brien, B.V. Rodriguez-Molina, N. Nazarian, M.A. Garcia-Garibay

Section D

Boston Convention & Exhibition Center
Room 204A

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*

M. N. Grayson, *Presiding*

- 1:00 ORGN 365.** Stereospecific photochemistry of crystalline Δ^2 -1,2,3-triazolines to form aziridines. **T. Chung**, M.A. Garcia-Garibay
- 1:20 ORGN 366.** Mechanistic details of Pd(II)-catalyzed C-H iodination with molecular I_2 : Oxidative addition vs. electrophilic cleavage. **B. Haines**, X. Wang, J. Yu, J. Musaev
- 1:40 ORGN 367.** Nucleofugality in oxygen and nitrogen derived pseudohalides in Menshutkin reactions: The Importance of the intrinsic barrier. **G. Spahlinger**, J.E. Jackson
- 2:00 ORGN 368.** Exploring excited-state catalyzed 1,3 dipolar cycloaddition reactions. **J. Ortiz Sanchez**, T.J. Heavey, N. Lajkiewicz, J.A. Porco, D. Coker
- 2:20 ORGN 369.** The two sides of dynamic covalent exchange at nanoscale interfaces: Structural effects on molecular reactivity, molecular effects on nanostructure properties. **E.R. Kay**

2:40 ORGN 370. Mechanistic insights into ruthenium-catalyzed asymmetric butadiene hydrohydroxyalkylation. **M.N. Grayson**, M.J. Krische, K.N. Houk

- 3:00 ORGN 371.** Developing new Schiff bases for fluorescent detection of aluminum cation and their potential applications. **L. McDonald**, J. Wang, N. Alexander, H. Li, Y. Pang
- 3:20 ORGN 372.** Optical and photoacoustic properties of quadrapolar curcuminoid dyes. **S. Bellinger Buckley**, M. Frenette, M. Hatamimoslehhabadi, S. Laoui, S. Bag, F. Mathila, C. Yelleswarapu, J.J. Rochford
- 3:40 ORGN 373.** Solution and solid state photochromism of spiropryrans. **V.M. Breslin**, M.A. Garcia-Garibay
- 4:00 ORGN 374.** Quinoline based $\sigma, \sigma, \sigma, \sigma$ -tetradiradical: Synthesis and gas phase reactivity by using a linear quadrapole ion trap (LQIT) mass spectrometer. **R.R. Kotha**, H.I. Kenttamaa
- 4:20 ORGN 375.** Heteroatom-substituted BDPA: Tuning radicals for use as dynamic nuclear polarization agents. **G.T. Sazama**, J.J. Walsh, D. Frantz, T.V. Can, V. Michaelis, E.G. Keeler, R.G. Griffin, T.M. Swager
- 4:40 ORGN 376.** Reactive intermediate study of solution and solid state [2+2] photodimerization of cyclopentenones. **R. Ranaweera**, G.K. Weragoda, K. Griffin, R. Robinson, J. Coffman, E.J. Kidd, F. Jasuthasan, J.A. Krause, A.D. Gudmundsdottir

Section E

Boston Convention & Exhibition Center
Room 204B

New Reactions and Methodology

M. C. McIntosh, *Organizer*

P. S. Hanley, *Presiding*

- 1:00 ORGN 445.** Suzuki-Miyaura cross-coupling of aryl fluorosulfonates derived from phenols and sulfonyl fluoride. **P.S. Hanley**, A. Krasovskiy, M. Ober, C. Clark, G. Whiteker, W.J. Kruper
- 1:20 ORGN 446.** NHC-Cu-catalyzed nucleophilic fluorination of propargylic electrophiles. **L. Cheng**, C. Cordier
- 1:40 ORGN 447.** Withdrawn.
- 2:00 ORGN 448.** Hypervalent activation as key step in accessing the *ortho*-CH position of iodoarenes. **Y. Wu**, I. Arenas, L. Broomfield, **A. Shafir**
- 2:20 ORGN 449.** Rhodium-catalyzed intermolecular hydroamination. **A. Ickes**, S. Ensign, A.K. Gupta, K.L. Hull
- 2:40 ORGN 450.** Copper-catalyzed SP^3 C-H etherification via acyl protected phenols. **T.K. Salvador**, C.A. Arnett-Guardado, N. Sapiezynski, T.H. Warren
- 3:00 ORGN 451.** Inter- and intramolecular decarboxylation of bis-allylic esters lacking anion-stabilizing groups. **I.D. Hyatt**, M.P. Croatt
- 3:20 ORGN 452.** Selective functionalizations of tetracoordinated sulfur derivatives. **R.A. Bohmann**, C. Bolm
- 3:40 ORGN 453.** Organic, oxygen tolerant photocatalyst: Design and application in radical dehalogenations. **E. Discekici**, N. Treat, S. Oh, K.M. Mattson, Z.M. Hudson, Y. Luo, C.J. Hawker, J. Read De Alaniz
- 4:00 ORGN 454.** Metal free C-H coupling of aromatic compounds by graphene oxide activated by acidic additives. **Y. Nishina**, N. Morimoto, K. Morioku
- 4:20 ORGN 455.** Modified Friedländer quinoline synthesis in water. **F. Li**

Section F

Boston Convention & Exhibition Center
Room 206A

Total Synthesis of Complex Molecules

M. C. McIntosh, *Organizer*

Z. Zhang, *Presiding*

- 1:00 ORGN 456.** Progress towards the total synthesis of (-)-mandelalide A employing anion relay chemistry tactic. **M.H. Nguyen**, M. Imanishi, T. Kurogi, A.B. Smith
- 1:20 ORGN 457.** Gold-catalyzed approach to the synthesis of Echinopines A and B. **R. Dorel**, E. Coya, A.M. Echavarren
- 1:40 ORGN 458.** Versatility of gold(I)-catalysis applied to the total syntheses of (-)-nardoaristolone B and lundurine C. **M.E. Muratore**, M.S. Kirillova, A. Homs, R. Dorel, A.M. Echavarren
- 2:00 ORGN 459.** Asymmetric [2+2] cycloaddition of ketenes: Toward the total synthesis of (+)-lactacystin and (-)-salinosporamide A. **P. Rulliere**, S. Carret, J. Poisson
- 2:20 ORGN 460.** C7-derivatization of tryptophans and tryptamines for the synthesis of complex alkaloids. **R.P. Loach**, O.S. Fenton, K. Amaike, D.S. Siegel, E. Ozkal, M. Movassaghi
- 2:40 ORGN 461.** Gold-catalyzed approach for the synthesis of cannabimovone and anhydrocannabimovone. **J. Carreras**, M.S. Kirillova, A.M. Echavarren
- 3:00 ORGN 462.** General, practical, and diversifiable synthetic route to new macrolide antibiotics. **I.B. Seiple**, **Z. Zhang**, P. Wright, A. Langlois, K. Yabu, D. Hog, P. Jakubec, A.G. Myers
- 3:20 ORGN 463.** Synthetic studies towards spiroindimicins B-D. **L.M. Blair**, J. Sperry
- 3:40 ORGN 464.** Synthesis and structural assignment of Astrilobin A, an *Annonaceae* acetogenin from the seeds of *Asimina triloba*. **J. van Kempen**, H. Schimanski, G. Haufe
- 4:00 ORGN 465.** Mechanistic evaluation of the interrupted Bischler-Napieralski reaction and its application to the total synthesis of the aspidosperma alkaloids. **K. White**, M. Movassaghi
- 4:20 ORGN 466.** Application of assembly-line synthesis to natural product synthesis. **T. Bootwicha**, V.K. Aggarwal

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Section G

Boston Convention & Exhibition Center
Room 206B

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*

J. S. Fossey, *Presiding*

1:00 ORGN 401. Organotransition metal catalysts confined in dispersible macromolecules. V.O. Rodionov

1:20 ORGN 402. Propargyl radical chemistry: Unlocking the potential. G.G. Melikyan, R. Davis, S. Cappuccino, M. Mouselli

1:40 ORGN 403. Direct, efficient, and general gold-catalyzed synthesis of fused-imidazo heterocycles. M. Garzón Sanz, P.W. Davies

2:00 ORGN 404. Imaging single molecule oxidation reactions in an environmentally controlled liquid-STM. D. den Boer, L. Thomas, M. Li, S. Wezenberg, D. Amabilino, A.W. Kleij, S. De Feyter, J.A. Elemans

2:20 ORGN 405. Rapid Cu(II)-mediated formation of 5,5'-bis(1,2,3-triazole)s from organic azides and terminal alkynes. C.J. Brassard, X. Zhang, R.J. Clark, L. Zhu

2:40 ORGN 406. Withdrawn.

3:00 ORGN 407. Preparation of propargylic sulfonates and their [2,3]-sigmatropic rearrangement to allenic sulfones. C.S. Hampton, R. Tata, M. Harmata

3:20 ORGN 408. 2,4-*cis*-Azetidines: Development of synthesis and applications to catalysis. J.S. Fossey, A. Yoshizawa, A. Feula

3:40 ORGN 409. Mild deoxygenation of aromatic ketones and aldehydes over Pd/C using polymethylhydrosiloxane as the reducing agent. A. Volkov, K. Gustafson, C. Tai, O.O. Verho, J.E. Backvall, H. Adoffsson

4:00 ORGN 410. Iron (II)-catalyzed stereoselective intramolecular olefin aminofluorination and aminochlorination. C. Zhu, D. Lu, J. Tian, H. Xu

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Designs: From Molecules to Functional Materials

Glycolipid Immunostimulants

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TUESDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Biologically-Related Molecules and Processes; Innovation from Discovery to Application; Metal-Mediated Reactions and Syntheses; Molecular Recognition and Self-Assembly; Peptides, Proteins, and Amino Acids

R. D. Broene, *Organizer*

8:00 - 10:00

ORGN 476. Development and optimization of a medium-throughput synthesis workflow for process development. J.A. Jurica

ORGN 477. Binding analysis of Xe-129 with cyclotrimeratrylenes (CTV) compounds. J. Rhoat

ORGN 478. Studies toward a convenient and inexpensive synthesis of D-vinylglycine. E. DeCicco, L. Sanchez

ORGN 479. Recent advances in automated solubility and crystallization screening in pharmaceutical development. J. Qiu

ORGN 480. Novel synthesis of modified nucleic acids and nucleoside analogs for solid phase synthesis of ribonucleic guanidine (RNG). A. Chavez, A. Awad, C. Stringer

ORGN 481. Toward the non-invasive detection of hypoxic tumors by monitoring reductase activity with catalyCEST MRI. S.C. Gilmore, I. Daryaei, M. Pagel

ORGN 482. Lanthanide assisted ring distortion of medium-sized cyclic peptide. G.G. Simpson, S. Hamedzadeh, K. Ha

ORGN 483. Discovery of noncovalent small molecule inhibitors of APOBEC3 enzymes. A.L. Perkins, M.E. Olson, M. Li, R.S. Harris, D.A. Harki

ORGN 484. Synthesis and biological evaluation of pharbinilic acid and derivatives as NF- κ B pathway inhibitors. J. Annand, P. Bruno, A.K. Mapp, C. Schindler

ORGN 485. Synthesis of small molecule conjugated near-infrared fluorescent probes and their application in selective cancer cell staining. S. König, R. Krämer

ORGN 486. Methodology facilitating library synthesis of C1-substituted carbapenems. T.Q. Nguyen, C. Edwards, P. Nguyen, M. Cox, D. Le, E. Kim, M. Alqurafi, S. Smriti, P. Oelschlaeger, J.D. Buynak

ORGN 487. Design, synthesis, and testing of linear multivalent constructs targeted to melanocortin receptors. D.C. Dehigaspitiya, B.L. Anglin, C.S. Weber, R.M. Lynch, E.A. Mash

ORGN 488. Development of acridon-2-yl-alanine-specific aminoacyl tRNA synthetases for in vivo incorporation. I. Sungwienwong, E. Petersson

ORGN 489. First synthesis of penicillenol B₁, B₂, C₁ and of a bisazide analog for photoaffinity labeling. K. Kempf, O. Kempf, M. Ullmann, R. Schobert

ORGN 490. Synthetic lectins for the diagnosis of breast cancer. K.M. O'Connell, E. Gatrone, A.A. Veldkamp, J.J. Lavigne

ORGN 491. Synthesis of low-molecular weight chiral compounds for fragment-based lead discovery. S.D. Nelson, L. Furst, S. Haftchenary, S.J. Ferrara, Z.V. Boskovic, S. Dandapani, S.L. Schreiber

ORGN 492. Synthesis and crystal structure studies of 2'-5'-linked RNA duplexes. F. Shen, R. Wang, S.M. Magliocco, V. Valsangkar, J. Sheng

ORGN 493. Development of cobalamin-conjugated nanoparticles as photochemotherapeutic agents. T.A. Shell, J.R. Shell, H.L. Nowotarski, D.S. Lawrence

ORGN 494. Design, synthesis, and evaluation of novel guanidinium-rich, glycerol-derived oligocarboxylates for the complexation, delivery, and release of siRNA. M. Huttner, P.A. Wender

ORGN 495. Improving the equilibrium of iminoboronate formation via substituent effects. S. Cambray, J. Gao, A. Bandyopadhyay

ORGN 496. Synthesis of a chemiluminescent cyclosporine conjugate. J. Grote

ORGN 497. Fluorescent labeling of RNA using biorthogonal chemistry. E. Agustin, P. Asare Okai, M. Royzen

ORGN 498. Synthesis and base pairing studies of geranylated DNA and RNA. R. Wang, S.M. Magliocco, V. Valsangkar, F. Shen, J. Sheng

ORGN 499. Broad-based synthesis of glycomimetics from glycosyl crotylstananones. D.R. Mootoo, A.S. Altiti, S. Bachan

ORGN 500. Synthesis and medicinal chemistry of the daphnane diterpene carbon skeleton. L. Nguyen, A.B. Beeler

ORGN 501. Using small molecules to solve big problems. J.E. Stokes, D.R. Spring

ORGN 502. Metal-free and recyclable synthesis of benzothiazoles using thiourea as a sulfur surrogate. Y. Ying, F.H. Wu

ORGN 503. Improved synthesis of single isomers of 5-carboxy-fluorescein, 5-carboxy-rhodamine 110 and Alexa Fluor® 488. B.N. Blackman, R.E. Swenson

ORGN 504. Gossypolone and gossypol-hemiquinone: Biological activity of terpenoids found in cotton (*Gossypium*). R.D. Stipanovic, L. Puckhaber, J. Frelchowski, Jr., J. Esquivel, J. Westbrook, M. O'Neil, A. Bell, J. Lopez, Jr., M.K. Dowd, K.D. Hake, S. Duke

ORGN 505. Photochemically-generated fragment collections: A better starting point for discovery of biologically active molecules. Z.V. Boskovic, C. Gerry, B. Hua, O. Verho, S. Haftchenary, S.L. Schreiber

ORGN 506. Optimized modular diazo compound for bioreversible protein esterification. K. Mix, R.T. Raines

ORGN 507. Improved and optimized syntheses of fentanyl and related analogs. S. Hok, R.N. Leif, B.P. Mayer, C.A. Valdez

ORGN 508. Design, synthesis, and biological evaluation of β -carboline dimers based on the structure of neokaulamine. J. Chatwchien, J.D. Winkler, M.E. Murphy, M.T. Hamann, S. Basu

ORGN 509. Synthesis and structure determination of diastereomeric phenyl indanes dimerized from ferulic acid. E. Nomura, T. Noda, Y. Kakimoto, T. Yamamoto, H. Mori, Y. Miyake

ORGN 510. Comparison of phosphines reactivity with nitroxyl (HNO) and S-nitrosothiols. Z. Miao, S.B. King

ORGN 511. Synthesis of electron rich pseudoazulenyl dinitrones exhibiting low oxidation potential. N. Birudukota, D.A. Becker

ORGN 512. No-wash Luciferin-based assay for transporter activity detection. D. Mustafa, D. Ma, W. Zhou, P. Meisenheimer, J. Cali

ORGN 513. New approach to click-chemistry: Photolysis of the triazene functional group. A. Gann, A.M. Hussey, V.J. Emck, N.A. Schnarr, J.J. Chambers

ORGN 514. Impacts of pH/latents on disinfected drinking water. M. Neyrat, H. Kim, T. Corbet, L. Li, C. Tsui, K.L. Yeung

ORGN 515. Metal-catalyzed, microwave-mediated, intramolecular aziridination: Synthesis of benzoxazine and benzoxazinone derivatives. E.B. Atuk, S.M. Shahid, E.C. McLaughlin

ORGN 516. Synthesis of the phenylalanine derived lactones using a zinc mediated HCRL reaction. R.K. Chhetri, C. Zercher

ORGN 517. Alkyl-aryl and alkyl-alkyl cross coupling reactions catalyzed by iron bis(imino)pyridine complexes. T. Mako, J.L. Drake, J.A. Byers

ORGN 518. Access to tetrahydroisoquinolines via intramolecular direct functionalization of alpha-cyclopropyl amino acid-derivatives. C.L. Ladd, A.V. Belouin, A.B. Charette

ORGN 519. Metal cluster-enhanced propargyl radicals: Expanding a substrate base. G.G. Melikyan, S. Cappuccino, M. Mouselli

ORGN 520. New ligand design for copper mediated diaryl C-O bond formation. F. Damkaci, C. Sigindere, J. Malone, E.C. Vik

ORGN 521. Stereoselective amination of thioesters: Mechanistic studies. H. Piras, H. Lebel

ORGN 522. Copper-mediated halogenation of aryl-nitroso compounds. A. van der Werf, N. Selander

ORGN 523. Regioselective C-N bond formation via gold catalysis. L. Marchetti, A. Kantak, R. Davis, B.L. DeBoef

ORGN 524. Development of N-heterocyclic carbene complexes for 1,3-halogen migration. S. Schmid, R. Van Hoveln, J. Rigoli, J.M. Schomaker

ORGN 525. C-C bond and C-X bond formation via copper catalyzed/mediated C(sp²)-H activation. M. Shang, J. Yu

ORGN 526. Development of metal-catalyzed oxidative biaryl coupling reactions for the synthesis of potential NF- κ B inhibitors. E.J. Groso, C. Schindler

ORGN 527. Propargyl radicals: From transiency to persistency to reaction site projection. G.G. Melikyan, R. Davis

ORGN 528. Complementary synthesis of borylated N-heterocycles. C.A. Merlic, R. Tobolowsky

ORGN 529. Computational chemical analysis for Ru(II)-Pheox catalyzed enantioselective intramolecular cyclopropanation. Y. Nakagawa, S. Chanthamath, N. Nakayama, H. Gotoh, K. Shibatomi, S. Iwasa

ORGN 530. 1,6-Cycloisomerization to give 2,3-disubstituted indole catalyzed by ruthenium hydride with N-heterocyclic carbene ligand. K. Takamoto, N. Hyogo, H. Fujioaka, M. Arisawa

ORGN 531. Catalytic hydration of nitriles to amides in water. F. Li

ORGN 532. Rhodium-catalyzed oxidative coupling of 2-aryl-imidazopyridines with internal alkynes via double C-H activation. S.K. Kotta

ORGN 533. Synthesis of 2,4,6-trisubstituted pyridines using palladium-catalyzed cross-coupling reaction. P.J. Trejo, A. Hernandez Campos, R. Castillo-Bocanegra

ORGN 534. Investigation into the synthesis of small indoline compounds for biological screening. **B. MacLeod**, J. Pienkos, W.H. Myers, W.D. Harman

ORGN 535. New diastereoselective synthesis of (E)₃-trisubstituted alkenes containing a trimethylsilylmethyl and biphenyl moieties via organoboranes. **N.G. Bhat**

ORGN 536. Better route to the key intermediate toward C-19 methyl substituted macroline-sarpagine indole alkaloids. **M. Rahman**, R. Jahan, R.V. Edwankar, J.R. Deschamps, J.M. Cook

ORGN 537. Selective cross-coupling of 2,6-dihaloopyridines with alkylboronic esters. **S. Laulhe**, J. Roizen

ORGN 538. Withdrawn.

ORGN 539. Diastereoselective RCM to bicyclo[4.3.1]phosphite-boranes: Tunable *P*-tether systems for the synthesis of complex polyols. **J.L. Markley**, P.R. Hanson

ORGN 540. Toward an efficient screening method for organophosphonate encapsulation. **P.W. Peterson**, A.J. Franjesevic, J.D. Badjic, C.M. Hadad

ORGN 541. Benzoxaboroles as new heterocyclic pharmacophore: Study of open/close structure and reactivity. **S. Vshyvenko**, I. Suzuki, M. Clapson, D.G. Hall

ORGN 542. Stepwise self-assembly of heteronuclear coordination cages by control of metal coordination geometry at specific sites. **A. Metherell**, M. Ward

ORGN 543. Characterization of halogen bond interactions in thiophene-based building blocks. **J.S. Williams**, J. Wilson, C. Petkoveski, P. Reeves, N. Hammer, A. Antonyamsy, D. Watkins

ORGN 544. 3D-supramolecular self-assemblies selectively binding C₆₀ over C₇₀. **K. Paek**, Y.S. Park, J. Lee, H. Koo

ORGN 545. Novel highly sensitive method for the detection of self-assembly and determination of critical assembly concentration. **S.G. Tarasov**, Y. Chen, N.I. Tarasova

ORGN 546. 2D bricklayer packing in conjugated systems through halogen bonding. **F. Frausto**, Z. Smith, T. Haas, S.W. Thomas

ORGN 547. Multivalent glycopeptide nanostructures for enhanced lectin binding. **M. Sardan**, M.O. Guler

ORGN 548. Introducing linear and branched perfluoroalkylated side chains to control the self-assembly of hexa-peri-hexabenzocoronene and its thermotropic properties. **B.A. Alameddine**, B. Heinrich, D. Guillon, B. Donnio, T. Jenny

ORGN 549. Self-assembly of the polystyrene rod-coil block copolymers derived from helical (*R*)- and (*S*)-triazolepolycarbodiimides inspected by TMAFM and SEM. **O.V. Kulikov**, D. Siriwardane, G.T. McCandless, J.F. Reuther, B.M. Novak

ORGN 550. A [2]Rotaxane from a [2]catenane via dynamic ring-chain equilibration: Scope and optimization. **M.M. Cetin**, D.B. Cordes, M.F. Mayer

ORGN 551. Design and synthesis of cyclic peptides inhibitors of EHD1 and long-loop recycling. **R. Eisert**, A. Kamens, J. Kritzer

ORGN 552. Microwave-promoted Eschweiler-Clarke reaction of amino acids. **H.S. Barcena**, S. Kranston

ORGN 553. Reaction optimization for the synthesis of novel vinylglycine derivatives. **E. York**, S. Isa, L. Sanchez

ORGN 554. Investigating the trimethylamine N-oxide (TMAO) induced structure of α -synuclein. **J.J. Ferrie**, R.F. Wissner, E. Petersson

ORGN 555. Withdrawn.

ORGN 556. Withdrawn.

ORGN 557. Broadening the utility scope of thioamides. **D.M. Szantai-Kis**, Y.J. Wang, E. Petersson

ORGN 558. Assessing aberrant glycosylation with synthetic lectins to detect and stage prostate cancer. **A.A. Veldkamp**, K.M. O'Connell, E.E. Gatrone, J.J. Lavigne

ORGN 559. Synthesis of protected L-tryptophan derivatives incorporating nitriles for use in 2D IR studies. **P.H. Gilmartin**, A.R. Cunningham, M. Tucker, **M.W. Fennie**

ORGN 560. Synthesis and characterization of an unnatural boron-nitrogen isostere of tryptophan. **K. Boknevtz**, S. Liu

ORGN 561. Chiral phosphoryl chlorides and phosphoramides: Catalysts for aza-Henry reaction. **J. Almalet**, V. Datilus, P. Kaur

ORGN 562. Using synthetic lectins to investigate metastatic potential in colon cancer. **E.E. Gatrone**, K.M. O'Connell, J.J. Lavigne, A.A. Veldkamp

ORGN 563. Solid phase peptide synthesis of a photoreactive collagen-mimicking peptide by incorporation of N-glycyl-7-nitroindoline moieties. **K. Williams**, A. Ornelas, A. Rahaman, S. Aghvami, C. Li, T. Boland, K. Michael

ORGN 564. Versatility of N-peptidyl nitroindolines for the formation of peptide/glycopeptide acids, amides, and thioesters. **L. Barrera**, K. Michael

ORGN 565. Prolinomyacin-based peptide scaffolds for lipid recognition. **A. Hosseini**, J. Gao

ORGN 566. Reversible cyclization and bicyclization of peptides via iminoboronate chemistry. **L. Blair**, S. Daley, J. Gao

ORGN 567. Development of a biocompatible peptide ligand for CuAAC. **L.C. Dahora**, A. Geoghan, M.G. Finn

ORGN 568. Design and synthesis of constrained peptides for the induction of autophagy. **L. Peraro**, Z. Zou, B. Levine, J. Kritzer

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center Ballroom East

On the Importance of Synthetic Organic Chemistry in Drug Discovery
J. A. Ellman, V. Mascitti, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 569. Bringing the full power of chemical synthesis to bear on the discovery of new antibiotics. **A.G. Myers**

8:50 ORGN 570. Ledipasvir for the treatment of chronic hepatitis C infection: A potent NS5A antiviral drug and component of the oral once-daily single-tablet regimen Harvoni®. **J.O. Link**, G. Cheng, M.C. Desai, H. Guo, D. Kato, T. Kirschberg, H. Liu, M.L. Mitchell, E. Mogalian, J. Parrish, R.W. Scott, N.H. Squires, J. Sun, J.G. Taylor, Y. Tian, C. Yang, L. Xu

9:35 ORGN 571. Heterocycles and medicinal chemistry: The importance of innovative synthesis. **A. Wood**

10:20 ORGN 572. Potentiating the activities of monoclonal antibodies for cancer and inflammatory disease treatment. **P.D. Senter**

11:05 ORGN 573. Beyond Darunavir: Backbone binding in molecular design to combat drug-resistance. **A.K. Ghosh**

Section B

Boston Convention & Exhibition Center Room 205B/C

Technical Achievements in Organic Chemistry Symposium

K. L. Lee, *Organizer, Presiding*

T. D. White, *Presiding*

9:00 Introductory Remarks.

9:10 ORGN 574. Grignard reagent formation in continuous stirred tank reactors with sequestered magnesium. **T. Braden**, M.D. Johnson, S.A. May, M.E. Kopach

9:40 ORGN 575. Harnessing the power of C-H functionalization in drug discovery. **S. Tyagarajan**, S.B. Boga, L.C. Campeau, T. Cernak, R.K. Dermerjian, D. Dirocco, G.A. Doss, S. Dreher, K.D. Dykstra, R.M. Helmy, S.W. Kraska, R. Kurukulasuriya, Y. Liu, M. Maletic, K. Moore, C.A. Parish, M. Reibarkh, E. Streckfuss, P. Vachal, T. Williamson, H. Yao

10:10 ORGN 576. Triflumezopyrim: A new class of nicotinic acetylcholine receptor inhibiting insecticides. **T.F. Pahutski**, G.P. Lahm, C.W. Holyoke, W. Zhang, D. Cordova, K.A. Hughes, M.T. Tong, D.R. Vincent, R.M. Leighty, E. Benner

10:40 ORGN 577. Flow chemistry: A technology for control freaks. **M.W. Bundesmann**, J.E. Davoren, M.S. Lall, C. Li, J. Yan, Q. Yan

11:10 ORGN 578. New streamlined methods of sulfone and sulfonamide synthesis from aromatic halides and boronic acids. **A. Shavnya**

Section C

Boston Convention & Exhibition Center Room 203

Frontiers of Functional Interfaces

A. Cattani-Scholz, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ORGN 579. Atomically thin free-standing 2D carbon materials and their hybrids for engineering of functional interfaces. **A. Turchanin**

8:50 ORGN 580. Accessing energetic reactions via diamond electrochemistry and photoelectrochemistry. **R.J. Hamers**, G.M. Nathanson, D. Zhu, L. Zhang, J.R. Schmidt, J. Bandy

9:30 Intermission.

9:40 ORGN 581. Electron transport across protein-modified interfaces. **D. Cahen**

10:20 ORGN 582. Interface chemistry in EGaIn-based molecular junctions. **K. Liao**, G.M. Whitesides

11:00 ORGN 583. Electronic properties and applications of functionalized semiconductors. **M. Stutzmann**

11:40 Concluding Remarks.

Section D

Boston Convention & Exhibition Center Room 204A

Heterocycles and Aromatics

M. C. McIntosh, *Organizer*

B. L. DeBoef, *Presiding*

8:00 ORGN 584. Green synthesis of diverse heterocyclic scaffolds. **W. Zhang**

8:20 ORGN 585. Progress towards the synthesis of a bowl-shaped fragment of C₂₄₀. **N. Dodge**, A. Whalley, D.P. Sumry

8:40 ORGN 586. High mobility organic semiconductors: Simple and effective synthesis and functionalization of benzothieno[3,2-b]benzothio-
phene. **J. Hollin**, A. Whalley

9:00 ORGN 587. One-pot synthesis of 3,4,5-trisubstituted 1,2,4-triazoles via the addition of hydrazides to activated secondary amides. **W.S. Bechara**, I.S. Khazhieva, E. Rodriguez, A.B. Charette

9:20 ORGN 588. Synthesis of C–C and C–N bonds via oxidative C–H activation. **B.L. DeBoef**

9:40 ORGN 589. Thiohydroxamic acids as versatile reagents for heterocycle synthesis. **B.C. Lemerrier**, J.G. Pierce

10:00 ORGN 590. Catalytic functionalization of unactivated sp³ C–H bonds through intramolecular oxygen nucleophiles affording cyclic ethers. **S. Thompson**, G. Dong

10:20 ORGN 591. Synthesis of highly twisted porphyrin oligomers base on aniline oxidation. **S. Hiroto**, S. Ito, H. Shinokubo

10:40 ORGN 592. Mechanistic studies to enable a scalable Friedel-Crafts reaction. **J. Albrecht**, **G. Beutner**, B. Cohen, D.A. Conlon, J. Fan, D. Fantair, M. Lawler

11:00 ORGN 593. Synthesis of new heterocyclic fused 3-aminoazepinones. **B. Schurgers**, G. Van Lommen, G. Verniest

11:20 ORGN 594. Quinoline-annulated porphyrins as NIR dyes for bioimaging. **M.P. Luciano**, J. Akgigbe, M. Zeller, Q. Zhu, C. Bruckner

Section E

Boston Convention & Exhibition Center Room 204B

New Reactions and Methodology

M. C. McIntosh, *Organizer*

N. Zheng, *Presiding*

8:00 ORGN 595. Reactivity of photochemically derived tricyclic vinyl aziridines. **E.E. Blackham**, K. Booker-Milburn, J. Knowles

8:20 ORGN 596. Access to nitriles mediated by Bobbitt's salt, an environmentally benign and recyclable oxidant. **K.M. Lambert**, S.A. Eldirany, W.F. Bailey

8:40 ORGN 597. New rearrangement and substitution reactions of ethenylbenzylamines. **X. Shi**, A.C. Chon, A. Hou, W.F. Kiesman

9:00 ORGN 598. Unexpected retroaldol-aldol reaction during O-alkylation of hydroxylated Vince lactam derivatives. **J. BrÄNalt**

9:20 ORGN 599. Withdrawn.

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9:40 ORGN 600. Synthesis of (2,4)-pyrrolophanes via a [3+2] cycloaddition of functionalized donor-acceptor cyclopropanes and nitriles. **N. Vemula**, B.L. Pagenkopf

10:00 ORGN 601. Unprecedented reactivity of the donor-acceptor cyclopropanes in cycloadditions with nitrosoarene. **N. Vemula**, T. Chidley, B.L. Pagenkopf

10:20 ORGN 602. Investigating the anomerisation of selenium glycosides. **A.W. McDonagh**, P.V. Murphy

10:40 ORGN 603. Mechanochemical ruthenium-catalyzed olefin metathesis: From small molecules to polymers. **L. Do**, T. Friscic

11:00 ORGN 604. Metallacyclie-mediated synthesis of highly functionalized decalins. **H. Mizoguchi**, G.C. Micalizio

11:20 ORGN 605. Nickel-catalyzed allylation of imines generated in situ from α -amido sulfones. **J.A. Caputo**, M. Naodovic, D.J. Weix

11:40 ORGN 606. Modulating the reactivity of HF through Laurence's hydrogen bond basicity scale. **O.E. Okoromoba**, G.B. Hammond, B. Xu

Section F

Boston Convention & Exhibition Center Room 206A

Biologically-Related Molecules and Processes

M. C. McIntosh, *Organizer*

D. H. Appella, *Presiding*

8:00 ORGN 657. Bisubstrate analogs and inhibitors of farnesyl diphosphate synthase: Synthesis and enzymatic studies. **G. Ramamoorthy**

8:20 ORGN 658. Evolutionary significance of RNA 2'-5' linkage. **R. Wang**, F. Shen, S.M. Magliocco, V. Valsangkar, **J. Sheng**

8:40 ORGN 659. Synthesis and chemical biology of the morpholinone fragment of the monanchocidins. **Y. Shi**, J.G. Pierce

9:00 ORGN 660. Natural products with the 6-7-5 ring scaffold. **A.S. Bayden**

9:20 ORGN 661. Total synthesis of the potent immunoresolvents Resolvin D3 and Resolvin D4. **J.W. Winkler**, J. Dalli, S. Glynn, C.N. Serhan, N.A. Petasis

9:40 ORGN 662. Diastereoselective design of privileged structures: Forward chemical genetics for phenotypic screening of chemical probes. **T.H. Altel**

10:00 ORGN 663. Copper-catalyzed synthesis of 2-arylpyrrolidines. **C. Um**, S.R. Chemler

10:20 ORGN 664. Multivalent display using a synthetic, PNA-based scaffold to characterize ligand-receptor interactions of α V β 3 integrin, adenosine A2A, and dopamine D2. **D.H. Appella**

10:40 ORGN 665. Late-stage introduction of a diverse variety of heteroaryls into a thioamidine series of BACE inhibitors. **J.C. Murray**, B.T. Oneill, P.J. Mikochnik, K. Ogilvie, J.K. Dutra, L.M. Buzon, L.A. Martinez-Alsina, K.E. Henegar, S.M. Sakyra

11:00 ORGN 666. Fast-click, slow-release strategy to improve solid phase synthesis of RNA. **M. Royzen**, E. Agustini, P. Asare Okai

11:20 ORGN 667. Expansion of bio-orthogonal space: Development of biocompatible reactions with new functionalities. **J. Kim**, C.R. Bertozzi

11:40 ORGN 668. Copper catalyzed benzylic C-H amination using simple amination reagents. **A. Wang**, M. Emmert

Section G

Boston Convention & Exhibition Center Room 206B

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*

A. Buitrago Santanilla, *Presiding*

8:00 ORGN 669. Stereoselective alkoxide-directed metallacycle-mediated annulation reactions and application toward the synthesis of cortistatins. **C. Aquino**, G.C. Micalizio

8:20 ORGN 670. Regio- and stereoselective synthesis of six-membered heterocycles by Lewis acid catalysis. **S. Pathipati**, V. Singh, N. Selander

8:40 ORGN 671. Electroactivated transition-metal catalyzed C-H activation to promote C-N bond formation. **S. Bhatia**, J.E. Jackson

9:00 ORGN 672. Nanomole-scale high-throughput chemistry for the synthesis of complex molecules. **A. Buitrago Santanilla**, E. Regalado, T. Pereira, M. Shevlin, B. Kevin, L.C. Campeau, J. Schneeweis, S. Berritt, Z. Shi, P.G. Nantermet, Y. Liu, R.M. Helmy, C.J. Welch, P. Vachal, I.W. Davies, T. Cernak, S. Dreher

9:20 ORGN 673. Light-switchable catalysis: Molecular-motor-based rhodium complex for asymmetric Alder-ene reaction. **W. Chen**, B. Feringa

9:40 ORGN 674. Copper-catalyzed oxidative coupling between ethers and salicylaldehydes for the selective synthesis of acetals. **B.D. Barve**, Y. Wu, M. El-Shazly, M. Korinek, Y. Cheng, J. Wang, F. Chang

10:00 ORGN 675. Ruthenium-catalyzed tandem-isomerization/asymmetric transfer hydrogenation of allylic alcohols. **T. Slagbrand**, H. Lundberg, H. Adolfsen

10:20 ORGN 676. Pyridine *N*-oxide vs. pyridine substrates for Rh(III)-catalyzed C-H bond functionalization. **S.R. Neufeldt**, G. Jimenez-Oses, J.R. Huckins, O.R. Thiel, K.N. Houk

10:40 ORGN 677. Ene-type cyclization chemistry from cyclohexadiene-tricarbonyliron derivatives. **K.B. Beach**, A.J. Pearson

11:00 ORGN 678. Copper-catalyzed coupling of *N,N*-dimethylaminobenzyl boronate esters with amines. **K.A. McGarry**, A. Duenas, T.B. Clark

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Energy Storage, Solar Fuels, and Biofuels: Satisfying the Energy Needs While Decreasing the Carbon Footprint

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WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center Room 205B/C

Technical Achievements in Organic Chemistry Symposium

K. L. Lee, *Organizer, Presiding*

T. D. White, *Presiding*

2:00 Introductory Remarks.

2:10 ORGN 624. Formation of acyl imidazoles using *N,N*-carbonyldiimidazole — increasing reaction robustness through mechanistic understanding. **K. Engstrom**

2:40 ORGN 625. Forward and reverse chemical genetic approaches toward selective kinase modulation. **E. Harrington**

3:10 ORGN 626. Process development/optimization on the synthesis of an intermediate leading to baricitinib (LY3009014). **M.E. Kobierski**, K. Seibert, E.W. Crick, D.L. Varie, C.V. Luciani, A.L. Fields, T.M. Wilson, M. Lovette, R. Memmer

3:40 ORGN 627. Synthesis of macrocyclic inhibitors for the EML4-ALK project: Route optimization and scale-up of clinical candidate PF-06463922. **J. Hoffman**, M.R. Collins, J. Cui, J.G. Deal, M. He, R.L. Hoffman, Q. Huang, T.W. Johnson, J.C. Kath, P. Le, C. Palmer, P. Richardson, N. Sach, G. Smith, J. Zhu, P. Zhu

Section B

Boston Convention & Exhibition Center Room 203

Materials, Devices and Switches

M. C. McIntosh, *Organizer*

E. S. Sterner, *Presiding*

1:30 ORGN 628. Designing organic materials for humidity-resistant volatile aromatics sensing. **E.S. Sterner**, F. Bertani, J. Im, T.M. Swager

1:50 ORGN 629. Molecular design and synthesis of donor-acceptor type organic molecules for organic light-emitting diode (OLED) applications. **W. Huang**, S.L. Buchwald

2:10 ORGN 630. Polar liquid crystals derived from sulfonium zwitterions of [*closo*-1-CB₁₁H₁₂]⁺. **J. Pecyna**, P. Zagórski, P. Kaszynski

2:30 ORGN 631. Room-temperature red phosphorescence of structurally simple benzo[2,1,3]thiadiazoles. **G.D. Gutierrez**, G.T. Szazama, T.M. Swager

2:50 ORGN 632. Healable polyhydroxyurethane thermosets. **D. Fortman**, J. Brutman, M.A. Hillmyer, W. Dichtel

3:10 ORGN 633. Facile synthesis of substituted iptycenes. **G. Vadehra**, X. Jiang, M.A. Garcia-Garibay

3:30 ORGN 634. Tuning optoelectronic properties of core-substituted naphthalene diimides by the selective conversion of imides to monoimides. **F.S. Etheridge**, R. Fernando, J.A. Golen, A.L. Rheingold, G. Sauvé

3:50 ORGN 635. Crystalline, oriented thin films of a redox-active covalent organic framework for efficient energy storage. **C.R. DeBlase**, K. Hernandez, K. Silberstein, G. Rodriguez-Calero, R.P. Bisbey, H.D. Abruna, W. Dichtel

4:10 ORGN 636. Interplay of molecular packing and electronic coupling: How chemistry can tune the charge-carrier transport properties of organic semiconductors. **K. Thorley**, C. Risko, J.E. Anthony

Section C

Boston Convention & Exhibition Center Room 204A

Heterocycles and Aromatics

M. C. McIntosh, *Organizer*

W. Zhang, *Presiding*

1:00 ORGN 637. Rapid synthesis and SAR studies of antitumor alkaloids in the sempervirine family. **T.D. Bannister**, X. Pan, C. Yang, J. Cleveland

1:20 ORGN 638. Chemistry of six-membered mesoionic 4,6-dioxo-1,3-diazones. **W. Zhang**, C.W. Holyoke, K.A. Hughes, M.T. Tong

1:40 ORGN 639. Azetidine and pyrrolidine derivatives with biological activity in a zebrafish embryo developmental assay. **J.S. Fossey**, A. Feula, S. Dhillon, F. Müller, M. Hama Salih, L. Male

2:00 ORGN 640. Nucleophilic reactions of few selected heterocyclic systems with dibenzoylacetylene. **M. Muneer**

2:20 ORGN 641. Binding of azaborine heterocycles inside the modular cavity of T4 lysozyme mutants. **H. Lee**, T. He, S.Y. Liu

2:40 ORGN 642. Synthetic strategies for water-soluble PEGylated hydrophyrins. **M. Liu**, N. Zhang, J. Jiang, C. Chen, J.S. Lindsey

3:00 ORGN 643. Conformationally assisted lactamizations for the synthesis of protected marine-derived hetero-2,5-diketopiperazines. **J.W. McDaniel**, K. Ha, C.D. Hall

3:20 ORGN 644. Flying molecules: Synthesis of multiporphyrin-systems for quantum interference experiments. **L. Felix**, U. Sezer, M. Arndt, M. Mayor

3:40 ORGN 645. Palladium-catalyzed intermolecular [3+2] cycloaddition reactions of iminoacetoneitriles with trimethylenemethane. **I. Korboukh**, M. Hermsen, R.L. Danheiser

4:00 ORGN 646. Utilizing palladium-catalyzed cyclopropanations to create contorted aromatics. **S.R. Bheemireddy**, K.N. Plunkett

Section D

Boston Convention & Exhibition Center Room 204B

New Reactions and Methodology

M. C. McIntosh, *Organizer*

D. Robbins, *Presiding*

1:00 ORGN 647. Development and application of new methods for nickel-catalyzed amination of phenol derivatives. **D. Robbins**

1:20 ORGN 648. Identifying lead hits in catalyst discovery by screening and deconvoluting complex mixtures of catalyst components. **E. Wolf**, E. Richmond, J. Moran

1:40 ORGN 649. Diversity oriented synthesis of macrocycles using a build/couple/pair/diversity strategy. **F. Nie**, D.L. Kuciw, J.E. Stokes, D.R. Spring

2:00 ORGN 650. Highly selective reductive amination of cycloaliphatic dialdehydes to diamines via macrocyclic polyimine intermediates. **M.L. Tulchinsky**, B.B. Fish

2:20 ORGN 651. Polyepoxide cascade reactions under basic conditions: Progress toward a synthesis of brevisulcinal F. **M.H. Katcher**, T.F. Jamison

2:40 ORGN 652. Study of a one-pot intramolecular sequence of Vilsmeier-Haack reaction and azomethine ylide cycloaddition towards the tricyclic core of the *Aspidosperma* alkaloids. **P. Boissarie**, G. Belanger

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

3:00 ORGN 653. Polyketide-inspired method development: Diastereoselectivity control. **R. Hong**

3:20 ORGN 654. Synthetic strategies toward alotamide **A. M.W. Boudreau, J.G. Pierce**

3:40 ORGN 655. Withdrawn.

4:00 ORGN 656. Withdrawn.

Section E

Boston Convention & Exhibition Center Room 206A

Biologically-Related Molecules and Processes

M. C. McIntosh, *Organizer*

D. A. Harki, *Presiding*

1:00 ORGN 607. Synthesis of 2',3'-modified Uridine/5-methyluridine derivatives. **I. Mohammad, L. McLaughlin**

1:20 ORGN 608. Catch and release DNA decoys. **D.A. Harki, N.B. Struntz, J.K. Hexum**

1:40 ORGN 609. High-throughput palladium quantification using catalysis-based colorimetric detection method for pharmaceutical compounds. **X. Bu, J. Jo, M.P. Tracey, K. Koide, C.J. Welch**

2:00 ORGN 610. Quinoline-based photoremovable protecting groups for activating biologically relevant phenols. **D.E. McLain, A.P. Muliawan, J. Huang, M. Widegren, A.C. Rea, L. Vandenberg, R.E. Ball, A.G. Hudson, Y. Zhu, L.L. Johnston, J.D. Lauderdale, M. Levin, D.L. Phillips, T.M. Dore**

2:20 ORGN 611. Polyvalent catalysts operating on polyvalent substrates: A model system for surface controlled reactivity. **C.S. McKay, M.G. Finn**

2:40 ORGN 612. Photoactivatable mitochondrial specific fluorescent probes. **M.N. Tran, D.M. Chenoweth**

3:00 ORGN 613. P450 BM3 monooxygenase variants as versatile catalysts in organic chemistry. **C. Holec, K. Neufeld, J. Pietruszka**

3:20 ORGN 614. Effects of fatty acyl moieties on antibacterial activities of peptide-immobilized cellulosic materials. **A. Opitakorn, M. Rauytanapanit, T. Praneenararat**

3:40 ORGN 615. Polymorphs, solvates, and hydrates of brexpiprazole. **T.A. Zeidan, P. Navare, J.T. Trotta, M.B. Hickey, M. Oliveira, R.A. Chiarella**

4:00 ORGN 616. Fluorescent sensors for minimally invasive monitoring of blood analytes in vivo. **N.P. Cooley, S.C. Bustamante Lopez, S.C. Rittler, M.A. Milanick, K.E. Meissner, T.E. Glass**

4:20 ORGN 617. Characterizing the prenylome using alkyne-containing isoprenoid probes. **M.D. Distefano, V. Diaz-Rodriguez, C. Palsuledesai**

Section F

Boston Convention & Exhibition Center Room 206B

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*

R. D. Broene, *Presiding*

1:00 ORGN 618. Iridium catalyzed carbocyclizations: Efficient (5+2) cycloadditions of vinylcyclopropanes and alkynes. **M. Melcher, D. Strand**

1:20 ORGN 619. Effective conversion of heteroaromatic ketones into primary amines via hydrogenation of intermediate ketoximes. **K. Baucom, A.S. Guram, C.J. Borths**

1:40 ORGN 620. Unified reaction conditions for the mild and selective Pd-catalyzed C2-arylation of tryptophans and tryptophan-containing peptides. **A. Reay, T. Williams, A. Hammarback, A. Whitwood, I. Fairlamb**

2:00 ORGN 621. Synthesis of quinoxalin-4(3H)-ones in aqueous media catalyzed by a Cp*Ir complex. **L. Lu, F. Li**

2:20 ORGN 622. Fluorous Grubbs metathesis catalysts: Applications in phase transfer activation. **H.S. Bazzi, J. Balogh, H. Su, J.A. Gladysz**

2:40 ORGN 623. C-H propargylic amination using rhodium dimers. **J. Bartholomeus, H. Lebel**

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Artificial Photosynthesis: Challenges and Strategies to Meet Energy Needs in an Environmentally Benign Manner

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WEDNESDAY EVENING

Section A

Boston Convention & Exhibition Center Ballroom

Heterocycles and Aromatics; New Reactions and Methodology

R. D. Broene, *Organizer*

7:00 - 9:00

ORGN 679. Divergent synthesis of aziridines by functionalization of the intact ring. **J.A. Bull, T. Boulton, D.P. Affron**

ORGN 680. Preparation of some aromatic thiols. **H. Hu, T.P. Vaid**

ORGN 681. Chlorin-bacteriochlorin energy transfer dyads with deep-red absorption and near-IR emission. **J. Akhigbe, M. Ptaszek**

ORGN 682. Domino reactions involving dihydrooxazinone precursors affording pyridone and pyridine products. **J. Williamson, J.R. Scheerer**

ORGN 683. Bacteriochlorin dyads with solvent polarity dependent singlet oxygen photosensitization properties. **N.A. Esemoto, Z. Yu, L. Wiratan, M. Ptaszek**

ORGN 684. Synthetic investigations of 3,4-dihydroquinoxalin-2(1H)-one and quinoxalin-2(1H)-one under varied experimental conditions. **J. Kurttila, T. Emery, C.J. Kellen-Yuen**

ORGN 685. Synthesis of highly functionalized 5,5- and 5,6-trans-fused bicyclic heterocycles from anhydro-sugar derivatives. **J. Panteleev, B. Samas, D.W. Kung**

ORGN 686. Protecting group strategy for the boron position in 1,2-azaborines: Copper (I) catalyzed oxidation of 1,2-azaborine. **A. Baggett, S.Y. Liu**

ORGN 687. Ozonation of β -octaalkylporphyrins. **M. Sharma, E. Meehan, C. Bruckner**

ORGN 688. Introduction of carboxyl functionalities to meso-tetrakis(pentafluorophenyl)porphyrins and -hydroporphyrins using S₂Ar chemistry. **N. Hewage, B. Yang, A.G. Agrios, C. Bruckner**

ORGN 689. Cycloaddition — reduction strategies for formation of heterocycles and new carbon-carbon bonds. **D.J. Martynowych, J.M. Roth, J. Stash, E. Holland, M.W. Fennie**

ORGN 690. Copper-catalyzed hydroamination of propargyl imidates. **P.J. Fricke, M.W. Fennie**

ORGN 691. Benzylic cyclizations of alkylpyridines and alkylimidazoles. **M. Joshi, F.C. Pigge**

ORGN 692. Synthesis and characterization of phenylene-containing oligoacenes. **S.P. Luppino, R. Parkhurst, T.M. Swager**

ORGN 693. BN-isosteres of anthracene and tetracene via 2,3-unsymmetrically substituted acenes. **J.S. Ishibashi, S.Y. Liu**

ORGN 694. Building blocks for the synthesis of oligopyrroles and indole analogs. **R. Xiong, E. Borbas**

ORGN 695. Irreversible endo-selective Diels-Alder reactions of substituted alkoxyfurans: A general synthesis of endo-cantharimides. **R. Foster, T.D. Sheppard, H. Hailes, C. Tame, M. Porter, L. Benhamou, K. Bucar**

ORGN 696. Reductive decomposition of triaryl isocyanurates. **M.A. Servos, S.J. Peters**

ORGN 697. Novel synthesis of diaryl heterocycles. **A.N. Thaxton, M. Trudell**

ORGN 698. Diaminoaceneaphthylene, a key but elusive intermediate toward carbonyl-substituted perimidinespirohexadienone photochromes. **A. Prins, J.G. Gillmore**

ORGN 699. Rapid access to 3-aminoinadazoles from aromatic tertiary amides. **P. Cyr, S. Regnier, W.S. Bechara, A.B. Charette**

ORGN 700. Octaethyl-1,3-oxazinochlorin: Expanding octaethylporphyrin. **R. Li, E. Meehan, M. Zeller, C. Bruckner**

ORGN 701. Model studies toward synthesis of xestoproxamine C via intramolecular cyclization of substituted pyridines. **A.I. Lansakara, F.C. Pigge**

ORGN 702. Efficient synthesis of 5-hydroxy-tryptophol and derivatives. **K.G. Henry, J.A. Wisniewski, E.A. Colby Davie**

ORGN 703. Application of Charge-accelerated Claisen rearrangements of N-aryl-2-vinyl aziridines for synthesis of benzazepinones. **S. Rasapalli, U. Javed, J. Kenmoe, A. Atitebi**

ORGN 704. Revisiting the synthesis of quinoxalin-4(3H)-ones by carbonyl functional group removal and via ring contractions of benzodiazepinones. **S. Rasapalli, V. Sammeta, U. Javed, J.A. Boerth, E. Tsogtgerel**

ORGN 705. Biomimetic synthetic studies towards aromatic cores of juanlimycins A-B and divergolides C-D. **S. Rasapalli, A. Wolf, U. Javed, H. Ijaz, P. Exavier**

ORGN 706. Multicomponent green synthesis of aminopyrazoles from oxo-nitriles and their heterocyclic annulations. **S. Rasapalli, R. Mastrolia, M. Caswell, N. Vantangoli**

ORGN 707. Cross-coupling type tandem chloropalladation/dearomative cyclization toward functionalized bridged [3.2.1] skeleton compounds. **G. Liu, Y. Dong**

ORGN 708. Synthesis and in vitro biological evaluation of N-aryl-3-pyrrolyl- β -lactams against cancer cells. **D. Bandyopadhyay, J. Cruz, B.K. Banik**

ORGN 709. Organocatalyzed multicomponent synthesis of pyranopyrazoles: A green approach. **D. Bandyopadhyay, J. Salinas, V.M. Cano, A. Velasco**

ORGN 710. Acid- and base-induced conformational alteration of N,N-diarylamides bearing tropolone. **A. Ito, M. Sato, R. Yamasaki, I. Okamoto**

ORGN 711. Efficient and regioselective halogenation of pyridine N-oxide. **Y. Chen**

ORGN 712. Novel potential bioactive 4-amino substituted 1,2,4-triazolo[4,3-a]quinoxalines: Synthesis and unexpected results by derivatization. **B. Matuszczak, C. Jud, V. Kahlenberg**

ORGN 713. Synthesis of 2-amino-3-cyanopyridine derivatives of dehydroabietic acid catalyzed by ytterbium triflate [Yb(OTf)₃]. **M. Shen, D. Wang, J. Song, S. Shang, S. Liao, Z. Song**

ORGN 714. Concise synthesis of highly functionalized pyrimidine-2,4-(1H,3H)-dione derivatives. **G.C. Sati, D. Crich, E.C. Böttger, A. Vasella**

ORGN 715. Synthesis of 1,2,4-triazines via an intramolecular Staudinger aza-Wittig reaction. **J.K. Johnson, D. Fu, S. Elzner, D. Amantini, P. Wipf**

ORGN 716. Multigram synthesis of α -carboline. **C.A. Zifcsak, B.J. Dugan, L. He, G.R. Ott, B.D. Dorsey**

ORGN 717. Molecular diversity from Ugi 4-CR: Synthesis and biological evaluation of pyrazinoisoquinolines and pyrroloisoindolones. **E. Hernández-Vázquez, L.D. Miranda**

ORGN 718. Tale of two protecting groups — BOC vs. SEM — for directed lithiation and C-C bond formation on a pyrrolopyrimidine core. **R.N. Nair, T.D. Bannister**

ORGN 719. Synthesis of novel hybrid flavones for chemotherapeutic applications. **T. Sum**

ORGN 720. Synthesis of naturally occurring flavonoids and novel biflavonoids for medicinal applications. **T. Sum**

ORGN 721. Design and synthesis of long-wavelength and tumor-selective photodynamic therapy agent. **C. Liu, C. Scott**

ORGN 722. Regio- and stereospecific synthesis of C-3 functionalized proline derivatives by palladium catalyzed directed C(sp³)-H arylation¹. **D.P. Affron, O.A. Davis, J.A. Bull**

ORGN 723. Turning spiroketals inside-out: A rearrangement triggered by an enol ether epoxidation. **C. Lorenc, M. Pecuh, A.J. Williams, G. Martin, A. Moser, A. Buevich, T. Williamson**

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- ORGN 724.** Cyclic *N*-acyliminium ions for the diversity-oriented synthesis of functionalized γ -lactams. **P. Wu**, T.E. Nielsen, M. Clausen
- ORGN 725.** Electron deficient phthalocyanines as solid-state surface complexing agents. **P. Heintz**, C. Colomier, S. Gorun, G. Graffius
- ORGN 726.** Synthesis of benzoxaz-olthioly and benzthiazolthioly fused 3-alkylquinazolin-4(3H)-ones. **C. Venkata Ramana Reddy**, R. Mohammad
- ORGN 727.** Metallo-radical catalysis for stereoselective intramolecular C–H radical amination. **K. Lang**, H. Lu, P.X. Zhang
- ORGN 728.** β -Heteroatom-stabilized carbenes. **G.C. Lada**, L. Terrab, S. Moss, A. Mellinger, J. Unger
- ORGN 729.** Pd-catalyzed hydrogations using water as a solvent as well as hydrogen source. **C.J. Ellstrom**, H. Cho, B. Torok
- ORGN 730.** Lithium in alumina: A new approach to organolithium reagents. **F. Jaliloh**
- ORGN 731.** Stereodivergence in intermolecular [4+3] cycloadditions of bicyclic methylene aziridines. **N. Gerstner**, C. Adams, J.M. Schomaker
- ORGN 732.** Metal mediated condensation reactions of phenols with aldehydes as reactive intermediates in multicomponent reactions. **E. Allen**, S. Schaus
- ORGN 733.** Intramolecular cyclizations of alcohols with rhodium(II) azavinyl carbenoids generated in situ from *N*-sulfonyl-1,2,3-triazole intermediates. **J.M. Bennett**, K.N. Choinski, S.M. Aulita, J.D. Shapiro, Y. Mei, M.M. Majireck
- ORGN 734.** Divergent reactions of indolyl- and pyrrolyl-tethered 1-sulfonyl-1,2,3-triazoles: Efficient synthesis of polycyclic spiroindolines and tetrahydrocarbolines by rhodium(II)-catalyzed intramolecular annulations. **L. Fu**, H.M. Davies
- ORGN 735.** Phosphate-tether mediated ring-closing metathesis to bicyclo[3.1] phosphates: Effects of ring size and stereochemical complexity in the formation of medium and large rings. **J.L. Markley**, S. Maitra, R. Chegondi, P.R. Hanson
- ORGN 736.** Development of a lignin depolymerization strategy using visible-light photoredox catalysis. **G. Magallanes**, B.S. Matsuura, C. Stephenson
- ORGN 737.** Photocatalytic oxidation of lignin model systems by merging palladium and visible-light-induced photoredox catalysis. **M.D. Kaerkaes**, B.S. Matsuura, C. Stephenson
- ORGN 738.** General, high yielding, and green method for the preparation of heterocyclic fused aminoisoxazoles. **W. Yu**, K. Maloney, P. Bulger
- ORGN 739.** Investigating visible light enabled ketyl radical fragmentations, couplings, and cyclizations. **T. Monos**, C. Stephenson
- ORGN 740.** Palladium-catalyzed (hetero) arylation of α - β unsaturated lactams. **D. Canterbury**, K. Hesp, J. Polivkova
- ORGN 741.** Synthesis of some aryl amides — potential double-acting inhibitors — under microwave irradiation. **S.A. Santo**, L.S. Longo Jr, **A.C. Reis**
- ORGN 742.** Flexible synthetic entry into the diterpene class of natural products. **S. Bar**, C. Schindler
- ORGN 743.** Refinement of a biaryl coupling reaction. **S. Corning**
- ORGN 744.** Design of small molecule libraries. **T. Flagstad**, T.E. Nielsen, M. Clausen
- ORGN 745.** Cinchona alkaloid-catalyzed synthesis of chiral trifluoromethylated dihydropyrans. **K. Kasten**, A.D. Smith
- ORGN 746.** Isothiourea-mediated one-pot synthesis of functionalized pyridines. **D.G. Stark**, L.C. Morrill, A.D. Smith
- ORGN 747.** Photocatalytic smiles rearrangement for the construction of the benzylic difluoro functionality. **M.J. Sevrin**, H. Albright, J.J. Douglas, C. Stephenson
- ORGN 748.** Scope of enantioselective homocrotolboration of aldehydes. **L. Tian**, H. Lin, I.J. Krauss
- ORGN 749.** Unsymmetrical 1-halopolyynes — synthesis, structure, and reactivity. **B.Z. Pigulski**, N. Gullia, S. Szafert
- ORGN 750.** Nickel-catalyzed decarboxylative C–H arylation of azoles with perfluoro- and nitrobenzoates. **J. Crawford**, K. Shelton, B. Sadarananda, E. Reeves, D. Kalyani
- ORGN 751.** Nickel-catalyzed decarboxylative cross-coupling of perfluorobenzoates with aryl halides and sulfonates. **L.W. Sardzinski**, W.C. Wertjes, **A.M. Schnaith**, D. Kalyani
- ORGN 752.** Efficient method for the preparation of styrene derivatives via Rh(III)-catalyzed direct C–H vinylation. **K. Otley**, J.A. Ellman
- ORGN 753.** Transition metal catalyzed functionalization of alkynes. **B. Catano**, Y. Xing, C.C. Kim, J. Lee
- ORGN 754.** Ruthenium catalyzed C–H silylation of unprotected gramines, tryptamines, and their congeners. **K. Devaraj**, C. Sollert, C. Juds, P. Gates, L.T. Pilarski
- ORGN 755.** Novel anionic cascade for synthesis of chiral 3-pyrrolones. **I. Chogii**
- ORGN 756.** Palladium catalyzed direct arylation of nitroaromatics. **A.M. Schnaith**, S.B. Davick, D. Kalyani
- ORGN 757.** Selective access to heterocyclic sulfonyl halides in a parallel medicinal chemistry platform. **J. Tucker**, L. Chenard, J.M. Young
- ORGN 758.** Toward the development of a general transannular hydroamination strategy for the synthesis of pyrrolizidine and indolizidine alkaloids. **E.E. Cleary**, K.E. Allen, K.E. Weinert-Stein, A.B. Kaplan, C.C. Williams, B.C. Schafer, B.K. Wesley, C.J. Whiting, M.M. Majireck
- ORGN 759.** Catalytic turnover in Friedel-Crafts arylation of tertiary aliphatic fluorides. **M. Dryzhakov**, J. Moran
- ORGN 760.** Mild and metal-free *N*-arylation of secondary acyclic amides at room temperature. **G. Tinnis**, E. Stridfeldt, H. Lundberg, H. Adolfsson, B. Olofsson
- ORGN 761.** Redox neutral alkylation of electron rich heterocycles using photoredox catalysis. **T.M. Williams**, E. Swift, C. Stephenson
- ORGN 762.** Withdrawn.
- ORGN 763.** Development of a biomimetic biaryl coupling reaction to access strained cyclophanes. **R. Watson**, C. Schindler
- ORGN 764.** Mild and direct lactamization protocol for the synthesis of pyridopyrazine-1,6-diones. **D. Rankic**, C.M. Stiff, C. am Ende, J.M. Humphrey
- ORGN 765.** Catalytic asymmetric synthesis of α -amino acid derivatives through [2,3]-rearrangement. **T. West**, A.D. Smith, D.S. Daniels
- ORGN 766.** Design, synthesis, and anticancer evaluation of diversely substituted 2-azetidinones. **D. Bandyopadhyay**, F. Olazarán-Santibanez, A.K. Contreras, I.M. Chapa, I. Balderas-Rentería, G. Rivera, B.K. Banik
- ORGN 767.** Palladium-catalyzed α -arylation of aryl nitromethanes. **K. VanGelder**, M. Kozłowski
- ORGN 768.** Effective nitrogen radical reactions via Co(II)-based metallo-radical catalysis. **L. Jin**, J. Tao, H. Lu, X. Cui, P.X. Zhang
- ORGN 769.** Improved general synthetic route to dialkylphosphino-alkanes: Featuring the first synthesis of Me-DIOP. **A.J. Kendall**, D.T. Seidenkranz, D. Tyler
- ORGN 770.** Development of predictive models to elucidate the roles of ligand and substrate in tunable silver-catalyzed nitrene transfer. **R.J. Scamp**, R.C. Johnston, S. Hare, P. Cheong, D.J. Tantillo, J.M. Schomaker
- ORGN 771.** Development of a novel Bronsted acid composite material and study of its catalytic performance using cloud computing. **H. Wang**
- ORGN 772.** Metalloalkyl radical-mediated stereoselective radical reactions via Co(II)-based metallo-radical catalysis. **X. Cui**, X. Xu, L. Jin, P.X. Zhang
- ORGN 773.** Route to polysubstituted β -naphthols from coumarins by the directed remote metalation reaction. **J. Patel**, J. Board, **M. Hossain**, V. Snieckus
- ORGN 774.** Taming chlorine azide: Access to 1,2-azidochlorides from alkenes. **R.A. Valiulin**, S.K. Mamiyala, M.G. Finn
- ORGN 775.** Ruthenium-catalyzed cross coupling reaction of 1-naphthylsilanes with internal alkynes via C–H activation. **K. Sugita**, Y. Tokoro, S. Fukuzawa
- ORGN 776.** Regioselective acetylation of TMS ethers: Application toward carbohydrates, glycolipids, and their conjugates. **S.S. Park**, J. Gervay-Hague
- ORGN 777.** Conversion of aldehydes to β -hydroxyboronate esters by diboration/homologation sequences. **C.J. Ferber**, C.M. Moore, C.R. Medina, P. Cannamela, T.B. Clark
- ORGN 778.** *N*-alkylation of anilines and sulfonamides with trichloroacetimidates. **D. Wallach**, P. Stege, J.D. Chisholm
- ORGN 779.** Platinum carbon-catalyzed efficient H–D exchange reaction in 2-propanol/D₂O mixed solvent. **T. Yamada**, K. Morita, Y. Monguchi, Y. Sawama, H. Saijki
- ORGN 780.** Triazabutadiene chemistry in organic synthesis and chemical biology. **F.W. Kimani**, J.C. Jewett
- ORGN 781.** Development of directed photocatalytic C–H and sulfide functionalization with iron catalysts. **H. Albright**, C. Schindler
- ORGN 782.** Zirconium (IV) catalyzed ring opening of on-DNA epoxides in water and its application in DNA-encoded library (DEL) synthesis. **L. Fan**, C.P. Davie
- ORGN 783.** Structural requirements for diastereoselectivity in aza-Cope rearrangement: Mannich cyclizations leading to 2,2-disubstituted-4-acylpyrrolidines. **H.A. Lindsay**, J. Hunt
- ORGN 784.** Aza-Cope rearrangement—Mannich cyclizations of imines: A protecting-group free route to acyl pyrrolidines. **A. Oudeif**, J.M. Reder, B. Yambrosic, P. Pineau, H.A. Lindsay
- ORGN 785.** Palladium-catalyzed synthesis of sulfones by the alkylation of (hetero)aryl boronic acids. **K. Hesp**, A. Shavnya, V. Mascitti, A.C. Smith
- ORGN 786.** Three-component coupling approach for the synthesis of diverse heterocycles utilizing reactive nitrilium trapping. **A. Varadi**, T.C. Palmer, P.R. Notis, G.N. Redel-Traub, D. Afonin, J. Subrath, G.W. Pasternak, C. Hu, I. Sharma, S. Majumdar
- ORGN 787.** Effective synthesis of 3-amino-2-alkenones. **J.M. Young**, B. Torok, R. Dembinski
- ORGN 788.** Bis-imidazolium dicationic ionic liquids as alternative solvents for metal triflate-catalyzed Gröbe-Blackburn-Bienamy multi-component reaction. **L.S. Longo Jr**, P. Licence
- ORGN 789.** Synthesis of trifluoroethyl amines as new, stable scaffolds for lead structure research. **A. Deusch**, A. Hoffmann-Röder
- ORGN 790.** Progress toward an asymmetric [2+2] photocycloaddition: Investigation of ureas and thioureas as H-bonding chiral hosts. **A. Shrestha**, N. Camasso, M. Shinn, E.C. McLaughlin
- ORGN 791.** Photolabile protecting group for hydroxamic acid. **K.T. Mortensen**, L.B. Olsen, T.E. Nielsen, K. Qvortrup
- ORGN 792.** Tactic for the installation of sulfonamide pharmacophores on biaryls via palladium-catalyzed oxidative coupling: Access to functionalized 2-arylindoles, rarely explored in drug discovery. **N. Dayal**, K.P. Jethava, D.V. Prajapati, J. Laha
- ORGN 793.** Isothiourea mediated surface modification of self-assembled monolayers on SiO₂. **R. Chisholm**, J.D. Parkin, G. Haehner, A.D. Smith
- ORGN 794.** Erbium triflate catalyzed allylation of cyclic acetals. **R.S. Mohan**, K.G. Nottingham, N.C. Lazzara
- ORGN 795.** Oxidation and functionalization of methane via palladium(II) catalysis and a free radical process. **N. Zargari**, J. Lee, J. Chen, A. Coward, K.W. Jung
- ORGN 796.** Bimetallic cross-coupling of unactivated alkenes. **N. Zargari**, **G. de Prevoisin**, G. Ahn, Y. Kim, K. Kaneshiro, R. Runberg, J. Park, K.W. Jung
- ORGN 797.** Thioetherification and etherification under neutral conditions using trichloroacetimidates. **B. Duffy**, K. Howard, J.D. Chisholm
- ORGN 798.** Thermally induced C–H functionalization by donor/acceptor carbenes. **C. Tortoreto**, H.M. Davies

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

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Using Passive Sampling Techniques to Detect Organic Contaminants

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THURSDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 203

Chemistry of Fullerenes, Carbon Nanotubes, and Graphene

M. C. McIntosh, *Organizer*

G. Han, *Presiding*

8:00 ORGN 799. Interior functionalization of fullerene fragments: Geometry transformation and solid state aggregation patterns upon addition of dihalocarbenes to a π-bowl. C. Dubceac, A.S. Filatov, A. Zabula, M.A. Ptrukhina

8:20 ORGN 800. Withdrawn.

8:40 ORGN 801. Covalent functionalization of carbon nanotubes with iodonium salts. M. He

9:00 ORGN 802. Rapid synthesis of crowded aromatic architectures from silyl acetylenes. S. Hein, H. Arslan, I. Keresztes, W. Dichtel

9:20 ORGN 803. Electrochemical route to generate self-assembled graphene-like structures from aromatic hydrocarbons. M. Marcaccio, E. Ussano, G. Valentini, L.T. Scott, C. Fontanesi, F. Paolucci

9:40 ORGN 804. Ambient-processed transition metal oxide free-Perovskite solar cells enabled by a new organic charge transport layer. G. Han, S. Chang, S. Gradecak, T.M. Swager

Section B

Boston Convention & Exhibition Center
Room 204A

Heterocycles and Aromatics

M. C. McIntosh, *Organizer*

Y. Lian, *Presiding*

8:00 ORGN 805. Synthesis and functionalization of highly substituted oxetanes: Molecular scaffolds for drug discovery. O.A. Davis, J.A. Bull

8:20 ORGN 806. Stereoselective functionalization of saturated heterocycles by palladium catalyzed C(sp³)-H arylation. J.A. Bull, D.P. Affron

8:40 ORGN 807. Design, syntheses, and characterizations of [4,4,4]tridecastarphenes. H. Geng, G.P. Miller

9:00 ORGN 808. Reaction of diaminopyrimidines with aldehydes: A new mode of reactivity and a highly fluorescent product. G.E. Greco, Z.A. Conrad, A.M. Johnston, Q. Li, E.L. Timothy

9:20 ORGN 809. Directed ortho-metalation (DoM) and directed metalation group (DMG) — dance strategies for the synthesis of C-7 (C-4) substituted benzimidazoles. S. Singh, A. Friedman, S. Gomes, M. Kitching, V. Snieckus

9:40 ORGN 810. Iron trichloride-catalyzed biaryl synthesis via ring-opening Friedel-Crafts arylation of 1,4-epoxy-1,4-dihydronaphthalenes. S. Asai, T. Kawajiri, Y. Monguchi, H. Sajiki, Y. Sawama

10:00 ORGN 811. Expedient synthesis of gem-dialkylbenzyl heterocycles through olefinic hydroarylation. Y. Lian, K. Burford, A.T. Londregan

10:20 ORGN 812. Synthesis and antioxidant properties of anthocyanidins. A. Tuuchi, P. Chen, H.S. Barcena

Section C

Boston Convention & Exhibition Center
Room 204B

Flow Chemistry and Continuous Processes

M. C. McIntosh, *Organizer*

E. Levesque, *Presiding*

8:00 ORGN 813. On-demand diattenuator diazo reagents: In-flow generation and purification. E. Levesque, S.T. Laporte, S. Vanier, A.B. Charette

8:20 ORGN 814. Dynamic systems in flow: A new approach toward the synthesis of porous organic cages. M.E. Briggs, N. Lunt, A.G. Slater, R.L. Greenaway, A.I. Cooper

8:40 ORGN 815. Development of efficient flow reactions using heterogeneous catalysts. T. Hattori, A. Tsubone, T. Ida, Y. Sawama, Y. Monguchi, H. Sajiki

9:00 ORGN 816. Continuous flow halogenation: Challenges and opportunities. R.V. Jones, L. Kocsis, T. Sipocz, F. Darvas

9:20 ORGN 817. Polystyrene-supported 9-amino(9-deoxy)epi quinine derivative for continuous flow asymmetric Michael reactions. J. Izquierdo-Ferrer, C. Ayats, A. Henseler, M.A. Pericas

Section D

Boston Convention & Exhibition Center
Room 206A

Biologically-Related Molecules and Processes

M. C. McIntosh, *Organizer*

M. D. Distefano, *Presiding*

8:00 ORGN 818. Natural product-inspired fragment-based drug discovery: Development of *M. tuberculosis* CYP121 inhibitors. M. Kavanagh, J.L. Gray, A.G. Coyne, H. Davis, K. McLean, A.W. Munro, C. Abell

8:20 ORGN 819. Discovery and optimization of peptide-based ligands for the CuAAC reaction. A. Geoghan, L.C. Dahora, M.G. Finn

8:40 ORGN 820. Probes to perturb the protein-protein interface in α-antithrombin. D. Xin, K. Burgess

9:00 ORGN 821. Application of 1,3-dipolar cycloaddition reaction for protein labeling. Z. Wang, A. Leverette, A. Daughtry

9:20 ORGN 822. Synthesis of phospholipid analogs for real-time monitoring of lipolysis by phospholipase A₂ enzymes. J. Hajdu, D. Trinh

9:40 ORGN 823. Marine very long-chain methoxylated Δ5,9 fatty acids are effective inhibitors of topoisomerases IB. N.M. Carballeira, N. Montano, A. Rodriguez, L.A. Amador, R. Balana-Fouce, R. Reguera

10:00 ORGN 824. Drug discovery: From computational screening to synthesis of lead compounds. J. Brown, J. Sirois, B.L. DeBoef

10:20 ORGN 825. Maltose containing a thioacetal linkage is resistant to hydrolysis and efficiently targets bacteris in vivo. X. Wang, N. Murthy

10:40 ORGN 826. Theoretical modeling of (An)ion transport in liposomes. S.A. Kostina

11:00 ORGN 827. New fluorescence turn-on and turn-off probe for biological investigations. X. Shang, R. Lai, X. Zhou, J. Guo

11:20 ORGN 828. Compatibility of non-REACH restricted solvents with chemiluminescent labeling processes. J. Grote

11:40 ORGN 829. Chemical synthesis and biological investigation of roccaglate analogs. W. Wang, J.A. Porco

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Designs: From Molecules to Functional Materials

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PHYS

Division of Physical Chemistry

E. Sibert, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Accelerated Discovery of Chemical Compounds: Design New Polymers & Inorganic Materials from Integration of Polymer Science, Materials Science, & Informatics (see COMP, Sunday, Monday)

Calculating pK_a's & Redox Potentials (see COMP, Sunday, Monday, Tuesday)

Molecular Dynamics Simulations in Drug Discovery (see COMP, Monday, Tuesday)

Quantum Chemistry (see COMP, Monday, Tuesday, Wednesday, Thursday)

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials (see ENVR, Tuesday, Wednesday, Thursday)

Computational Study of Water (see COMP, Wednesday, Thursday)

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 251

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

Interfacial Phenomena

Cosponsored by COLL

A. E. Bragg, *Organizer*

A. T. Krummel, P. B. Petersen, *Organizers, Presiding*

8:00 PHYS 7. New vibrational probes of H-bonding at aqueous interfaces. A.V. Benderskii

8:35 PHYS 2. Freezing reactive ions in time: Nonlinear optical imaging of X-ray induced photoelectrons. G.J. Simpson

8:55 PHYS 3. Ultrafast structural dynamics of interfacial water molecules revealed by 2D sum frequency generation vibrational spectroscopy. R. Livingstone, M. Bonn, E. Backus

9:30 PHYS 4. Accurate lineshapes from sub-1 cm⁻¹ resolution sum frequency generation vibrational spectroscopy of alpha-pinene at room temperature. F. Geiger

9:50 Intermission.

10:10 PHYS 5. Complex water solutions: Organization and intermolecular interactions revealed for water, ions, and lipids at surfaces. H.C. Allen, D. Verreault

10:45 PHYS 6. Investigation of synchrotron induced local electric fields produced by second harmonic generation microscopy. J.A. Newman, C.M. Dettmar, S. Toth, M. Becker, R.F. Fischetti, G.J. Simpson

11:05 PHYS 1. Revealing H-bond structure at the aqueous interface and in confined environments. M.J. Shultz, A. Brumberg, P.J. Bisson, R.M. Shultz, T.H. Vu

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

Novel Architectures and Representations for Large-Scale Calculations

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*

E. F. Valeev, *Presiding*

8:00 PHYS 8. Using next-generation architectures to model large and complex molecular environments. W. Dejong

8:40 PHYS 9. Multiconfigurational quantum chemistry on graphical processing units. E.G. Hohenstein

9:00 PHYS 10. Electronic structure theory as generalized N-body problem: Strong scaling for fast solvers. M. Challacombe

9:40 PHYS 11. New algorithm for general tensor contractions on GPUs, accelerators, and multicore CPUs. I. Kaliman, E. Epifanovsky, A. Krylov

10:00 PHYS 12. Withdrawn.

Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENVR

D. A. Knopf, S. Lee, *Organizers, Presiding*

8:00 PHYS 13. Atmospheric fate and effects of organic aerosol particles: An interplay between natural sources and human activities. I. Riipinen, B. Murphy, S. Häme, M. Dalirian, N. Rastak, J. Werner, J. Julin, S. Pandis, V.F. McNeill, O. Björneholm, A. Ekman

8:30 PHYS 14. Chemical imaging of atmospheric particles. A. Laskin

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- 9:00 PHYS 15.** Diversity of oxygenated organic compounds in atmospheric particles during SOAS. **K.A. Pratt**, E. Boone, A. Laskin, J. Laskin, M. Riva, J. Surratt, M. Nhiziyo, A.P. Ault, S.B. Bertman
- 9:30 PHYS 16.** Detection and quantification of reactive oxygen species in ambient and laboratory-generated organic aerosols. **M. Shiraiwa**, A. Arangio, H. Tong, U. Pöschl
- 10:00 PHYS 17.** H₂O uptake on atmospheric aerosols from microscopy and quartz crystal microbalance methods. **M.K. Gilles**, T.H. Harder, D. Farland, N. Vezina, D. Yancey Pien, R. O'Brien, S.T. Kelly, M.D. Petters, B. Wang, A. Laskin
- 10:30 PHYS 18.** Need for accurate chemistry in aerosol models: Aerosols effects on deep-convective clouds and lightning. **J. Pierce**, D.C. Stolz, S.A. Rutledge
- 11:00 PHYS 19.** Influence of water vapor near UV absorption on solar irradiance: Laboratory studies and model simulation. **L. Zhu**
- 11:15 PHYS 20.** Bimolecular reactions of dicarbon radicals with C_s, C_n, and C_s unsaturated hydrocarbons: Energetics and dynamics of combustion intermediates. **B.B. Dangji**, D.S. Parker, R. Kaiser, A. Landera, D. Belisario-Lara, A.M. Mebel

Section E

Boston Convention & Exhibition Center
Room 254B

Materials for Heat to Energy Conversion

M. G. Kanatzidis, *Organizer*

R. Seshadri, *Organizer, Presiding*

- 8:00 PHYS 21.** Zintl phases as electron-crystal phonon-glass materials. **S. Kazlarich**
- 8:30 PHYS 22.** Materials genome approach to computational design of nanostructured thermoelectrics. **C. Wolverton**
- 9:00 PHYS 23.** Tailoring electronic transports in bulk nanostructured half-Heusler alloys. **P.F. Poudeu**
- 9:30** Intermission.
- 9:50 PHYS 24.** Thermoelectric power enhancement and anisotropic thermoelectric property of ordered PEDOT:PSS films. **T. Ishida**, M. Mukaida, Q. Wei, K. Kirihara
- 10:10 PHYS 25.** Semiconducting polymer-inorganic microstructure dopant thermoelectric composites. **H.E. Katz**, R.M. Ireland, X. Guo, D. Madan
- 10:25 PHYS 26.** Structure, bonding, and anharmonicity in tetrahedrite-based thermoelectrics. **D. Morelli**
- 10:55 PHYS 27.** Charge transfer in the lithium-benzene complex via Density Functional Theory. **C.H. Borca**, L.V. Slipchenko, A. Wasserman

Section F

Boston Convention & Exhibition Center
Room 255

Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact Fundamentals and Applications

Cosponsored by COLL

C. Burda, *Organizer*

K. Hamad-Schifferli, W. Parak, *Organizers, Presiding*

- 8:00 PHYS 28.** Nanoparticle-lipid coronas. **C.J. Murphy**
- 8:30 PHYS 29.** Fabrication and applications of corona-free nanoparticles. **V.M. Rotello**
- 9:00 PHYS 30.** Controlling biomolecular structure and function at the bio/abio interface. **L.J. Webb**
- 9:30 PHYS 31.** Role of the protein corona in mediating nanoparticle targeting. **W. Chan**
- 10:00 PHYS 32.** Development of a physiologically-relevant multivariate nanoparticle molecular interaction fingerprint: Updates on the Biological Surface Adsorption Index (BSAI). **J. Riviere**
- 10:30 PHYS 33.** Biological identity of nanomaterials: Mapping the protein corona. **P.M. Kelly**, K.A. Dawson

Section G

Boston Convention & Exhibition Center
Room 256

Physical Chemistry of Clusters & Nanoparticles

Catalysis

Financially supported by Mantis Deposition, Ltd.
D. Jiang, G. E. Johnson, *Organizers, Presiding*

- 8:00 PHYS 34.** Size and temperature window for efficient hydrogenation of ethylene on platinum clusters. **U. Heiz**
- 8:30 PHYS 35.** Effect of reaction induced nanoparticle restructuring on coke deposition as probed by operando spectroscopy and microscopy. **S. Zhao**, Y. Li, Q. Wu, A. Orlov, E. Stach, A. Frenkel, R.G. Nuzzo
- 8:50 PHYS 36.** Cluster size matters: Size-dependent performance of subnanometer clusters in heterogeneous catalysis, electrocatalysis, and Li-air batteries. **S. Vajda**
- 9:20** Intermission.
- 9:40 PHYS 37.** New approaches for the acceleration of catalytic processes for solar fuel generation. **I. Hod**, O.K. Farha, J.T. Hupp
- 10:00 PHYS 38.** Catalytic subnano clusters: A playground of chemical bonding. **A. Alexandrova**
- 10:30 PHYS 39.** Temperature-dependent evolution of the oxidation state of cobalt and platinum in Co_{1-x}Pt_x bimetallic clusters under H₂ and CO + H₂ mixture. **B. Yang**, G. Khadra, J. Tuaille-Combes, E. Tjo, S. Seifert, X. Chen, V. Dupuis, S. Vajda

Section H

Boston Convention & Exhibition Center
Room 257A

Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability, & Spectroscopic Signatures What Astrochemistry has Taught Chemists

M. S. El-Shall, *Organizer*

R. C. Fortenberry, *Organizer, Presiding*

- 8:00** Introductory Remarks.
- 8:10 PHYS 40.** How astrochemists add to our knowledge of chemistry. **E. Herbst**
- 9:00 PHYS 41.** Computing the spectroscopic signatures of molecules in various astrophysical environments: Rotational, rovibrational, and electronic spectroscopy. **T.J. Lee**, X. Huang, P. Bera, R.C. Fortenberry, C. Mackie, A. Candian, A. Tielens
- 9:35** Intermission.
- 10:05 PHYS 42.** Curious case of NH₂OH: Hunting a direct amino acid precursor species in the interstellar medium. **B. McGuire**, B. Carroll, K. Dollhopf, G.A. Blake, A. Remijan
- 10:40 PHYS 43.** Interplay between ice chemistry and desorption in the dense interstellar medium. **E. Fayolle**, K. Oberg, J. Bergner, D. Graninger, M. Rajappan, M. Bertin, J. Fillion, X. Michaut, C. Romanzin, R. Garrod, E. van Dishoeck
- 11:05 PHYS 44.** Formation pathways, reactivity, stability, and structure of astrophysically relevant organic ions. **M.S. El-Shall**

Section I

Boston Convention & Exhibition Center
Room 257B

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Cosponsored by COMP

M. Kertesz, C. A. Parish, *Organizers*

H. Lischka, *Organizer, Presiding*

A. Krylov, *Presiding*

- 8:00 PHYS 45.** Diradicals, lurking. **R. Hoffmann**, T. Zeng, P. Xu, Y. Tsuji
- 8:40 PHYS 46.** Enhanced electrical conductivity in substitutionally doped organic molecular solids based on spiro-bis(phenalenyl)boron radicals. **R.C. Haddon**
- 9:20** Intermission.
- 9:50 PHYS 47.** Experimental and theoretical studies of quinonimides and quinonimidyl radicals. **P. Wenthold**
- 10:30 PHYS 48.** Effect of the substitution of oxygen for CH₂ on the singlet-triplet energy differences (ΔE_{ST}) in trimethylenemethane \rightarrow oxyallyl, *meta*-benzoquinodimethane \rightarrow *meta*-benzoquinone and 1,2,4,5-tetramethylenebenzene \rightarrow 1,2,4,5-tetraoxatetramethylenebenzene. **X. Wang**, B. Chen, D.A. Hrovat, **W.T. Borden**

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 251

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

Interfacial Phenomena in Materials

Cosponsored by COLL

A. E. Bragg, A. T. Krummel, P. B. Petersen, *Organizers*

C. G. Elles, *Presiding*

- 1:30 PHYS 49.** Free energies of the hydrated electron: Understanding the electron's temperature dependence and behavior at the air/water interface. **B.J. Schwartz**, W.J. Glover, J.R. Casey
- 2:05 PHYS 50.** Finding conical intersections in condensed phase systems via quantum dynamics of model system-bath Hamiltonians. **M. Mavros**, D. Hait, V. Vaissier, T.A. Van Voorhis
- 2:25 PHYS 106.** In vivo 2D electronic spectroscopy. **G.S. Engel**, P.D. Dahlberg, S. Chamberlin, C. Hunter
- 3:00** Intermission.
- 3:20 PHYS 52.** Ultrafast vibrational spectroscopy (2D-IR) of solutes in ionic liquids. **Z. Ren**, T. Brinzer, S. Dutta, E. Berquist, D. Lambrecht, **S. Garrett-Roe**
- 3:55 PHYS 53.** Watching molecules jump: Ultrafast nonlinear terahertz spectroscopy of liquids and binary mixtures. **M.A. Allodi**, I. Finneran, G.A. Blake
- 4:15 PHYS 54.** Dynamics and spectroscopy of water, alcohols, and carbon dioxide in ionic liquids. **S. Corcelli**

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

Massively Parallel Electronic Structure

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*

D. Lambrecht, *Presiding*

- 1:30 PHYS 55.** Massively scalable coupled cluster codes using data-flow-based execution. **T.L. Windus**, K. Kowalski, A. Danalis, H. McCraw
- 2:10 PHYS 56.** Massively parallel fragment based methods as implemented in Psi4. **R. Richard**, D. Sherrill
- 2:30 PHYS 57.** Algorithmic and software techniques for scaling quantum chemistry on massively parallel computers. **J.R. Hammond**
- 3:10 PHYS 58.** Scalable electronic structure methods based on block-sparse and general compressed tensor representations. **E.F. Valeev**
- 3:50 PHYS 59.** Large-scale real-time TDDFT simulation: Plane-wave implementation and applications to condensed phase systems. **A. Schleife**, K.G. Reeves, A.A. Correa, **Y. Kanai**
- 4:10 PHYS 60.** Beyond "biologically relevant": Applying computationally tractable standards for noncovalent interactions to develop next-generation chemical databases. **L.A. Burns**, J. Faver, D. Sherrill, K.M. Merz

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

4:30 PHYS 61. First principles spectroscopy of heterogeneous systems: Recent advances in GW and hybrid functional calculations. G.A. Galli

Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENVR

D. A. Knopf, S. Lee, *Organizers*

N. M. Donahue, L. Zhu, *Presiding*

1:30 PHYS 62. Measurement and modeling of site-specific nitrogen and oxygen isotopic composition of atmospheric nitrous oxide at Mace Head, Ireland. M.J. McClellan, E. Harris, W. Olszewski, S. Ono, R. Prinn

1:45 PHYS 63. Ambient and modified atmospheric ion chemistry: From top to bottom. A.A. Viggiano, N. Shuman, D. Hunton

2:15 PHYS 64. Insights into the chemistry and impacts of peroxyxynitric acid (HO₂NO₂) and nitrous acid (HONO) on wintertime ozone formation in the Uintah Basin. P. Veres, J. Roberts, S. Alvarez, T. Bates, S.S. Brown, F. Colosimo, P. Edwards, J. Flynn, J. de Gouw, J. Johnson, B. Lefer, J. Liggio, K. Min, P.K. Quinn, J. Stutz, C. Tsai, J.J. Wentzell, R. Wild, B. Yuan

2:45 PHYS 65. Observations of gaseous organic acids from oceanic sources in the summertime Arctic. J.J. Wentzell, A.K. Lee, J. Liggio, E.L. Mungall, J.L. Thomas, J.P. Abbatt

3:00 PHYS 66. On the lifetime of nitrogen oxides in the continental boundary layer. R.C. Cohen

3:30 PHYS 67. New approaches to sticky molecules: Advances in detection of ammonia and nitric acid on short timescales suitable for eddy covariance flux measurements. J. Roscioli, S.C. Herndon, J.B. Nowak, D. Jervis, M.S. Zahniser, D. Nelson, J.B. McManus

3:45 PHYS 68. Identification and characterization of ammonia sources in the front range of Colorado and their influence on particle composition. J.B. Nowak, J. Roscioli, S.C. Herndon, M.S. Zahniser, D. Nelson, J.B. McManus, R. Bahreini, K.K. Vu, J. Dingle, G. Huey, D. Tanner, M. Frank, T. Campos, F. Flocke

4:00 PHYS 69. Precise determination of methane isotopes from direct absorption spectroscopy: Measurement of small samples. J.H. Shorter, T.I. Yacovitch, D. Nelson, M.S. Zahniser, D. Jervis, J.B. McManus, S.C. Herndon, C. McCalley

4:15 PHYS 70. Laser based, ultra-high precision isotope monitor for carbon dioxide. D. Nelson, J.B. McManus, S.C. Herndon, M.S. Zahniser

Section D

Boston Convention & Exhibition Center
Room 254A

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Proteins

Cosponsored by COMP

E. Alexov, R. Luo, *Organizers*

M. Feig, *Presiding*

1:30 PHYS 71. Structure, function, and inhibitors of the acid-gated *Helicobacter pylori* urea channel, an essential component for acid survival and chronic infection. H. Luecke

2:10 PHYS 72. Massively-parallel pipeline to investigate structure-to-function relationships for human disease mutations. H. Yu

2:50 Intermission.

3:10 PHYS 73. Complex energy landscape of the protein IscU. I.K. Ali, J.R. Bothe, Z. Dai, J.H. Kim, R.O. Frederick, M. Tonelli, W.M. Westler, J.L. Markley

3:50 PHYS 74. IR probes of protein electrostatics and dynamics. F.E. Romesberg

4:30 PHYS 75. Membrane protein folding. J.E. Kim

Section E

Boston Convention & Exhibition Center
Room 254B

Materials for Heat to Energy Conversion

M. G. Kanatzidis, R. Seshadri, *Organizers*

E. Toberer, *Presiding*

1:30 PHYS 76. Effect of the spin degree of freedom on solid-state heat-to-electricity converters. J.P. Heremans, H. Jin, S. Watzman, S.R. Boona

2:00 PHYS 77. Investigation of the thermoelectric properties in some oxides, sulfides, and selenides. S. Hebert

2:30 PHYS 78. Exploring the interplay between chemical bonding and magnetic interactions in layered AlFe₂B₂ compounds. R. Barua, B. Lejune, L. Lewis

2:45 Intermission.

3:05 PHYS 79. Material descriptors for predicting thermoelectric performance. E. Toberer

3:35 PHYS 80. Engineering figure of merit as a direct indicator of thermoelectric conversion efficiency and power generation. Z. Ren

4:05 PHYS 81. All-scale hierarchical thermoelectrics based on SnTe. M.G. Kanatzidis, G. Tan, L. Zhao, F. Shi, S. Hao, V.D. Draid, C. Wolverton

Section F

Boston Convention & Exhibition Center
Room 255

Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Fundamentals and Applications

Cosponsored by COLL

C. Burda, *Organizer*

K. Hamad-Schifferli, W. Parak, *Organizers*, *Presiding*

1:30 PHYS 82. Coating and labeling gold nanoparticles for biotargeting. L. Liz Marzan

2:00 PHYS 83. Pyridine-modified amphiphilic polymer: Strategy to improve the performance of polymer-coated quantum dots in diverse analytical and bio-applications. C. Carrillo-Carrion, W. Parak

2:20 PHYS 84. Loading and releasing payloads from protein coronas surrounding gold nanoparticles. H. de Puig Guixé, A. Cifuentes, J. Kah, S. Borros, K. Hamad-Schifferli

2:40 PHYS 85. Microscopic understanding of nanoparticle biological interactions. K.A. Dawson

3:10 PHYS 86. Biocompatible nanoparticles with a polypeptide corona by emulsion polymerisation. M. Klapper, R. Dorrestein, F. Karagoz, S. Parekh, K. Muellen

3:40 PHYS 87. Influence of nanoparticle physicochemical properties on diamond and gold nanoparticle interaction with soluble proteins. E. Melby, H. Abbott, T. Kuech, M.D. Torelli, A. Vartanian, L.M. Jacob, M. Tonelli, R.J. Hamers, C.J. Murphy, J.A. Pedersen

Section G

Boston Convention & Exhibition Center
Room 256

Physical Chemistry of Clusters & Nanoparticles

Catalysis

Financially supported by Extrel CMS

D. Jiang, *Organizer*

G. E. Johnson, *Organizer, Presiding*

A. C. Reber, *Presiding*

1:30 PHYS 88. Influence of support effects on the catalytic activity of graphene-supported platinum nanoclusters for CO oxidation. A. Ramasubramaniam

2:00 PHYS 89. Reactivity and solvation of redox products in mixed molecular-RTILs solvents: Nanodomains partition. A. Atifi, M.D. Ryan

2:20 PHYS 90. Cluster catalysis: Gas phase and surface clusters. X. Tang, X. Zhang, Z. Hicks, G. Liu, K.H. Bowen

2:50 Intermission.

3:10 PHYS 91. Catalytic nanoparticles in solid oxide fuel cells based on triode operation. D. Joyce, V. Broadley

3:40 PHYS 92. Average physical enhancement of OH radical production in water by nanomaterials under hard X-ray irradiation. T. Guo

Section H

Boston Convention & Exhibition Center
Room 257A

Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability, & Spectroscopic Signatures Inorganic Astrochemistry

M. S. El-Shall, R. C. Fortenberry, *Organizers*

N. J. Reilly, *Presiding*

1:30 PHYS 93. Crossed molecular beams and computational study on the formation of organosilicon molecules in the interstellar medium. R. Kaiser, T. Yang, B.B. Dangi, L. Bertels, M.P. Head-Gordon

2:05 PHYS 94. Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology? N.J. Deyonker, T.N. Brown, K.O. Brown

2:40 PHYS 95. Laser detection and characterization of transient gas phase silicon species. D. Kokkin, T. Steimle

3:15 Intermission.

3:45 PHYS 96. Spectroscopic and photochemical properties of the nitrogen oxide sulfide (SNO) radical and its isomer. J.S. Francisco, R.C. Fortenberry

4:20 PHYS 97. Spectroscopic, structural, and energetic analysis of noble gas cations. R.C. Fortenberry, R.A. Theis

Section I

Boston Convention & Exhibition Center
Room 257B

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Cosponsored by COMP

H. Lischka, C. A. Parish, *Organizers*

M. Kertesz, *Organizer, Presiding*

P. Wenthold, *Presiding*

1:30 PHYS 98. High-spin organic molecules. A. Rajca

2:10 PHYS 99. Diradicals, triradicals, and polyradicals the easy way: The spin-flip approach. A. Krylov

2:50 Intermission.

3:20 PHYS 100. Multireference coupled cluster theory applied to problematic radical-radical abstraction reactions. W.D. Allen, B. Magers, C. Wu, L.B. Harding, S.J. Klippenstein

4:00 PHYS 101. Highly correlated multireference studies of aromatic polyradicals. C.A. Parish

4:25 PHYS 102. Approximate projection as an efficient approach for studying challenging electronic structures: From metal oxide clusters to non-innocent ligands. H.P. Hratchian

4:50 PHYS 103. Extended multireference characterization of naphthalene- and fulvalene-derived tetraradicals. J. Schriber, C.A. Parish

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 251

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

Liquid Environments

Cosponsored by COLL

A. E. Bragg, A. T. Krummel, P. B. Petersen, *Organizers*

S. Garrett-Roe, *Presiding*

8:00 PHYS 104. Light, molecules, action: Broadband UV-visible transient absorption studies of excited state dynamics in photoactive molecules. R.J. Sension, B. Arruda, T.E. Wiley, K.G. Spears, N.A. Miller

8:35 PHYS 105. Ultrafast vibrational dynamics of hydrogen-bonded complexes. A.M. Stingel, B.L. Van Hoozen, P.B. Petersen

8:55 PHYS 51. Dynamics in the isotropic phase of liquid crystals — 2D IR experiments and mode coupling theory. M.D. Fayer, K.P. Sokolowsky, H.E. Bailey

9:30 PHYS 107. Coupled electron-proton dynamics measured by ultrafast spectroscopy in solids and molecular models. A. Rury, E. Driscoll, S. Sorenson, J.M. Dawlaty

9:50 Intermission.

- 10:10 PHYS 108.** Two color nonlinear spectroscopy for the rapid acquisition of coherent dynamics: Applications to photosynthetic systems. J.P. Ogilvie, S.S. Senlik, V. Policht
- 10:45 PHYS 109.** Vibronic couplings in multichromophores: Application to tricyclopentane. C.H. Borca, L.V. Slipchenko
- 11:05 PHYS 110.** Elucidating molecular fluorescence mechanisms of fluorescent protein based biosensors: Insights from femtosecond stimulated Raman spectroscopy. B. Oscar, W. Liu, L. Tang, Y. Wang, Y. Zhao, R.E. Campbell, C. Fang

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

Fragment-Based Approaches

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*

E. G. Hohenstein, *Presiding*

8:00 PHYS 111. Molecules-in-molecules (MIM) and many-overlapping-body (MOB) expansion: Fragment-based methods for calculating accurate energies and spectroscopic properties of large molecules. K. Raghavachari

8:40 PHYS 112. Fragment-based methods for non-covalent interactions: From molecular clusters to crystals. K. Lao, J. Herbert

9:00 PHYS 113. Modeling molecular crystals: From fragment interactions to NMR crystallography. G.J. Beran

9:40 PHYS 114. Electronic energies and molecular properties from systematic molecular fragmentation. M.A. Collins, D.M. Reid

10:20 PHYS 115. Naturally parallel, fragment based approach to computing collective excitations in crystals and aggregates based on an ab-initio implementation of a Frenkel-Davydov exciton model. A. Morrison, J. Herbert

10:40 PHYS 116. Cluster based approximation of tensors: Fast reduced-scaling exact exchange and MP2 for 3D systems. C. Lewis, E.F. Valeev

11:00 PHYS 117. Condensed-phase chemistry with the Effective Fragment Potential method. L.V. Slipchenko

Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENVR

D. A. Knopf, S. Lee, *Organizers*

N. Ng, J. A. Thornton, *Presiding*

8:00 PHYS 118. Atmospheric hydroxyl in forests: What recent measurements are telling us. W. Brune, P.A. Feiner, D.O. Miller, L. Zhang

8:30 PHYS 119. Quantifying regional OH concentrations using airborne measurements of isoprene and its oxidation products. A.B. Guenther, D. Gu, H. Yu, J. Shilling, M. Shrivastava, T. Karl, P. Artaxo, L. Kaser, F. Santos, K. Longo, S.T. Martin, B. Yuan, S. Kim, R. Seco

9:00 PHYS 120. Ultrafast dynamics of far-UV excited states of acetone using angle-resolved electron-ion coincidence detection. D.E. Couch, W.K. Peters, H. Kapteyn, M.M. Murnane

9:15 PHYS 121. Chemical nucleation by acid-base reactions: Discoveries from laboratory experiments enabled by instrumental developments. P.H. McMurry, D.R. Hanson, C.N. Jen

9:45 PHYS 122. New insights on isoprene suppression of biogenic new particle formation. S. Lee, J. Uin, A.B. Guenther, J. de Gouw, A. Koss, A.H. Goldstein, G. Isaacman-VanWertz, K. Olson, L. Yee, N. Ng, L. Xu, W. Brune, K. Baumann, V. Kanawade, F. Keutsch, A. Nadykto, J. Herb

10:00 PHYS 123. Withdrawn.

10:30 PHYS 124. Molecular dynamics of clusters formed from ammonia, sulfuric acid, and water. N. Chon, A.W. Duster, H. Lin

11:00 PHYS 125. Growth mechanisms of ambient nanoparticles. M.V. Johnston

11:30 PHYS 126. Water + oil: How do particles form? B.E. Wyslouzil

Section D

Boston Convention & Exhibition Center
Room 254A

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Membrane Proteins, Nano Systems, and Motors

Cosponsored by COMP

E. Alexov, R. Luo, *Organizers*

H. Zhou, *Presiding*

8:00 PHYS 127. Modeling nanotoxicity: Molecular simulation of protein-nanoparticle interactions and their implications in nanomedicine. R. Zhou

8:40 PHYS 128. Reducing membranes to what really matters: Modeling membranes implicitly. M. Feig

9:20 Intermission.

9:40 PHYS 129. Molecular simulation of protein interactions with material surfaces: Challenges and solutions. R.A. Latour

10:20 PHYS 130. Molecular mechanism of the bidirectional motility of yeast kinesin-5/Cin8. W. Qiu

11:00 PHYS 131. Tracking viral membrane molecular dynamics through temporally-resolved plasmon coupling microscopy. A. Feizpour, H. Akiyama, S. Gummuluru, B.M. Reinhard

Section E

Boston Convention & Exhibition Center
Room 254B

Hydrophobicity, Ion Solvation, & Interfaces: Theory, Simulations, & Experiments

Interfaces & Ions

D. Ben-Amotz, S. Garde, *Organizers*

A. P. Willard, *Presiding*

8:00 Introductory Remarks.

8:10 PHYS 132. Dimensional control of chemical interfaces using polymerizable amphiphiles. S.A. Clairidge

8:40 PHYS 133. Insights from X-ray surface scattering on the interfacial transport of ions from aqueous to organic phases. M.L. Schlossman

9:10 PHYS 134. Simulation of IRRAS and other infrared spectra for molecules on metal oxide surfaces. K. Hermansson, P.D. Mitev, L. Österlund, S. Hu

9:30 Intermission.

9:45 PHYS 135. Seeing the Stern layer at the silica/aqueous interface using nonlinear optical spectroscopy. J. Gibbs-Davis

10:15 PHYS 136. Interactions and competitions at small molecule - mineral interfaces. D. Wu, X. Guo, H. Sun, A. Navrotsky

10:35 PHYS 137. Photochemistry of OH radical at the air-water interface: A QM/EFP study. P. Gurunathan, L.V. Slipchenko

Section F

Boston Convention & Exhibition Center
Room 255

Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Applications and Consequences

Cosponsored by COLL

C. Burda, *Organizer*

K. Hamad-Schifferli, W. Parak, *Organizers, Presiding*

8:00 PHYS 138. Layer-by-layer complex surfaces modulate protein adsorption and cell interactions. P.T. Hammond

8:30 PHYS 139. Observing real time cargo delivery and protein expression in primary cells using a AuNP-SET based cargo delivery vehicle. G.F. Strouse

9:00 PHYS 140. TiO₂ nanoparticles and the protein corona: Importance for oxidative stress-related gene expression. C.K. Payne

9:30 PHYS 141. Uptake and localization properties of polyester based nanoparticles in response proteins, pH and charge. A.M. Nystrom

10:00 PHYS 142. Localisation and properties of nanoparticle conjugates after cell entry... and why it matters. D.N. Mason, J. Comenge, G. Carolan, R. Levy, M. Held

10:30 PHYS 143. In vivo integrity of polymer-coated inorganic colloidal nanoparticles. W. Parak

Section G

Boston Convention & Exhibition Center
Room 256

Materials for Heat to Energy Conversion

R. Seshadri, *Organizer*

M. G. Kanatzidis, *Organizer, Presiding*

8:00 PHYS 144. Efficient thermoelectric energy conversion in Te-free I-V-VI₂ metal chalcogenides. K. Biswas

8:30 PHYS 145. Power of perovskite-structure solid solutions to tune solar thermochemical fuel production: Accessing a strongly lowered thermal operation range. J.L. Rupp

9:00 PHYS 146. Thermionic and photon-enhanced emission energy conversion. N.A. Melosh, D. Riley, K. Sahasrabudde, Z. Shen, J. Schwede, R. Howe

9:30 Intermission.

9:50 PHYS 147. Raman and infrared absorption studies of the photopolymerization of 1,4-dihydrobuta-1,3-diene in crystalline urea inclusion complex. S. Dinca, D.G. Allis, M.B. Sponsler, B.S. Hudson

10:05 PHYS 148. Extremely low thermal conductivity of thermoelectric thallium tellurides. H. Kleinke

10:35 PHYS 149. Zintl-chemistry for half-Heusler thermoelectric materials. G. Snyder

Section H

Boston Convention & Exhibition Center
Room 257A

Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability, & Spectroscopic Signatures

Laboratory Techniques

R. C. Fortenberry, *Organizer*

M. S. El-Shall, *Organizer, Presiding*

8:00 PHYS 150. Selected-ion infrared spectroscopy of small organic cations. M.A. Duncan

8:35 PHYS 151. Silicon and sulfur analogs of well-known astronomical molecules: Exploring chemistry beyond the first row. M. McCarthy, S. Thorwirth

9:10 PHYS 152. Laser spectroscopy of interstellar molecules in the laboratory. T. Schmidt

9:45 Intermission.

10:15 PHYS 153. Electronic spectroscopy of astrophysically relevant silicon-containing species: Si-terminated carbon chains SiC_nH (n=3-5), rhomboidal Si₃C, and Si₂C. N.J. Reilly, D. Kokkin, P.B. Changala, J. Baraban, R.C. Fortenberry, M. Stiglich, T. Crawford, J. Maier, J. Stanton, M. McCarthy

10:50 PHYS 154. Ultrafast dynamics of methyl azide photodissociation in the far UV. W.K. Peters, D.E. Couch, H. Kapteyn, M.M. Murnane

11:15 PHYS 155. CPUP: Chirped-pulse microwave spectroscopy in uniform supersonic flows to probe molecular reaction dynamics and photochemistry under astrophysical conditions. L.N. Zack, C.S. Abeysekera, N. Ariyasingha, B.Y. Joalland, B. Park, R. Field, I.R. Sims, A.G. Suits

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

Section I

Boston Convention & Exhibition Center
Room 257B

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Cosponsored by COMP

M. Kertesz, H. Lischka, *Organizers*
C. A. Parish, *Organizer, Presiding*
J. Musfeldt, *Presiding*

8:00 PHYS 156. Molecular dynamics on reactions involving diradicals: Concerted and stepwise. K.N. Houk

8:40 PHYS 157. Radicals, diradicals, polyradicals — controlling spin and reactivity in organic high spin molecules. W.W. Sander, E. Mendez Vega, J. Mieres Perez, Y. Tsegaw

9:20 Intermission.

9:50 PHYS 158. Gas-phase studies on charged aromatic di-, tri-, and tetraradicals. H.I. Kenttamaa

10:30 PHYS 159. Complete active space spin-flip methods for the electronic structure of molecules with strongly correlated electrons. M.P. Head-Gordon

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 251

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies Biological Interfaces and Interactions

Cosponsored by COLL

A. E. Bragg, A. T. Krummel, P. B. Petersen, *Organizers*

C. Fang, *Presiding*

1:30 PHYS 160. Electrostatic and electrodynamic fields at the protein-protein interface. L.J. Webb

2:05 PHYS 161. Experimental and molecular dynamics simulation studies on Terahertz spectra of biomolecules. D. Wei, M. Zhang, S. Yan, M. Tang, C. Shi, Z. Yang, L. Xia, C. Du, H. Cui

2:25 PHYS 162. Laser spectroscopy of structure and dynamics at bio-interfaces. K.B. Eissenthal, S. Kazer, S. Kwok, B.I. Doughty, Y. Rao

3:00 Intermission.

3:20 PHYS 163. Probing ultrafast structure and dynamics of preferential solvation using ultrafast 2D-IR in systems ranging from biophysics to photocatalysis. K.J. Kubarych

3:55 PHYS 164. Structure and dynamics of biological tryptophan radicals. J.E. Kim

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

Embedding Methods

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*
D. Zgid, *Presiding*

1:30 PHYS 165. Embedding theories for chemical reactions in the condensed phase. T.F. Miller

2:10 PHYS 166. Bootstrap embedding: An internally consistent fragment-based approach to large systems. M. Welborn, T. Tsuchimochi, T.A. Van Voorhis

2:30 PHYS 167. Reduced-scaling electronic structure theory approaches for simulating responsive organic materials. D. Lambrecht

3:10 PHYS 168. Electronic structure methods for large systems: Recent developments and applications. S. Li

3:50 PHYS 169. Embedded mean-field theory: Toward a large-scale ab-initio molecular dynamics. J. Lee, K. Miyamoto, M.E. Fornace, F.R. Manby, T.F. Miller

4:10 PHYS 170. Electronic spectra of explicitly solvated bulk systems using coupled cluster theory. R. Molt, J.N. Byrd, N.G. Richards

4:30 PHYS 171. There seem only two truly scalable algorithms for electron correlation in large systems. S. Hirata

Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENVR

D. A. Knopf, S. Lee, *Organizers*

K. Lehtipalo, K. R. Wilson, *Presiding*

1:30 PHYS 172. Size distribution characteristics of organosulfates in the Pearl River delta region. B. Kuang, P. Lin, M. Hu, J. Yu

2:00 PHYS 173. Impacts of various pollution sources on aerosol formation and optical extinction in the Front Range of Colorado. R. Bahreini, K.K. Vu, J. Dingle, E. Apel, T. Campos, R.C. Cohen, C. Eben, F. Flocke, A. Fried, R. Hornbrook, G. Huey, D. Montzka, J.B. Nowak, D. Richter, R. Roscioli, M. Stell, D. Tanner, G.S. Tyndall, J. Walega, P. Weibring, A. Weinheimer

2:30 PHYS 174. Multiphase chemical kinetics between OH and biomass burning surrogate species: The role of particle phase state and implications for cloud formation. D.A. Knopf, J.H. Slade, A. Arangio, R. Thalman, J. Wang, U. Pöschl, M. Shiraiwa

2:45 PHYS 175. Investigating the links between ozone and organic aerosol chemistry in biomass burning smoke plumes. M. Alvarado, C. Lonsdale, R. Yokelson

3:00 PHYS 176. Evolution of functional group composition in organic aerosols. S. Takahama, G. Ruggeri, B. Henderson

3:30 PHYS 177. New metrics to quantify aerosol mixing state. N. Riemer, M. West

4:00 PHYS 178. Evidence of sea spray aerosols enriched in organic pollutants. X. Wang, M. Pendergraft, K.A. Prather

4:15 PHYS 179. Distinct organic containing particle types in sea spray aerosols as a function of biological activity. C. Sultana, X. Wang, J. Trueblood, T. Hill, C. Lee, O. Laskina, C. Bealle, K. Moore, P.J. DeMott, V.H. Grassian, K.A. Prather

Section D

Boston Convention & Exhibition Center
Room 254A

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Protein Stability, Folding, and Aggregation

Cosponsored by COMP

E. Alexov, R. Luo, *Organizers*

R. Zhou, *Presiding*

1:30 PHYS 180. Electrostatic interactions in protein structure, folding, binding, and assembly. H. Zhou

2:10 PHYS 181. Encounter state plays a prominent role in weak protein interactions. M. Ubbink

2:50 Intermission.

3:10 PHYS 182. Origins of metamorphic folding in the human chemokine XCL1/lymphotactin. B.F. Volkman, R.C. Tyler, J.C. Fox

3:50 PHYS 183. Paradyamics: A new approach for modeling enzymatic reactions. I. Kupchenko, A. Warshel

4:10 PHYS 184. Aggregation dynamics of α -synuclein monitored by Raman spectroscopy. J.D. Flynn, J.C. Lee

Section E

Boston Convention & Exhibition Center
Room 254B

Hydrophobicity, Ion Solvation, & Interfaces: Theory, Simulations, & Experiments

Interfaces & Ions

D. Ben-Amotz, S. Garde, *Organizers*

K. Hermansson, *Presiding*

1:30 PHYS 185. What can interfacial water molecules tell us about solute structure? A. Willard

2:00 PHYS 186. Hydration mimicry: A strategy for ion permeation? M. Chaudhari, J.M. Vanegas, S.L. Rempe

2:30 PHYS 187. Exploring specific ion effects on the hydrophobic hydration of macromolecules. P.S. Cremer

2:50 PHYS 188. Is water behaving symmetrically to charge? S. Roke

3:20 PHYS 189. Charge hydration asymmetry: New twists to the old story. A.V. Onufriev

3:40 PHYS 190. Loosening the grip of polymer electrolytes: How the asymmetry of ion diffusion in conventional polyethers reveals a new design paradigm. B.M. Savoie, T.F. Miller

4:00 PHYS 191. Electrostatic embedding schemes for the many-body approximation of classical polarizable models. T.L. Head-Gordon

Section F

Boston Convention & Exhibition Center
Room 255

Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact Applications and Consequences

Cosponsored by COLL

K. Hamad-Schifferli, *Organizer*

C. Burda, W. Parak, *Organizers, Presiding*

1:30 PHYS 192. Biomaterials interfaces. G.M. Whitesides

2:00 PHYS 193. Bionic supraparticles. N. Kotov

2:30 PHYS 194. Applicability and limitations of safety corona data for preclinical safety assessment of engineered nanomaterials. M.A. Dobrovoskaia, S.E. McNeil, B. Neun, S. Man, J. Clogston, A. Patri, M. Hansen, R. Crist, X. Ye

3:00 PHYS 195. Virus-like particles: Targeted diagnostic imaging and directed immune responses. T. Douglas

3:30 PHYS 196. Multifunctional nanoprobes for cancer diagnosis and drug delivery. J. Zhu

4:00 PHYS 197. Understanding the impact of glycosylation at the bionano interface. M. Monopoli, S. Wan, P. Kelly, Y. Yan, K.A. Dawson

Section G

Boston Convention & Exhibition Center
Room 256

Physical Chemistry of Clusters & Nanoparticles

Structural Properties

Financially supported by Mantis Deposition, Ltd. G. E. Johnson, *Organizer*

D. Jiang, *Organizer, Presiding*

A. Alexandrova, *Presiding*

1:30 PHYS 198. Size-selected gold clusters: Solving the atomic structure of model nanoparticles and prospects for scale-up. R.E. Palmer

2:00 PHYS 199. Stability and atomic segregation phenomena in size and shape selected PtNi nano particles: CO effect. M. Ahmadi, C. Cui, P. Strasser, B. Roldan-Cuenya

2:20 PHYS 200. Cluster films by helium droplet mediated cluster assembly: Growth and characterization. C.J. Ridge, S. Emery, K.B. Rider, C.M. Lindsay

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2:40 PHYS 201. Predicting structures of semiconducting nanoparticles: An ab initio computational study. H.J. Kulik, Q. Zhao, L. Xie

3:00 Intermission.

3:20 PHYS 202. In-situ detection of hydrogen-induced phase transitions in individual palladium nanocrystals. J.A. Dionne, A. Baldi, T. Narayan, A. Koh

3:40 PHYS 203. Understanding early-stage growth of indium phosphide quantum dots using first principle calculations. L. Xie, K.F. Jensen, H.J. Kulik

4:00 PHYS 204. Accurate characterization of nanoscale interfaces. Nature of interactions between inherent carbonaceous clusters and underlying arc-discharge carbon nanotubes. A. Furmanchuk, Z. An, R. Ramachandramoorthy, T. Filleter, M.R. Roenbeck, H.D. Espinosa, G.C. Schatz, S.T. Nguyen

4:20 PHYS 205. Closo-Si₁₂C₁₂ molecule from cluster to crystal: A theoretical prediction. X.F. Duan, L.W. Burggraf

Section H

Boston Convention & Exhibition Center
Room 257A

Materials for Heat to Energy Conversion

M. G. Kanatzidis, R. Seshadri, *Organizers*
E. Toberer, *Presiding*

1:30 PHYS 206. Superdiffusive thermo-electric transport and energy conversion. A. Shakouri, A. Mohammed, Y. Koh, B. Vermeersch, K. Yazawa

2:00 PHYS 207. Effect of dislocations on optical and transport properties of organometal halide perovskites. P. Tyagi

2:15 PHYS 208. Thermal conductivity of nanocrystalline and nanocomposite bulk materials. C. Dames

2:45 Intermission.

3:05 PHYS 209. Open-framework and other low thermal conductivity materials: New materials research and theoretical guidance for thermo-electrics applications. G.S. Nolas

3:35 PHYS 210. Thermodynamics of CO₂ capture in metal-organic frameworks. D. Wu, J.J. Gassensmith, T. McDonald, X. Guo, Z. Quan, S.V. Ushakov, P. Zhang, J.R. Long, A. Navrotsky

4:05 PHYS 211. Engineering the thermal phonon spectrum for thermoelectric energy conversion. A. Minnich

Section I

Boston Convention & Exhibition Center
Room 257B

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Cosponsored by COMP

M. Kertesz, C. A. Parish, *Organizers*

H. Lischka, *Organizer, Presiding*

H. I. Kenttamaa, *Presiding*

1:30 PHYS 212. Revealing the singlet-triplet equilibrium in photochemically activated organic biradicals. J. Mustfeldt, A. Clune, J. Fasso-Tande, R. Harrison, P. Lahti

2:10 PHYS 213. Revisiting the chemistry of the phenalenyls. T. Kubo, K. Uchida

2:50 Intermission.

3:20 PHYS 214. Extraordinary long, 3.04-Å 2e/6c bond and triplet excited state observed for π-[TCNE]₂²⁻ in [NMe₄]₂[TCNE]₂ (TCNE = tetracyanoethylene). J.S. Miller, J.J. Novoa, A. Graham, F. Mota, E. Shurdha, A.L. Rheingold, A. Simonson, P. Stephens

4:00 PHYS 215. Theoretical molecular design for singlet fission based on the diradical character: Tetrathiafulvalene and bisimidazol diradicals. S. Ito, N. Ito, M. Nakano

4:25 PHYS 216. Theoretical investigation of singlet fission using spin/charge cumulants and one-particle density matrix. A. Luzanov, D. Casanova, X. Feng, A. Krylov

4:50 PHYS 217. Ab initio wave function studies of organic photovoltaic systems. I. Borges, E. Uhl, L. Modesto-Costa, A. Aquino, H. Lischka

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

E. L. Sibert, *Organizer*

8:00 - 10:00

62, 120, 142, 147, 152, 177-178, 184, 190, 192, 211. See previous listings.

PHYS 218. Solar fuels from light and heat: Activating small polaron hopping. W. Chueh
337, 340, 349, 379, 398, 469, 512, 631. See subsequent listings.

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 257B

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

Photophysical Dynamics of Biological and Biomimetic Systems

Cosponsored by COLL

A. E. Bragg, A. T. Krummel, *Organizers*

P. B. Petersen, *Organizer, Presiding*

8:00 PHYS 219. When complicated things happen to simple liquids: Nitriles at silica interfaces. J.T. Fourkas

8:35 PHYS 220. Electronic-vibrational coupling for dyes at the TiO₂ interface measured by heterodyne detected doubly resonant sum frequency generation spectroscopy. C. Rich, M.A. Mattson, A.T. Krummel

8:55 PHYS 221. Nonlinear coherent vibrational spectroscopy of electrified interfaces. N. Garcia-Rey, B.G. Nicolau, B. Dryzhkov, D.D. Klott

9:30 PHYS 222. Effect of energy level alignment on heterogeneous electron transfer: Injection from porphyrinoids into TiO₂. J. Nieto-Pescador, B. Abraham, L. Gundlach

9:50 Intermission.

10:10 PHYS 223. Molecular structure and dynamics at electrode/catalyst interfaces probed by time-resolved vibration sum-frequency generation spectroscopy. T. Lian

10:45 PHYS 224. Probing excitonic interactions across interfaces in 2D/0D transition metal dichalcogenide/quantum dot hybrid structures using time-resolved optical spectroscopy. A.J. Goodman, F. Prins, W.A. Tisdale

11:05 PHYS 225. Charge dynamics and molecular intermediates of photocatalytic interfaces. T. Cuk, M. Waegle, X. Chen, D. Hérilhy

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

Excited States and Strongly Correlated Electrons

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*
R. A. DiStasio, *Presiding*

8:00 PHYS 226. Bioluminescence challenge: Simulating and exploring thermal nonadiabatic chemistry. R. Lindh

8:40 PHYS 227. On the nature of a large Stokes shift in mPlum fluorescent protein. S. Faraji, A. Krylov

9:00 PHYS 228. Computationally efficient approaches for molecular excited-state properties within the framework of time-dependent density functional theory. W. Liang

9:40 PHYS 229. Systematically improvable multiscale methods for correlated electron systems. D. Zgid

10:20 PHYS 230. Multireference excited state method applied to acenes and phenalenyl derivatives. S. Yost, N. Mayhall, M.P. Head-Gordon

10:40 PHYS 231. Electronically excited states of large atomic and molecular clusters using absolutely localized molecular orbitals with configuration interaction singles (ALMO-CIS). K.D. Closser, Q. Ge, M.P. Head-Gordon

11:00 PHYS 232. Modeling middle-size to large-size multireference molecular systems. R. Carlson, C. Hoyer, A. Sonnenberger, D.G. Truhlar, L. Gagliardi

Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENV/R

D. A. Knopf, S. Lee, *Organizers*

F. Geiger, P. Veres, *Presiding*

8:00 PHYS 233. Tracking aerosol chemical age through stable carbon isotope. A. Kiendler-Scharr, I. Gensch, X. Sang, A. Khan, W. Laumer, P. Schlag, S. Schmitt

8:30 PHYS 234. Using single particle mass spectrometry (SPMS) to characterize chemical composition of atmospherically-relevant aerosol particles. M.A. Zawadowicz, J.T. Jayne, P. Croteau, D.R. Worsnop, D. Cziczo

8:45 PHYS 235. Polycyclic aromatic hydrocarbon photolysis kinetics in aqueous, organic, and aqueous-organic environments. J. Grossman, A. Stern, M. Kirich, T.F. Kahang

9:00 PHYS 236. Characterization and quantification of nitrogen-containing aromatic compounds in atmospheric fine particulate matter in urban Hong Kong. K. Chow, X. Huang, J. Yu

9:15 PHYS 237. Direct views of the SOA aerosol particle/gas interface. F. Geiger

9:30 PHYS 238. Molecular probe for SOA precursors: The photochemical mechanism of sunlight irradiated aqueous pyruvic acid. A.J. Eugene, M.I. Guzman

9:45 PHYS 239. Computational screening of possible brown carbon compounds in the atmospheric aerosol. M. Caricato

10:00 PHYS 240. Dynamics of secondary organic aerosols: Are they gummy or just sticky. N.M. Donahue, W. Chuang, Q. Ye, P. Ye

10:30 PHYS 241. Large enhancement in the heterogeneous oxidation rate of organic aerosols by hydroxyl radicals in polluted regions. N.K. Richards-Henderson, A.H. Goldstein, K.R. Wilson

Section D

Boston Convention & Exhibition Center
Room 254A

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Proton and Electron Transport

Cosponsored by COMP

E. Alexov, R. Luo, *Organizers*

A. E. Roitberg, *Presiding*

8:00 PHYS 242. How proteins modulate proton affinity and pathway accessibility in proton pumps. M. Gunner

8:40 PHYS 243. Microstate model for describing charge transfer in proteins: From simple proteins to complex machineries. M. Ullmann, E. Bombarda

9:20 Intermission.

9:40 PHYS 244. Mimicking photosynthetic electron, energy, and proton transfer. J.D. Gust, T.A. Moore, A.L. Moore

10:20 PHYS 245. Proton transfer in cytochrome c oxidase. E. Knapp, A. Woelke

11:00 PHYS 246. Channelrhodopsin: Molecular dynamics studies of hydration and cation transport. M.R. VanGordon, S.W. Rick, S.L. Rempel

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

Section E

Boston Convention & Exhibition Center
Room 254B

Hydrophobicity, Ion Solvation, & Interfaces: Theory, Simulations, & Experiments

Nanoco confinement

D. Ben-Amotz, S. Garde, *Organizers*

S. L. Rempe, *Presiding*

8:00 *PHYS* **247**. Reversible control of nanoscale hydration. A. Luzar

8:30 *PHYS* **248**. Dispersion stability, phase partitioning, and ligand adsorption of plasmonic gold and silver nanoparticles. D. Zhang

9:00 *PHYS* **249**. What is the structure of aqueous-alkane nanodroplets? B.E. Wyslouzil, H. Pathak, A. Obeidat, G. Wilemski

9:20 *PHYS* **250**. Understanding freezing point deviations and the Gibbs-Thomson equation for fluids confined to nanopores. S. Shimizu, L. Drabushuk, N. Manohar, M. Strano

9:40 *PHYS* **251**. Experimental measurement of extreme phase transition temperatures for water confined inside carbon nanotubes. K. Agrawal, S. Shimizu, M. Strano

10:00 *PHYS* **252**. Understanding surfactants structure on the SWCNT sidewall via single molecule photoluminescence spectroscopy. R. Pramanik, S.K. Doorn, J. Duque

10:20 *PHYS* **253**. Simple ab initio model for the hydrated electron that agrees with experiment. D.M. Bartels, J.A. Walker, A. Kumar, M.D. Sevilla

Section F

Boston Convention & Exhibition Center
Room 255

Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Methods and Tools for Characterization

Cosponsored by COLL

W. Parak, *Organizer*

C. Burda, K. Hamad-Schifferli, *Organizers*,
Presiding

8:00 *PHYS* **254**. Intracellular localization and detection of biomolecules by surface enhanced Raman spectroscopy (SERS). H. Moehwald

8:30 *PHYS* **255**. Analytical ultracentrifugation as a tool for characterization of protein nanoparticles interactions. F. Stellacci

9:00 *PHYS* **256**. Characterising protein and peptide layers on gold nanoparticles. M. Volk

9:30 *PHYS* **257**. Protein- and DNA-imperceptible nanoparticle hard coating and 3D multiresolution study of nanoparticle-cell interactions. H. Yang, K. Welsher, S. McManus, C. Hsia, S. Yin

10:00 *PHYS* **258**. Multiplexing nanoparticle based SET and FRET to measure correlated distances on DNA. R.A. Riskowski, R. Armstrong, G.F. Strouse

10:20 *PHYS* **259**. Spectroscopic properties of semiconductor quantum dots embedded in biological medium. B. Ellis, W. Jiang, J. Elward, F. Irudayanathan, S. Nangia, A. Chakraborty

10:40 *PHYS* **260**. Protein corona formation around lipid wrapped nanoparticles. B.M. Reinhard

Section G

Boston Convention & Exhibition Center
Room 256

Physical Chemistry of Clusters & Nanoparticles

Structural Properties

Financially supported by Extrel CMS

D. Jiang, *Organizer*

G. E. Johnson, *Organizer, Presiding*

J. A. Dionne, *Presiding*

8:00 *PHYS* **261**. Controlling protein conformation on surfaces by soft-landing electrospray ion beam deposition. S. Rauschenbach

8:30 *PHYS* **262**. Capturing structural transitions during progression from nanoparticles to bulk crystals. G.J. Simpson

8:50 *PHYS* **263**. Hierarchical structural patterns in the Au₁₃₃(SR)₅₂ nanoparticle revealed by X-ray crystallography. C. Zeng, R. Jin

9:10 *PHYS* **264**. Core-shell metalloboranes: Property alteration and charge-control of structure. F.Y. Naumkin, R. Chelat, B. Irving

9:30 Intermission.

9:50 *PHYS* **265**. Gold nanoclusters with the protection involving alkynyl ligands. Q. Wang

10:20 *PHYS* **266**. Deconstructing the binding of citrate to gold nanoparticles. L. Cavallo, A. Jedidi

10:40 *PHYS* **267**. Tailoring characteristics of nanoparticles: Size, shape, composition, and environment matters. T.S. Rahman

11:10 *PHYS* **268**. Characterization of mixed-ligand phosphonic acid functionalized fumed silica nanoparticles using solid-state NMR. S.K. Davidowski, G.P. Holland, J.L. Yarger

Section H

Boston Convention & Exhibition Center
Room 257A

Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability, & Spectroscopic Signatures

Large Molecules

M. S. El-Shall, R. C. Fortenberry, *Organizers*

E. Fayolle, *Presiding*

8:00 *PHYS* **269**. Spectral features and nanostructuring of soot as analog of the carbonaceous cosmic dust. T. Pino, T. Le, L. Gavilan, I. Alata, D. Deldicque, J. Rouzaud, E. Dartois

8:35 *PHYS* **270**. Tackling the anharmonic spectrum of polycyclic aromatic hydrocarbons. A. Candian

9:10 *PHYS* **271**. PAH clusters and the interstellar infrared emission bands. J. Roser, A. Ricca Bauschlicher

9:45 Intermission.

10:15 *PHYS* **272**. Search for sugars and related compounds in residues produced from the UV irradiation of astrophysical ice analogs. M. Nuevo, S.A. Sandford, C.K. Materese, G.W. Cooper

10:50 *PHYS* **273**. Activation of two weak IR fundamentals of solid methane: The importance of amorphous ices. R.L. Hudson, P. Gerakines, M. Loeffler

Section I

Boston Convention & Exhibition Center
Room 251

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Cosponsored by COMP

H. Lischka, C. A. Parish, *Organizers*

M. Kertesz, *Organizer, Presiding*

P. Piecuch, *Presiding*

8:00 *PHYS* **274**. Plasmon resonances in acenes and silicenes. C.M. Aikens, E. Guidez, K.M. Weerawardene

8:40 *PHYS* **275**. Noncovalent interactions of pyrene groups with graphene in dispersions and polymer composites. M. Green, R. Hedden

9:20 Intermission.

9:50 *PHYS* **276**. Structure-Property relationships of curved aromatic materials from first principles. K.K. Baldrige

10:30 *PHYS* **277**. Radical and polycyclic aromatic hydrocarbons: A theoretical study. A. Das, H. Lischka

10:55 *PHYS* **278**. Oxygenated quad-vacancies in single graphene under aqueous conditions: The world's thinnest proton channel? F. Geiger

11:20 *PHYS* **279**. Electronic states of carbon vacancy defects in graphene: A pyrene model. F. Machado, A. Aquino, H. Lischka

11:45 *PHYS* **280**. Conduction and efficient rectification in unimolecular hemibiquinone self-assembled monolayers. J.E. Meany, M. Johnson, R.M. Metzger, S.A. Woski

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Sponsored by CHED, Cosponsored by ANYL‡, BIOL‡, BIOT‡, BMGT‡, CORP‡, DAC‡, ENFL‡, PHYS‡ and POLY‡

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Electron and Energy Transfer: From Molecular to Device Engineering for Minimizing Environmental Impacts

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 257B

Award Symposium

Financially supported by *The Journal of Physical Chemistry*

E. L. Sibert, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 *PHYS* **281**. Career highlights and what I learned from them. H. Metiu

2:05 *PHYS* **282**. Applications of optical cavity techniques to problems in atmospheric chemistry and spectroscopy. M. Okumura

2:35 *PHYS* **283**. Solid-state NMR structural studies of proteins using paramagnetic probes. C.P. Jaronic

3:05 *PHYS* **284**. New approaches to simulating biological and molecular catalysis. T.F. Miller

3:35 Intermission.

3:55 *PHYS* **285**. Understanding plasmon resonances using quantum mechanical methods. C.M. Aikens

4:25 *PHYS* **286**. Intuitive understanding of electronic relaxation in molecules. J.E. Subotnik

4:55 *PHYS* **287**. Hidden dynamics of complex solid-state reactions, Revealed one nanocrystal at a time. P.K. Jain

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

Ab Initio Molecular Dynamics

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*

W. Kim, *Presiding*

1:30 *PHYS* **288**. Complex molecular and ionic liquids from first-principles molecular dynamics simulations. B. Kirchner, D. Firaha, O. Holloczki, M. Thomas, I. Sancho Sanz

2:10 *PHYS* **289**. Active role of the substrate during catalysis by the therapeutic enzyme L-asparaginase II. J.M. Vanegas, A. Anishkin, D.M. Rogers, S. Sukharev, S.L. Rempe

2:30 *PHYS* **290**. Exploring the interface of electronic structure theory and molecular dynamics. R. Steele

3:10 *PHYS* **291**. Linear scaling first-principles molecular dynamics for very large systems with the CONQUEST code. T. Miyazaki

3:50 *PHYS* **292**. Combining linear-response and real-time time-dependent density functional theory for the simulation of excited state absorption. S. Fischer, C.J. Cramer, N. Govind

4:10 *PHYS* **293**. Enabling large-scale hybrid density functional theory calculations in condensed-phase systems. R.A. DiStasio

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Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENVR

D. A. Knopf, S. Lee, *Organizers*

K. Lehtipalo, K. R. Wilson, *Presiding*

1:30 PHYS 294. Sources and relationships between aerosols and trace gases in coastal Antarctica. P.F. DeCarlo, M. Giordano, L. Kalnajs, A. Johnson, S. Davis, T. Deshler

2:00 PHYS 295. Ozonolysis of catechol at the gas-solid interface. E.A. Pillar, M.I. Guzman

2:15 PHYS 296. Effect of oxidant concentration, exposure time, and seed particles on secondary organic aerosol chemical composition and yield. A. Lambe, P. Chhabra, T.B. Onasch, W. Brune, J. Hunter, J.H. Kroll, M. Cummings, J. Brogan, Y. Parmar, D.R. Worsnop, C.E. Kolb, P. Davidovits

2:30 PHYS 297. Oxidative aging of secondary organic aerosol within aqueous particles. J.H. Kroll, K. Daumit, A.J. Carrasquillo

2:45 PHYS 298. Atmospheric heterogeneous reaction kinetics related to organic aerosols. H. Akimoto

3:15 PHYS 299. Single particle time of flight mass spectrometry utilizing a femtosecond desorption and ionization laser. D. Cziczo, M.A. Zawadowicz, A. AbdElMonem, C. Mohr, H. Saathoff, D. Murphy, K.D. Froyd, T. Leisner

3:30 PHYS 300. Organosulfate formation in the secondary organic aerosol produced from photooxidation of various VOCs in the presence of NO_x and sulfuric acid aerosol using natural sunlight. M. Jang, H. Jiang, J. Park, R. Beardsley

4:00 PHYS 301. Chemical speciation of organic aerosol driven by phase partitioning. M.J. Walker, B.J. Williams, R. Martinez, D. Mitroo, C. Fortenberry

4:15 PHYS 302. Surface enhanced Raman spectroscopy (SERS) as a tool to improve detection limits of secondary organic aerosol components and probe hygroscopic and phase behavior. A.P. Ault, R.L. Craig, A. Bondy

4:45 PHYS 303. Comprehensive characterization of organic carbon through multiple generations of aging. G. Isaacman-VanWertz, J.P. Franklin, C. Lim, P. Massoli, A. Lambe, J.B. Nowak, T.B. Onasch, M. Canagaratna, S.C. Herndon, J.T. Jayne, D.R. Worsnop, L. Su, D.A. Knopf, P.K. Misztal, C.M. Arata, A.H. Goldstein, J.H. Kroll

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Sponsored by CHED, Cosponsored by ANYL†, BIOT†, BMGT†, CORP†, DAC†, ENFL†, PHYS† and POLY†

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Innovation in Materials for Emerging Uses

Sponsored by MPPG, Cosponsored by PHYS, PMSE and POLY

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Designs: From Molecules to Functional Materials

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 251

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

Structure, Dynamics, and Behaviors of Material Systems

Cosponsored by COLL

A. E. Bragg, A. T. Krummel, P. B. Petersen, *Organizers*

S. T. Roberts, *Presiding*

8:00 PHYS 304. Multidimensional kinetics: New processes, new timescales, and more dimensions. M. Berg, H. Wu, S. Verma

8:35 PHYS 305. Structural dynamics and heterogeneities of localized excited states in conjugated polymers. A.E. Bragg

8:55 PHYS 306. Exciton transport in carbon nanotube photovoltaic films using 2D white-light spectroscopy. M.T. Zanni

9:30 PHYS 307. Photoinduced charge transfer rates as a probe for characterizing donor-acceptor interfaces in polymer-based solar cells. J. Dasgupta

9:50 Intermission.

10:10 PHYS 308. 2D spectroscopy of quantum dots in the short-wave infrared. S.D. Park, D. Baranov, J. Ryu, D.M. Jonas

10:45 PHYS 309. 3D tracking of single guest molecules in polymer thin films toward the investigation of complex dynamics in micro-heterogeneous media. S. Ito, Y. Taga, K. Hiratsuka, S. Takei, D. Kitagawa, S. Kobatake, H. Miyasaka

11:05 PHYS 310. Mapping the nanoscale exciton diffusivity in heterogeneous electronically coupled materials with time-resolved super-resolution imaging. S.B. Penwell, L.D. Ginsberg, R. Noriega, B.D. Folie, N.S. Ginsberg

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

Correlated Wavefunction Approaches

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*

A. Chakraborty, *Presiding*

8:00 PHYS 311. Local correlation methods for molecules and solids. M. Schuetz

8:40 PHYS 312. Local orbitals and spin flip methods. P.M. Zimmerman

9:00 PHYS 313. From local correlated wavefunction theory to petascale orbital-free density functional theory. E.A. Carter

9:40 PHYS 314. Coupled cluster theory for large systems. G.E. Scuseria

10:20 PHYS 315. Molecular properties from multiconfiguration explicitly correlated wave functions. C. Peng, E.F. Valeev

10:40 PHYS 316. Anatomy of molecular properties evaluated with explicitly correlated coupled-cluster methods. J. Zhang, E.F. Valeev

11:00 PHYS 317. Energy decomposition analysis for second-order Møller-Plesset perturbation theory based on absolutely localized molecular orbitals. J. Thirman, M.P. Head-Gordon

11:20 PHYS 318. Fully relativistic quantum chemistry for open-shell complexes with heavy atoms. T. Shiozaki

Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENVR

D. A. Knopf, S. Lee, *Organizers*

F. Geiger, P. Veres, *Presiding*

8:00 PHYS 319. Effects of anthropogenic emissions on aerosol formation from isoprene and monoterpenes in the southeastern United States. N. Ng, L. Xu, H. Guo, C. Boyd, M. Klein, A. Bougiatioti, K. Cerully, J. Hite, G. Isaacman-VanWertz, N. Kreisberg, C. Knote, K. Kevin Olson, A. Koss, A.H. Goldstein, S.V. Hering, J. de Gouw, K. Baumann, S. Lee, A. Nenes, R. Weber

8:30 PHYS 320. Role of atmospheric heterogeneous reactions in the fast formation of secondary particles. S. Tong, M. Ge, Q. Liu, K. Li, S. Hou

8:45 PHYS 321. Highly functionalized particle-phase organic nitrates observed in temperature and boreal forest ecosystems: formation mechanisms, and contribution to secondary organic aerosol and reactive nitrogen budgets. J.A. Thornton, F. Lopez-Hilfiker, B. Lee, C. Mohr

9:15 PHYS 322. Production of reactive species during the interfacial oxidation of polyphenols. M.I. Guzman, E.A. Pillar

9:30 PHYS 323. Highlights from recent oxidation studies to determine the gas/particle, chemical/physical characteristics of reaction products from a range of sources spanning from individual VOCs to complex combustion emissions. B.J. Williams, D. Mitroo, M. Walker, C. Fortenberry, Y. Zhang, C. Oxford, W. Brune, M. Baasandorj, D. Millet

10:00 PHYS 324. Investigation of ozonolysis of unsaturated fatty acids using FIGAERO-HRTof-CIMS: Evidence for reactions of particulate stabilized Criegee intermediates. M. Wang, L. Yao, L. Wang

10:30 PHYS 325. Withdrawn.

10:45 PHYS 326. Absorption cross sections of surface adsorbed NO₂ in 290 – 350 nm region. M. Sangwan, L. Zhu

Section D

Boston Convention & Exhibition Center
Room 254A

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Modeling pH and Water Dependent Properties

Cosponsored by COMP

E. Alexov, R. Luo, *Organizers*

M. Gunner, *Presiding*

8:00 PHYS 327. Dynamics and conformational changes coupled to changes in protonation states: Should we always blame the histidines? A.E. Roitberg

8:40 PHYS 328. Mechanism of pH-triggered self-assembly of polysaccharide. J. Shen

9:20 Intermission.

9:40 PHYS 329. Constant-pH molecular dynamics simulations of membrane systems: Titrable lipids and proton pumps. S. Campos, A.F. Oliveira, P. Magalhaes, D. Vila-Viçosa, V.H. Teixeira, H.A. Santos, C. Soares, M. Machuqueiro, A.M. Baptista

10:20 PHYS 330. Molecular multipole models for water and biological macromolecules. T. Ichiye

11:00 PHYS 331. Electrostatic effects and spatially extended enzyme active sites. M.J. Ondrechen, P.J. Beuning, R. Parasuram, T. Coulther, L. Ngu, K.E. Ramos

Section E

Boston Convention & Exhibition Center
Room 254B

Hydrophobicity, Ion Solvation, & Interfaces: Theory, Simulations, & Experiments

Interfaces & Biology

D. Ben-Amotz, S. Garde, *Organizers*

R. W. Martin, *Presiding*

8:00 PHYS 332. Dynamics of water at protein surfaces. P. Brotzakis, A. Kumar, P.G. Bolhuis

8:30 PHYS 333. Efficient and accurate characterization of protein hydration and interactions. E. Xi, R. Remsing, A. Patel

9:00 PHYS 334. Role of charge screening on anionic phospholipid asymmetry and translocation in lipid membranes. J.C. Conboy

9:30 PHYS 335. Liquid liquid phase separation in dilute but highly supersaturated aqueous solutions of lipophilic drugs. L. Taylor

10:00 PHYS 336. Phase separation and size dependence in organic aerosol. M. Freedman

10:20 PHYS 337. Gas-liquid water nucleation in the presence of acidic defects. T. Loeffler, C. Bresnahan, B. Chen, R. Kumar

10:50 PHYS 338. Solvation structure and ion-pairing for biological relevant ions using density functional theory. M.D. Baer, C.J. Mundy

11:10 PHYS 588. Reactions in complex biomimetic media. C.D. Keating

Section F

Boston Convention & Exhibition Center
Room 255

Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Applications and Consequences

Cosponsored by COLL

C. Burda, *Organizer*

K. Hamad-Schifferli, W. Parak, *Organizers, Presiding*

8:00 *PHYS 339.* Competitive charge and energy transfer in quantum dot conjugates for biosensing. **A.M. Scott**

8:30 *PHYS 340.* Influence of the nanoparticle composition in the protein corona adsorption. **S. Borros, I. Morera**

9:00 *PHYS 341.* Putting the biology-nanoparticle interface in a multiscale perspective. **P. Bergese**

9:30 *PHYS 342.* Biomedical applications of magnetic nanoparticles for hyperthermia and drug delivery. **T. Pellegrino**

10:00 *PHYS 343.* Engineering the nano-bio interface for disease therapy. **J. Kah**

10:30 *PHYS 344.* Stable-on-the-Tale environmentally responsible biocatalysts: Rational control of nano-bio interfaces. **C.V. Kumar**

Section G

Boston Convention & Exhibition Center
Room 256

Physical Chemistry of Clusters & Nanoparticles

Optical Properties and Applications

G. E. Johnson, *Organizer*

D. Jiang, *Organizer, Presiding*

K. L. Knappenberger, *Presiding*

8:00 *PHYS 345.* Engineering ultrasmall metal nanoclusters for biomedical and environmental applications. **J. Xie**

8:30 *PHYS 346.* Withdrawn.

8:50 *PHYS 347.* Ratiometric sensor using single chirality near-infrared fluorescent carbon nanotubes: Application to in vivo monitoring. **M. Landry, J. Giraldo, S. Kwak, R. Jain, M. Wong, N. Iverson, M. Ben-Naim, M. Strano**

9:10 Intermission.

9:30 *PHYS 348.* Withdrawn.

10:00 *PHYS 349.* Dark to bright: Using colloidal nanocrystals to harvest non-emissive triplet excitons in the short-wave infrared. **M.W. Wilson, N.J. Thompson, D.N. Congreve, M. Wu, M.G. Bawendi, M.A. Baldo**

10:20 *PHYS 350.* Photon antibunching to investigate electronic energy transport in small aggregates of semiconductor nanocrystal quantum dots. **A.K. Van Orden, K.J. Whitcomb, D. Ryan, M.P. Gelfand**

10:40 *PHYS 351.* Effect of aliphatic vs. aromatic ligands on the structure and optical absorption of Au₂₀(SR)₁₆. **K.M. Weerawardene, C.M. Aikens**

Section H

Boston Convention & Exhibition Center
Room 257A

Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability, & Spectroscopic Signatures

Advances in Theory

M. S. El-Shall, R. C. Fortenberry, *Organizers*

T. J. Lee, *Presiding*

8:00 *PHYS 352.* High-level spectroscopic calculations of relevance to astrochemists. **J. Stanton, P.B. Changala, J. Baraban, N.J. Reilly, M. McCarthy**

8:35 *PHYS 353.* Unraveling intermolecular interactions using electronic structure calculations: Theory and applications to polycyclic aromatic hydrocarbon ion molecule complexes. **M.P. Head-Gordon, R. Peverati**

9:10 *PHYS 354.* Deep hydrogen tunneling as an isomerization mechanism in organic species of astrochemical significance. **W.D. Allen**

9:45 Intermission.

10:15 *PHYS 355.* Diffusion Monte Carlo approaches for studying rotation/vibration couplings astrochemical ions. **A.B. McCoy, J.E. Ford, Z. Lin, M. Marlett, A.S. Petit**

10:50 *PHYS 356.* Equation-of-motion coupled-cluster methods for metastable electronic states. **T.C. Jagau, A. Krylov**

11:15 *PHYS 357.* Photonization/photodetachment spectroscopy and Dyson orbitals: Theoretical tools to aid experimental studies. **A. Gunina, S. Gozem, A. Krylov**

Section I

Boston Convention & Exhibition Center
Room 257B

From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment

Cosponsored by COMP

M. Kertesz, H. Lischka, *Organizers*

C. A. Parish, *Organizer, Presiding*

C. M. Aikens, *Presiding*

8:00 *PHYS 358.* Single-reference coupled-cluster and equation-of-motion coupled-cluster theories for high-accuracy ab initio computations of chemical reaction profiles involving biradical transition states and electronic spectra of radical and polyradical species. **P. Piecuch, J. Shen, N.P. Bauman**

8:40 *PHYS 359.* Electron-vibron coupling effects on electron transport via single-molecule magnet Fe₄. **K. Park**

9:20 Intermission.

9:50 *PHYS 360.* Synthesis and characterization of ruthenium complexes of a verdazyl-based diradical ligand: Interplay between metal-ligand non-innocence and magnetic exchange. **R.G. Hicks, R. Higgins, C. Sanz, S. McKinnon**

10:30 *PHYS 361.* Nonlinear optical properties of open-shell molecular systems. **M. Nakano**

11:10 *PHYS 362.* π -Stacking pancake bonding. **M. Kertesz**

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Energy Storage, Solar Fuels, and Biofuels: Satisfying the Energy Needs While Decreasing the Carbon Footprint

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 251

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

New Techniques

Cosponsored by COLL

A. T. Krummel, P. B. Petersen, *Organizers*

A. E. Bragg, *Organizer, Presiding*

1:30 *PHYS 363.* Coherent chiroptical spectroscopy and quantum interference. **M. Cho**

2:05 *PHYS 364.* Measuring single nanocrystal properties in the ensemble. **J.R. Caram, M.G. Bawendi**

2:25 *PHYS 365.* Determining reaction intermediate structures with vibrational cross angle method. **J. Zheng**

3:00 *PHYS 366.* Tabletop extreme ultraviolet spectroscopy of element-specific organometallic photophysics. **J. Vura-Weis**

3:20 Intermission.

3:40 *PHYS 367.* Probing conical intersections by novel multidimensional Raman techniques. **S. Mukamel, K. Dorfman, B. Fingerhut, H. Ando, M. Kowalewski**

4:15 *PHYS 368.* Wide-field FTIR microscopy with mid-IR pulse-shaping. **A.L. Serrano, A. Ghosh, J.S. Ostrander, M.T. Zanni**

4:35 *PHYS 369.* Femtosecond stimulated Raman spectroscopy: A vibrationally specific probe of reactive nonadiabatic coupling. **R.A. Mathies**

5:10 *PHYS 370.* Isomerization of a single azobenzene molecule observed through tip-enhanced Raman spectroscopy. **N. Tallarida, J. Lee, L. Rios, V.A. Apkarian**

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

Novel Representations and New Contraction Schemes

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*

T. Shiozaki, *Presiding*

1:30 *PHYS 371.* Density functional calculations in a wavelet basis: The BigDFT code. **S. Goedecker**

2:10 *PHYS 372.* Large-scale DFT calculations on metallic systems. **C. Skylaris, J. Aarons, A. Ruiz Serrano, M. Sarwar, D. Thompsett**

2:50 *PHYS 373.* Lagrange-sinc basis set for efficient electronic structure calculations. **W. Kim**

3:30 *PHYS 374.* Compressed sensing for the fast computation of matrices: Application to molecular vibrations. **J. Sanders, X. Andrade, A. Aspuru-Guzik**

3:50 *PHYS 375.* Geminal-spanning orbitals in local explicitly correlated coupled-cluster methods for large molecules. **F. Pavosevic, F. Neese, E.F. Valeev**

4:10 *PHYS 376.* Sculpting wave functions with number counting Jastrow factors. **E. Neuscamman**

Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENVR

D. A. Knopf, S. Lee, *Organizers*

S. Takahama, B. J. Williams, *Presiding*

1:30 *PHYS 377.* New experimentally-based secondary organic aerosol paradigm. **A. Zelenyuk, D. Imre, J. Wilson, J. Beranek, M. Shrivastava, E. Abramson**

2:00 *PHYS 378.* Viscosity of secondary organic materials and atmospheric implications. **M. Song, S.J. Hanna, P.F. Liu, Y. You, S. Kamal, S.T. Martin, A.K. Bertram**

2:15 *PHYS 379.* Light scattered by ammonium nitrate as a function of crystalline phase. **A. Johnson, D. Cziczo, A.J. Bauer, S. Seager**

2:30 *PHYS 380.* Particle rebound and phase state in Amazonia. **A. Bateman, Z. Gong, R. Souza, A. Manzi, P. Artaxo, S.T. Martin**

2:45 *PHYS 381.* Measuring the surface tension of individual submicron sized sea spray aerosol particles with atomic force microscopy. **H. Morris, V.H. Grassian, A.V. Tivanski**

3:00 *PHYS 382.* Role of water, viscosity, and molecular structure on the chemistry and cloud condensation properties of organic aerosols. **K.R. Wilson**

3:30 *PHYS 383.* Chemical characterization of ambient atmospheric aerosol particles at high altitude in Tenerife, Spain, using an aerosol time-of-flight mass spectrometer. **F. Mahrt, B. Sierau, Y. Boose, I. Garcia Alvarez, S. Rodriguez-Gonzalez, U. Lohmann**

3:45 *PHYS 384.* Chemical and physical considerations for marine cloud condensation nuclei. **D.B. Collins, S. Schill, C. Sultana, C. Lee, J.L. Axson, T. Bertram, K.A. Prather, K. Moore**

4:00 *PHYS 385.* Complex refractive index retrievals for polystyrene latex spheres from 220-420 nm. **T. Galpin, R.T. Chartier, N.R. Levergood, M.E. Greenslade**

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- 4:15 PHYS 386.** Using mass spectrometry to determine residual chemical composition in coagulation experiment. **K. Ardon-Dryer**, Y. Huang, D. Cziczó
- 4:30 PHYS 387.** Equilibrium structure of liquid-liquid phase separated aerosols: Thermodynamic predictions and molecular simulations. **Y. Qiu**, V. Molinero
- 4:45 PHYS 388.** Quantitative comparisons of mineral-rich aerosol mass spectra and ice nucleating efficiency. **S. Garimella**, M. Zawadowicz, C. Christopoulos, D. Rothenberg, D. Cziczó

Section D

Boston Convention & Exhibition Center
Room 254A

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Macromolecular Interactions

Cosponsored by COMP

E. Alexov, R. Luo, *Organizers*

A. E. Garcia, *Presiding*

- 1:30 PHYS 389.** Exploring dimensionality reduction in protein-protein association. **S. Vajda**, D. Kozakov, P. Vakili, I.C. Paschalidis
- 2:10 PHYS 390.** Predicting molecular interactions by protein-protein and protein-RNA docking. **X. Zou**
- 2:50 Intermission.**
- 3:10 PHYS 391.** Measuring drug populations and their reactions with targets inside bacterial cells using Raman microscopy. **P. Carey**, H. Heidari Torkabadi
- 3:50 PHYS 392.** Structural modeling of interactome. **I. Anishchenko**, P. Kundrotas, **I. Vakser**
- 4:30 PHYS 393.** Investigating the role of electrostatic fields in the interfacial inhibition of protein complexes. **E.T. Novelli**, L.J. Webb

Section E

Boston Convention & Exhibition Center
Room 254B

Hydrophobicity, Ion Solvation, & Interfaces: Theory, Simulations, & Experiments

Hydrophobicity & Hydration

D. Ben-Amotz, S. Garde, *Organizers*

R. Kumar, *Presiding*

- 1:30 PHYS 394.** Temperature and pressure dependence of methane correlations and osmotic second virial coefficients in water. **S. Ashbaugh**
- 2:00 PHYS 395.** NMR studies of hydrophobic hydration, from model systems to proteins. **S. Sengupta**, C. Kingsley, J. Guo, D. Khago, **R.W. Martin**
- 2:30 PHYS 396.** Structure and dynamics of the quasi-liquid-layer on ice I_h. **T. Kling**, M. Sulpizi, D. Donadio

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

- 2:50 PHYS 397.** Effect of surface energy on freezing of water probed using surface sensitive sum frequency generation spectroscopy. **Y. Zhang**, E. Anim-Danso, A.N. Dhinjwala
- 3:10 PHYS 398.** Why do some salts accelerate water dynamics? **E. Pluharova**, G. Stirnemann, P. Jungwirth, D. Laage
- 3:30 PHYS 399.** Hydration of classic hydrophobic solutes, Kr and Ar. **M. Chaudhari**, L.R. Pratt, D. Sabo, D. Asthagiri, S.L. Remppe
- 3:50 PHYS 400.** Aqueous proton transfer through graphene. **F. Geiger**

Section F

Boston Convention & Exhibition Center
Room 255

Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Applications and Consequences

Cosponsored by COLL

W. Parak, *Organizer*

C. Burda, K. Hamad-Schifferli, *Organizers*, *Presiding*

- 1:30 PHYS 401.** Structure and charge of functionalized nanoparticles using electrophoresis. **R.J. Hill**
- 2:00 PHYS 402.** Exploiting protein coronas on nanoparticles for biomedical applications. **A. Cifuentes**, H. de Puig Guixé, J.C. Kah, S. Borros, **K. Hamad-Schifferli**
- 2:20 PHYS 403.** Optically probing the selective uptake and processing of bio-nano conjugates in human cell lines. **K.J. Carnevale**, G.F. Strouse
- 2:40 PHYS 404.** Hypoxia sensing enzymes: Toward enzyme delivery. **M. Knapp**, V. Chaplin
- 3:10 PHYS 405.** Exploiting the protein corona around DNA-conjugated gold nanoparticles for enhancement of insulin translation in vitro. **K. Chan**, G. Yang, D. Susanti, J.X. Goh, E. Yeo, J.S. Chao, **J. Kah**
- 3:30 PHYS 406.** Protein corona as a drug delivery vector to enable low-dose multimodal cancer therapy. **J. Kah**, E. Yeo, D.J. Neo, J.U. Cheah, W. Goh, P.S. Thong, P. Kanchanawong

Section G

Boston Convention & Exhibition Center
Room 256

Physical Chemistry of Clusters & Nanoparticles

Optical Properties and Applications

D. Jiang, G. E. Johnson, *Organizers*, *Presiding*

- 1:30 PHYS 407.** Understanding monolayer-protected clusters using theoretical methods. **C.M. Aikens**, E. Guidez, K.M. Weerawardene
- 2:00 PHYS 408.** Ultrafast and nonlinear spectroscopy of colloidal plasmonic nanoparticles. **L.H. Haber**, T.E. Karam, R.R. Kumal, H.T. Smith
- 2:20 PHYS 409.** Optical properties and structural relationships of silver nanoclusters. **S. Yau**, B. Ashenfelter, O. Varnavski, T.P. Bigioni, T.G. Goodson
- 2:40 PHYS 410.** Withdrawn.
- 3:00 Intermission.**
- 3:20 PHYS 411.** Structural defects induced plasmon peak splitting in single bimetallic nanorods. **J. Zhao**, S. Thota, S. Chen, Y. Zhou, S. Zou

- 3:40 PHYS 412.** Multipolar Raman on chiral plasmonic nanennas. **M. Banik**, K. Rodriguez, E. Hultko, V.A. Apkarian

- 4:00 PHYS 413.** Synthesis and characterization of gallium doped CdSe quantum dots. **H. Luo**, C. Tuinenga, E. Guidez, C.A. Lewis, J. Shipman, S. Roy, C.M. Aikens, **V. Chikan**

- 4:20 PHYS 414.** Properties and processing of multi-layered chalcogenide glasses for direct laser writing of optically functional 3D nanostructures. **C.M. Schwarz**, C.N. Grabill, B. Gleason, G.D. Richardson, S. Labh, C. Rivero-Baleine, K. Richardson, A. Pogrebnyakov, T.S. Mayer, S.M. Kuebler

Section H

Boston Convention & Exhibition Center
Room 257A

Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability, & Spectroscopic Signatures

Spectroscopy

M. S. El-Shall, R. C. Fortenberry, *Organizers*

W. K. Peters, *Presiding*

- 1:30 PHYS 415.** THz time-domain spectroscopy of interstellar ice analogs. **S. Ioppolo**, B. McGuire, X. de Vries, B. Carroll, M.A. Allodi, G.A. Blake
- 2:05 PHYS 416.** Structural studies of reactive molecules by rotational spectroscopy: HOON, HOCOH, and C₆H₂. **K.N. Crabtree**, C. Wornack, O. Martinez, J. Stanton, M. McCarthy
- 2:40 PHYS 417.** Rotational effects in the reactions of OH+ and H₂O+ with H₂ and D₂. **N. Shuman**, S.G. Ard, O. Martinez, A.A. Viggiano
- 3:15 Intermission.**
- 3:45 PHYS 418.** Rotational spectroscopy and radio observations of exotic species created via novel laboratory synthesis. **D.T. Halfen**, L.M. Ziurys
- 4:20 PHYS 419.** Large amplitude motions and feasible proton permutations in the spectroscopy and dynamics of H₅⁺. **Z. Lin**, A.B. McCoy

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Artificial Photosynthesis: Challenges and Strategies to Meet Energy Needs in an Environmentally Benign Manner

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

WEDNESDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Poster Session

E. L. Sibert, *Organizer*

6:00 - 8:00

- PHYS 420.** Helical assemblies of CdTe nanoparticles induced by chiral amino acid ligand. **W. Feng**, J. Kim, N. Kotov
- PHYS 421.** Simulation of pump-probe spectra with an efficient, parallelized algorithm. **A. Markmann**, M. Soley, E. Nibbering, V.S. Batista

- PHYS 422.** Configuration interaction geminal screening on ground state and excited state energies for 10 electron systems and carbon dimer. **M.G. Bayne**, A. Chakraborty

- PHYS 423.** Reaction of CH₃ radicals with HO₂. **C. Yan**, L.N. Krasnoperov

- PHYS 424.** Protein corona formed from different blood plasma proteins affects the colloidal stability of nanoparticles differently. **G. Engudar**, **Y. Ho**, J. Kah

- PHYS 425.** Structure-function relationships of a natural nanoscale photonic device in cuttlefish chromatophores. **L. Deravi**

- PHYS 427.** Understanding the nature of hopping transport in conjugation-broken molecular wires. **D. Taherinia**, C.D. Frisbie

- PHYS 428.** Gas phase stereo chemistry of 2-phenylethyl methyl ether and its weakly bonded complexes from Fourier transform microwave spectroscopy. **R.M. Gurusingham**, M. Tubergen

- PHYS 429.** Elucidating structural features of molecular systems with quantum tunneling: Doubled rotational spectra of methylated indoles. **R.M. Gurusingham**, M. Tubergen

- PHYS 430.** Vascular margination and permeability of corona-coated polystyrene nanoparticles in microfluidic devices. **Y. Ho**, **S.W. Lee**, N.A. Azman, S. Beyer, G. Adriani, R. Kamm, J. Kah

- PHYS 431.** Study of gas phase CH₃ and HO₂ radicals at ambient temperature and pressure using laser photolysis coupled to transient UV - vis absorption spectroscopy. **M. Sangwan**, L.N. Krasnoperov

- PHYS 432.** Photochemical synthesis of Sn₃O₂/Ag and Sn₃O₂/Au nanostructures under the visible light illumination. **V.V. Shvalagin**, **N. Barashkov**, T. Sakhno, G. Grodzyuk, O. Shvets, V. Granchar

- PHYS 433.** Plasmonic coupling in random gold nanoparticle arrays. **J. Jenkins**, Y. Zhou, S. Thota, X. Tian, X. Zhao, S. Zou, J. Zhao

- PHYS 434.** Photoinduced electron transfer within conformationally flexible cytochrome c. **J. Gu**, T. Prytkova, E.V. Pletneva

- PHYS 435.** Heterogeneous chemistry of biologically-derived components of sea spray aerosol: The role of acid-base chemistry. **J. Trueblood**, A. Estillore, V.H. Grassian

- PHYS 436.** Raman spectroscopic study of TiO₂ electrodes and dye-sensitized solar cells. **Y. Northrup**, J.J. Rochford, M.C. Foster

- PHYS 437.** Surface reaction of carboxylic acids on titanium dioxide nanoparticles. **J.M. Marmolejos**, M. Kipreos, M.C. Foster

- PHYS 438.** Reactivity of vibrationally hot methane on Ir(110)-(1x2). **E. Nicotera**, E. Peterson, A. Utz

- PHYS 439.** Investigating gold nanoparticle surface charge density and photocleaving dynamics of miRNA mimics using second harmonic generation. **R.R. Kumal**, T.E. Karam, C.R. Landry, M. Abu-Laban, D. Hayes, L.H. Haber

- PHYS 440.** Optimizing gain in surface-enhanced femtosecond stimulated Raman spectroscopy via fully tunable pulses. **L.E. Buchanan**, M. McAnally, N.L. Gruenke, R.P. Van Duyne

- PHYS 441.** Direct observations of molecules at aerosol surfaces with second harmonic scattering. **Y. Wu**, B. Xu, W. Li, X. Li, H. Dai, V.F. McNeill, **Y. Rao**

- PHYS 442.** Small PbS quantum dots as a hole transport layer in planar perovskite solar cells. **W.R. Hess**, M.G. Bawendi

- PHYS 443.** Influence of quantum dot ligands on charge generation and recombination in hybrid organic/inorganic photovoltaics. **W. Wu, A. Colbert, D.S. Ginger**
- PHYS 444.** Determination of structural properties of fluorescent methane carbon nanodots. **R.D. Schmitz, J.O. Karolin, C.D. Geddes**
- PHYS 445.** Synthesis and spectrally resolved single particle photoluminescence imaging of CdS quantum dots. **R. C. A. Chowdhury**
- PHYS 446.** Nonlinear vibrational mid-infrared photothermal spectroscopy with a near-infrared fiber laser probe. **A. Totachawattana, H. Liu, S. Erramilli, M. Sander**
- PHYS 447.** Vibrational spectroscopy of benzene-(water)_n clusters with n=3-7. **D.P. Tabor, R. Kusaka, P.S. Walsh, E.L. Sibert, T.S. Zwier**
- PHYS 448.** Analysis of the intermolecular hydrogen bonding interactions of phenol derivatives in solution using infrared spectroscopy and density functional theory. **M.J. Toda, A.M. Fedor**
- PHYS 449.** Understanding CO₂ solvation in ionic liquids using energy decomposition analysis and vibrational spectroscopy. **E. Berquist, K.K. Bullard, Z.M. Campbell, D. Lambrecht**
- PHYS 450.** Measuring hygroscopic and liquid-liquid phase separation properties of organic/inorganic mixed phase atmospheric aerosols using FTIR. **S.S. Seppäläinen, M.A. Zawadzowicz, S.R. Proud, D. Cziczko**
- PHYS 451.** Computational study of the photochromism of nitrospiropyran and merocyanine. **S. Gurung, M.L. Mayes**
- PHYS 452.** Simulation of X-ray transient absorption spectroscopy for following vibrational motion. **A.D. Dutoi, S.R. Leone**
- PHYS 453.** Temperature-dependent measurements of charge organization in 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonate) ionic liquids obtained from vibrational spectroscopy. **L. Lowe-Thompson, C. Burba**
- PHYS 454.** Probing the surface chemistry of ALD reactions using in situ surface-enhanced Raman spectroscopy. **S. Masango, P.C. Stair, R.P. Van Duyne**
- PHYS 455.** Vibrational spectra of cyclodextrin-BPA host-guest complexes. **A. Shi, A. Palaksha, M.T. Buthelezi**
- PHYS 456.** Elucidating lipid structure on gold nanoparticle surfaces with surface-enhanced Raman spectroscopy. **K. Chang**
- PHYS 457.** Probing solvation dynamics at interfaces with surface bound azides and vibrational sum frequency generation spectroscopy. **M.A. Mattson, C. Rich, A.T. Krummel**
- PHYS 458.** Strong correlations and fractional electron errors in self-consistent second order Green's function theory. **J. Phillips**
- PHYS 459.** Calculation of ionization potentials and electron affinities within second order Green's function theory. **A. Welden, J. Phillips, D. Zgid**
- PHYS 460.** Active space EOM-CCSD approach with second-order perturbative correction: Theory and benchmarks. **A.A. Kunitas, K.B. Bravaya**
- PHYS 461.** Astrochemistry simulated in electron-irradiated CO₂/NH₃ ices. **S. Esmaili, A.D. Bass, P. Cloutier, L. Sanche, M. Huels**
- PHYS 462.** Replicating prebiotic astrochemistry through the use of a silicate grain surface analog. **A.N. Carey, M.C. Foster**
- PHYS 463.** Highly stable graphene oxide-polymer-protein composites for catalysis at thermally and chemically adverse conditions. **O.V. Zore, A. Pattammattel, S. Gnanaguru, C.V. Kumar, R. Kasi**
- PHYS 464.** Ultrafast spectroscopic characterization of an intensometric green fluorescent protein biosensor for Ca²⁺ imaging. **L. Tang, W. Liu, Y. Wang, Y. Zhao, B. Oscar, R.E. Campbell, C. Fang**
- PHYS 465.** Photothermal effect, optical enhancement, and catalytic activity of selected plasmonic nanoparticles. **T.E. Karam, H.T. Smith, R. Khoury, L.H. Haber**
- PHYS 466.** Dockground resource for protein recognition studies. **D. Singla, P. Kundrotas, I. Vakser**
- PHYS 467.** Statistical analysis of predicted vs. experimental interresidue contacts in protein-protein complexes from results of docking simulations. **L. Cavallo, R. Oliva, E. Chermak**
- PHYS 468.** Lysine becomes a heme ligand upon perturbation of the intraprotein hydrogen-bonding network in horse heart cytochrome c. **D. Shin, J. Gu, E.V. Pletneva**
- PHYS 469.** Exciton and charge transfer mechanism in proteins of the photosynthesis. **J.M. Foerster, L. Mueller, M. Ullmann**
- PHYS 470.** Computational study of nanoparticle catalysts in the water-gas shift reaction. **K. Haug**
- PHYS 471.** Stable-on-the-Table biocompatible electrocatalysts: Hemoglobin-poly(acrylic acid) nanogels. **A. Ghimire, O.V. Zore, R. Kasi, Y. Lei, C.V. Kumar**
- PHYS 472.** Surface TiO₂ mediated catalysis: A potential target for greenhouse gas reduction. **B. Mattingly**
- PHYS 473.** Proteasome noncovalent interactions in biology: Effective fragment potential (EFP) benchmarks on the protein database. **Y. Bui**
- PHYS 474.** Investigation of solvatochromic behavior of malononitrile-based merocyanine dye in polysiloxane films. **N. Barashkov, T. Sakhno, I. Irgibayeva, A. Mantel, A. Aldongarov, A. Ishchenko**
- PHYS 475.** Theoretical study on the structure and photoelectron spectrum of an allotrope of C₁₂₂. **Y. Wang, C. Huang, J. Chang**
- PHYS 476.** Highly luminescent quantum sized gold nanoclusters. **K. Pyo, D. Lee**
- PHYS 477.** Investigation of cyclodextrin complexes with PAHs using steady state fluorescence and parallel factor analysis. **J.W. Chiarelli, J. Kenny**
- PHYS 478.** Effect of pH on the intramolecular cyclization mechanism of aqueous 3a-substituted tryptophan. **M. Menéndez, R. Lopez, J. Méndez Hurtado**
- PHYS 479.** Characterizing a nonclassical carbene with coupled-cluster methods: The singlet potential energy surface of cyclobutylidene. **X. Wang, J. Agarwal, H.F. Schaefer**
- PHYS 480.** Spectroscopic maps for the IR spectroscopy of CO₂ in ionic liquids. **C.A. Daly, S.A. Corcelli**
- PHYS 481.** Study of the stability of 1-alkyl-3-methylimidazolium hexafluoroantimonate ionic liquids using X-ray photoelectron spectroscopy. **L.S. Longo Jr, P. Licence**
- PHYS 482.** Evaluating the structures and stabilities of D-mannitol polymorphs and hydrates. **T. Dierks, T.M. Korter**
- PHYS 483.** Calibration and utility of low-cost and highly-portable gas sensors for atmospheric composition measurement. **J.D. Shutter, O.A. Popoola, A.J. Durant, R.A. Freshwater, R.L. Jones**
- PHYS 484.** Topographical changes of liquid-metal alloys as a function of temperature. **N.J. Bello, I. Tevis, M. Thuo, M.C. Foster**
- PHYS 485.** FT-IR spectroscopy and DFT calculations of nearest neighbor ¹³C isotopologues of the helical peptide Z-Aib_n-OtBu. **M. Rotondaro, M.A. Kubasik**
- PHYS 486.** Investigations of ice-water interfaces with single-crystal ice I_h and matrix-isolated water. **A. Brumberg, P.J. Bisson, R.M. Shultz, M.J. Shultz**
- PHYS 487.** Nonlinear optical study of S-nitrosothiols using the Z-Scan technique. **D.R. Neiva Sonogo, A. Reis, S. Alves**
- PHYS 488.** Ab initio kinetic models for parallel addition reactions of the butadienyl radical. **P. Winter, R. LeCoulter, A.L. Cooksy**
- PHYS 489.** Carbon dioxide self-quenching rates measured with a quantum cascade laser. **K.J. Castle, C. Flynn**
- PHYS 490.** Investigation of the shock-sensitivity of HEDMs using DFT and bond order analysis. **A.L. Shoaf, L. Harper, C.A. Bayse**
- PHYS 491.** Photodissociation of methanol at 193.3 nm. **C. Yan, L.N. Krasnoperov**
- PHYS 492.** Molecularly engineered biographene interfaces: From columbic interactions to enzyme stabilization. **A. Pattammattel, M.J. Novak, C.V. Kumar**
- PHYS 493.** Control of nanoscale domain formation in polymer networks. **J. Jung, E. Jang, J. Kim**
- PHYS 494.** Nonlinear quantum transport in molecular junctions: A uniform theory bridging coherent tunneling and Coulomb blockade limits based on the Anderson's impurity model. **B. Jin**
- PHYS 495.** Computation of CH and NH isotopic exchange effects on ¹³C NMR spectra of small, rigid peptides. **E. Kleist, B.S. Hudson**
- PHYS 496.** Theoretical chemisorption studies on defect pyrene. **R. Nieman, A. Das, H. Lischka**
- PHYS 497.** Fundamental study of the metal insulator transitions dependency on morphology via vanadium pentoxide thin films grown by sol-gel and thermal evaporation. **B. Lamoureux**
- PHYS 498.** Study of thermal diffusivity of Sudan I derivatives by Z-Scan technique. **W. Kavassaki, L.S. Longo Jr, S. Alves**
- PHYS 499.** Explicitly correlated electron-hole method for calculating optical properties of semiconductor nanocrystals. **J.A. Scher, A. Chakraborty**
- PHYS 500.** Efficient hybrid bulk heterojunction solar cells: Understanding polymer diffusion within metal oxide nanostructures. **E. Sadler, A.J. Morris**
- PHYS 501.** Condensed-phase effects on the structural properties of C₆H₂CH₂CN-SiF₄ and CH₃CH₂CN-SiF₄. **N.J. Hora, J.A. Phillips**
- PHYS 502.** Withdrawn.
- PHYS 503.** Molecular surface area based predictive models for the adsorption and diffusion of disperse dyes on poly(lactic acid) fibers. **S. Xu, J. Chen, B. Wang, Y. Yang**
- PHYS 504.** Withdrawn.
- PHYS 505.** Molecular modeling of liquid pyrazole for next generation fuel cell membranes. **K.V. Greco, Q. Sun, S.M. Auerbach**
- PHYS 506.** Can disorder enhance incoherent exciton diffusion? **E.M. Lee, W.A. Tisdale, A. Willard**
- PHYS 507.** Generation of the sedimentation potential by rapid deceleration of a fluid jet. **H. Park, Z. Tang, G.J. Diebold**
- PHYS 508.** Machine learning approach to aerosol classification based on chemical analysis. **C. Christopoulos, S. Garimella, D. Cziczko**
- PHYS 509.** Withdrawn.
- PHYS 510.** DNA hydration dynamics: Detailed mapping and dynamics in the minor groove. **E. Duboue-Dijon, A.C. Fogarty, J.T. Hynes, D. Laage**
- PHYS 511.** Withdrawn.
- PHYS 512.** Evolving chemical complexity of sea spray aerosol particles and the effect on heterogeneous reaction with nitric acid. **C. Lee, J. Trueblood, V.H. Grassian, K.A. Prather**
- PHYS 513.** Magnetically induced polarization in chiral-ordered CaMn₇O₁₂. **J. Lim, D. Saldana-Greco, A.M. Rappe**
- PHYS 514.** Withdrawn.
- PHYS 515.** Synthesis of C-13 labeled ortho-carborane for solid-state NMR spectroscopy of thin films. **A.S. Alnafisah, C. Stirling, S. Purohit, B. Nordell, T. Nguyen, M. Paquette, N.A. Oyler**
- PHYS 516.** Withdrawn.
- PHYS 517.** Effects of cationic residues and base sequence in nucleic acid binding of histone-derived antimicrobial peptides. **S. Sim, K. Cutrona, B. Beyer, P. Wang, M. Radhakrishnan, D.E. Elmore**
- PHYS 518.** Heterogeneous oxidation of organic coatings on submicron aerosol particles. **C.Y. Lim, E.C. Browne, R.A. Sugrue, J.H. Kroll**
- PHYS 519.** Ultrafast terahertz Kerr effect spectroscopy of aromatic liquids. **I. Finneran, M.A. Alloodi, G.A. Blake**
- PHYS 520.** Structure of a single polymer chain confined in a dense array of nanoposts. **H. Joo, J. Kim**
- PHYS 521.** Light induced temperature increase of gold nanoparticles: Single and ensemble particle measurements. **K. Setoura, S. Ito, H. Miyasaka**
- PHYS 522.** Electron ionization and attachment energies of radicals using algebraic diagrammatic construction schemes. **M. Schneider, A. Dreuw**
- PHYS 523.** Membrane-bound structural distribution of alpha-synuclein determined via single-site thiocyanate infrared probe groups. **D.M. Konstantinovsky, C.H. Londergan, A.R. Vienneau**
- PHYS 524.** Single-enzyme meets single-polymer: Challenges of making 1:1 covalent adducts of enzymes with poly(acrylic acid). **K. Benson, C.V. Kumar**
- PHYS 525.** Withdrawn.

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- PHYS 527.** Automating kinetic solvent effects for mechanism generation. **B. Slakman, R.H. West**
- PHYS 528.** Synthesis of redox mediators for quantum dot sensitized solar cells. **R. Sturm**
- PHYS 529.** Interrogating the role of xCT in neuroregeneration through laser ablation of zebrafish neurons. **N.A. Ladd, A.P. Putzke, L. Chase, B.P. Krueger**
- PHYS 530.** Investigation of the thermostability of DNA polymerase using molecular dynamics simulations. **E. Modeste, L. Mawby, B. Miller, E. Wu, C.A. Parish**
- PHYS 531.** Predicting folding free energy changes caused by single point mutations via combined usage of MM-PBSA method and biophysical characteristics. **I. Getov, M. Petukh, E. Alexov**
- PHYS 532.** Detailed quantum studies on the m-benzyne and o-benzyne diradicals. **B. Zhang, C.A. Parish, C. Annas**
- PHYS 533.** Electrochemical sensors based on an ionic liquid of Au₂₅ nanocluster. **M. Jang, K. Kwak, D. Lee**
- PHYS 534.** Synthesis and characterization of highly purified bimetallic Au₂₅ nanoclusters. **M. Kim, K. Kwak, D. Lee**
- PHYS 535.** Computational study of intermolecular interactions between L-cysteine and 2-mercaptopyrimidine compounds using DFT, QTAIM, and NBO methods. **I.A. Morkan, A.U. Morkan, H.C. Yazici**
- PHYS 536.** Understanding the structural properties of anticancer drugs and DNA bases by employing surface-enhanced Raman scattering. **M. Torres, S. Khan, N. Mirsaleh-Kohan**
- PHYS 537.** X-ray absorption in insulators with non-Hermitian real-time time dependent density functional theory. **R.G. Fernando, M.C. Balhoff, K. Lopata**
- PHYS 538.** Valence bond theory study of charge-shift bonding resonance energy. **C. Laconsay, A. James, J.M. Galbraith**
- PHYS 539.** Cyclopropyl disrotatory ring opening reactions. **S. Houck, C.A. Parish, E. Speetzen**
- PHYS 540.** SERS studies of chemotherapeutic agents. **M. Duplanty, C. Madrid, N. Mirsaleh-Kohan**
- PHYS 541.** Energetics of methanol decomposition of graphene-supported Pt nanoclusters. **R.J. Gasper, A. Ramasubramanian**
- PHYS 542.** Mass and charge transport in pyrrolidinium cation-based and alkyltrimethylammonium cation-based ionic liquids. **A.M. Fleshman, A.J. Lowry**
- PHYS 543.** Application of the compensated Arrhenius formalism to temperature-dependent fluidity and self-diffusion coefficients of 1-alcohol and 3-alcohol systems. **G.E. Forsythe, A.M. Fleshman, M.A. Petrowsky, R. Frech**
- PHYS 544.** Electrochemical and photochemical studies of AuBr₃ for microscopic-photochemical-laser-traced-electrodeposition (μ PLATE). **C.N. Lafratta, C. Wheeler, E. Reed, P. Lawrence, C. Anyanwu**
- PHYS 545.** 3D discrete variable calculations for atom-asymmetric top complexes. **M.D. Marshall, H.O. Leung, G. Lupinski, J. Yu**
- PHYS 546.** Effect of substitution of fluorine by chlorine on the structures of protic acid-haloethylene heterodimers. **H.O. Leung, M.D. Marshall, F. Feng, N.D. Khan, J.P. Messinger**
- PHYS 547.** Systematically improvable exciton Hamiltonians in large-scale electronic structure calculations. **Y. Liu, A.D. Dutoi**
- PHYS 548.** Chemical characterization of ambient PM_{2.5} collected over Towson Maryland. **E. Meade, A. Brock, K.E. Kautzman, W. Wendt**
- PHYS 549.** Characterization of solvated and unsolvated fluorophores in vacuum. **V. Rajagopal, A.L. Ferzoco**
- PHYS 550.** Mapping chemical systems to model Hamiltonians for condensed phase dynamics. **M. Mavros, D. Hait, T.A. Van Voorhis**
- PHYS 551.** Measurement of IVOC and SVOCs as intermediates in SOA formation using online electron-impact mass spectrometry. **J.P. Franklin, G. Isaacman-VanWertz, J.H. Kroll**
- PHYS 552.** Surface thermodynamics of penta-graphene. **S. Chase, M. von Domaros, D. Bratko, A. Luzar**
- PHYS 553.** Conformational studies of N-chlorobenzenesulfonamides and N-chloro-2-nitrobenzenesulfonamides in the gas phase: Intramolecular hydrogen bonding. **H. Kim, M. DeRosa**
- PHYS 554.** Geometries of potential energy landscapes imply dynamical signatures for roaming reactions. **V. Cofer-Shabica, R.M. Stratt**
- PHYS 555.** Benchmark study of density functional theory for OH vibration frequency in water. **K. Jeon, M. Yang**
- PHYS 556.** Development of quantitative analysis methods of amyloid fibrils using atomic force microscopy. **C. Schifone**
- PHYS 557.** Photopolymerization of guest 1-iodo- and α,ω -diiodoalkanes in host urea inclusion compounds. **P. McLaughlin, B.S. Hudson**
- PHYS 558.** Withdrawn.
- PHYS 559.** Reaction mechanisms and branching ratios between CH(X²T) and C₂H₆, C₂H₄ and C₂H₂: An ab initio study. **J.L. Ribeiro, A.M. Mebel**
- PHYS 560.** Computational vibrational analysis of isomerization coordinates in combustion-related free radicals HCCCO and C8H7. **P. Zajac, G. Soriano, A.L. Cooks**
- PHYS 561.** Band gap formation in low dimensional heterostructures h-boron nitride and graphene. **P.A. Brown, C. Xu, K.L. Shuford**
- PHYS 562.** Structure-function relationships for graphene-supported Pt nanoclusters. **H. Shi, S.M. Auerbach, A. Ramasubramanian**
- PHYS 563.** Modeling nonradiative energy processes in quantum dot relaxation. **E.P. Aldrich, R. Beaulac**
- PHYS 564.** Structural control of non-adiabatic photochemical bond formation: Photocyclization dynamics of ortho-terphenyl and structural analogs. **M.S. Molloy, J. Snyder, J. DeFrancisco, A.E. Bragg**
- PHYS 565.** Green's function embedding in SCF calculations with periodic boundary conditions. **A.A. Rusakov, D. Zgid**
- PHYS 566.** Spectroscopic characterization of electron-lattice coupling in the cooperative proton-electron transfer material quinuhydrone. **A. Rury, S. Sorenson, E. Driscoll, J.M. Dawlaty**
- PHYS 567.** Modeling nonadiabatic energy transfer dynamics in photosynthetic complexes. **M. Lee, D. Coker**
- PHYS 568.** High-spin organic diradical incorporating the 1,2,4-benzotriazinyl radical. **N. Gallagher, A. Rajca**
- PHYS 569.** Fundamental characterization of 3,5-didehydropyrazine. **T. Scott**
- PHYS 570.** Phase-stabilized detection of heterodyne sum frequency generation for interfacial studies. **B. Xu, Y. Wu, D. Sun, H. Dai, Y. Rao**
- PHYS 571.** Coherence resonance in the transport of amino acids through carbon nanotube nanopores. **M.D. Ellison, L.M. Nebel, L.D. Bricker, S. Menges, M. Strano**
- PHYS 572.** Quantum mechanical study of tautomeric triggers of Bergman cyclization. **A.K. Jaini, C.A. Parish**
- PHYS 573.** Buzz on Bombolitin: Observing the structural and dynamic changes of bee venom with lipid matrices. **M.G. Roberson, S. White, K. Ketelaar, A. Leonard, I. Wallace, M. Tucker**
- PHYS 574.** Edible or digestible artificial light antennas: Hydrogels of dye-loaded bovine serum albumin and medium chain fatty acids. **J. Ding, J. He, C.V. Kumar**
- PHYS 575.** Electrocatalytic efficiency of functionalized multiwalled carbon nanotubes toward the removal of anti-inflammatory drug ibuprofen from aqueous solutions. **A. Bakr, M. Rahaman**
- PHYS 576.** Determining conformation and geometry of specific residues in a model peptide by ¹³C isotope-edited ATR-FTIR in H₂O. **J.D. Combs, C. Wang**
- PHYS 577.** Withdrawn.
- PHYS 578.** Timescale and energetics of hydration level change in an internal cavity of cytochrome c oxidase. **C. Son, A. Yethiraj, Q. Cui**
- PHYS 579.** Photochemistry of green fluorescent protein: A computational investigation. **P. Gurunathan, L.V. Slipchenko**
- PHYS 580.** Atomistic view of FUS N-terminal domain liquid-liquid phase separated states. **K.A. Burke, A. Janke, N. Fawzi**
- PHYS 581.** Application of a desolvation energy model to a two-state protein folding equilibrium. **D.K. Eggers, M.R. Gancayco, K. Choi**
- PHYS 582.** Intrinsic site-specific vibrational probe for infrared studies of protein dynamics. **F. Chalyavi, M.J. Tucker**
- PHYS 583.** Exploring the biochemical basis of composition and phenomena at the air-sea interface. **J. Michaud, C. Lee, C. Sultana, A. Rabines, M. Kim, R. Williams, F. Malfatti, F. Azam, R.S. Pomeroy, T. Bertram, A. Allen, K.A. Prather, M.D. Burkart**
- PHYS 584.** Testing atmospheric dispersion methods on emissions from Houston's chemical industries. **T. Yacovitch, G.R. Magoon, S.C. Herndon, J. Roscioli, C. Floerchinger, W.B. Knighton, C.E. Kolb**
- PHYS 585.** Photochemical production of hydroxyl radicals in indoor environments. **S. Kowal, T.F. Kahan**
- PHYS 586.** Changes in inorganic fine particulate matter sensitivities to precursors due to large-scale US emissions reductions. **J.I. Holt, N. Selin, S. Solomon**
- PHYS 587.** Probing molecular scale surface sites for ice nucleation on kaolinite and sodium chloride. **V. Alstadt, S.K. Sihvonen, G. Schill, R. Parker, J.D. Kubicki, M. Tolbert, M. Freedman**
- PHYS 589.** Scaled-ionic-charge simulation model that reproduces enhanced and suppressed water diffusion in aqueous salt solutions. **Z. Kann, J.L. Skinner**
- PHYS 590.** Extending correlated methods to large systems by exploiting advanced programming tools and new computer architectures. **E. Epifanovsky**
- PHYS 591.** SiC Porous materials derived from apple with high performance electromagnetic interference shielding. **Y. Xu, C. Liu**
- PHYS 592.** Quantum Control for Trapped Particles at Matter Surface. **Q. Wang**
- PHYS 593.** Gate-free electrical breakdown of metallic single-walled carbon nanotubes with high selectivity through cross-bar. **J. Li, J. Liu**
- PHYS 594.** Electronically excited states of helium clusters explored using ab initio quantum chemistry. **K.D. Closser, M.P. Head-Gordon**
- PHYS 595.** Ultrafast infrared and computational study of the formation of alkenylcarbenes from cyclopropanated phenanthrene derivatives. **J. Joseph, M. Chakraborty, J.M. Suzuki, N. Flanders, D.M. Thamattoor, C.M. Hadad**
- PHYS 596.** Steered classical density dynamics for energy minimization. **A. Markmann, M. Soley, V.S. Batista**
- PHYS 426.** Reaction CH₃ + CH₃ → C₂H₆ studied over the 292 – 714 K temperature and 1 – 100 bar pressure ranges. **M. Sangwan, C. Yan, C.N. Evgeni, L.N. Krasnoperov**

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

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THURSDAY MORNING

Section A

Boston Convention & Exhibition Center Room 251

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

Structure, Dynamics, and Behaviors of Material Systems

Cosponsored by COLL

A. E. Bragg, P. B. Petersen, *Organizers*

A. T. Krummel, *Organizer, Presiding*

8:00 **PHYS 597.** Investigating the influence of composition on exciton dynamics in organic thin films. **P. Goff, B. Caplins, D.A. Blank**

8:35 **PHYS 598.** Origins of recombination centers in organo-halide perovskites for solar photoconversion. **R.J. Stewart, J.B. Asbury**

8:55 **PHYS 599.** Role of conformational disorder in the electronic and structural dynamics of conjugated molecules. **T.J. Quinicy, M.S. Barclay, C.G. Elles**

9:30 **PHYS 600.** Molecular simulations of exciton transport in disordered organic films. **L. Shi, A.P. Willard**

9:50 Intermission.

10:10 **PHYS 601.** Ultrafast vibrational spectroscopy of electronic processes in solution processed photovoltaic materials. **R.J. Stewart, A. Rimshaw, C. Grieco, A.V. Larsen, J.B. Asbury**

10:45 **PHYS 602.** Working toward the development of singlet fission based light harvesting systems. **A. Le, J. Bender, S.T. Roberts**

11:05 PHYS 603. Ultrafast photophysics of chalcogenorhodamine dyes used in solar hydrogen production. **D.W. McCamant**, R. Sabatini, B. Zheng, M.W. Kryman, J.E. Hill, M. Mark, D. Mark, M.R. Detty, R. Eisenberg

11:40 PHYS 604. Probing nanoaggregate structures of polycyclic aromatic hydrocarbons with 2D IR spectroscopy. **J. Cyran, A.T. Krummel**

Section B

Boston Convention & Exhibition Center
Room 252A

Electronic Structure Methods for Large Systems

SCF Functionals and Algorithms

Cosponsored by COMP

M. P. Head-Gordon, J. Herbert, *Organizers*
R. Steele, *Presiding*

8:00 PHYS 605. Multipetaflops DFT calculations of electronic structure and electron transport. **J. Bernholc**

8:40 PHYS 606. Explicit two-component quasiparticle formulation for investigating excited electronic states of large finite-sized systems. **J. Scher, A. Chakraborty**

9:00 PHYS 607. Are users ready for the large-scale electronic structure methods we develop? **H.J. Kulik**

9:40 PHYS 608. Fast algorithms for Kohn-Sham density functional theory. **L. Lin**

10:20 PHYS 609. Generalizing the local density approximation. **P. Gill**

Section C

Boston Convention & Exhibition Center
Room 252B

Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Cosponsored by ENVR

D. A. Knopf, S. Lee, *Organizers*

J. H. Kroll, J. B. Nowak, *Presiding*

8:00 PHYS 610. Immersion ice nucleation properties of feldspar minerals. **Z.A. Kanji, A. Welti, U. Lohmann**

8:15 PHYS 611. Why does acid treatment inhibit ice nucleation on aluminosilicate clay minerals? **M. Freedman**

8:45 PHYS 612. Molecular study of the effects of chemical processing on heterogeneous ice nucleation: Role of active sites and product formation. **S. Sihvonen, K. Murphy, G. Schill, M. Tolbert, K.T. Mueller, M. Freedman**

9:00 PHYS 613. How important are glassy SOA ice nuclei for ice formation in cirrus clouds? **J. Penner, C. Zhou**

9:30 PHYS 614. Complexities of cloud condensation nuclei. **A. Asa-Awuku**

10:00 PHYS 615. Withdrawn.

10:15 PHYS 616. Hygroscopicity of organic aerosols and aerosol indirect effects on climate. **J. Wang, F. Mei, R. Thalman, P. Hayes, B. Palm, J.L. Jimenez, A. Setyan, S. Zhou, Q. Zhang, S. de Sa, S.T. Martin, P. Artaxo, X. Liu**

Section D

Boston Convention & Exhibition Center
Room 254A

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes

Nucleic Acids

Cosponsored by COMP

E. Alexov, R. Luo, *Organizers*

S. Vajda, *Presiding*

8:00 PHYS 617. Reversible folding of the GCAA hyperstable RNA tetraloop using molecular dynamics simulations. **A.A. Chen, J. Miner, A.E. Garcia**

8:40 PHYS 618. Exploring Coulombic and solvent polarization-mediated forces in nucleic acids folding: A Tightly Bound Ion (TBI) model approach. **S. Chen**

9:20 Intermission.

9:40 PHYS 619. Combining theory with experiments to attain deeper insight into ribozyme mechanism. **P. Bevilacqua, B.L. Golden, S. Hammes-Schiffer**

10:20 PHYS 620. Recognition of modified DNA bases. **W. Cao**

11:00 PHYS 621. Two ion binding shell mechanism of nucleic acid condensation. **I.S. Tolokh, A. Drozdetski, N.A. Baker, L. Pollack, A.V. Onufriev**

Section E

Boston Convention & Exhibition Center
Room 254B

Hydrophobicity, Ion Solvation, & Interfaces: Theory, Simulations, & Experiments

Hydrophobicity & Hydration

D. Ben-Amotz, S. Garde, *Organizers*

A. Patel, *Presiding*

8:00 PHYS 622. Structure and dynamics of hydrophobic hydration shells: A molecular description based on ab initio and classical molecular dynamics simulations. **E. Duboue-Dijon, G. Stirnemann, D. Laage**

8:30 PHYS 623. Quantifying hydrophobicity and solvation using Local Molecular Field Theory. **J.D. Weeks**

9:00 PHYS 624. Hydrogen bonding and aqueous interfacial structure: A mean-field model and its application to hydrophilic solvation. **S. Shin, A. Willard**

9:20 PHYS 625. Molecular understanding of water around hydrophobic solutes and at interfaces. **T. Ichiye**

9:40 PHYS 626. Hydrophobic hydration shell spectroscopy. **S. Zukowski, D. Ben-Amotz, B. Rankin, S. Pattanaude**

Section F

Boston Convention & Exhibition Center
Room 255

Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact

Fundamentals and Applications

Cosponsored by COLL

C. Burda, W. Parak, *Organizers*

K. Hamad-Schifferli, *Organizer, Presiding*

8:00 PHYS 627. Reversibly controlling the spacing and self-assembly of gold nanoparticles with computationally designed metal-coordinating proteins. **M.J. Eibling, C. MacDermaid, Z. Qian, C.J. Lanci, S. Park, J.G. Saven**

8:20 PHYS 628. Protein adsorption on nanocurved surfaces: Investigating the nanobio interaction by small angle scattering. **B. Bharti, J. Meissner, G.H. Findenegg**

8:40 PHYS 629. Shape matters for protein-nanoparticle interactions in biosensing. **D. Jana, J. He, E. Lehnhoff, C. Matti, L. Sagle**

9:00 PHYS 630. Engineered repeat-protein enabled synthesis of gold nanoparticles with tunable morphology. **T. Zarkovic Grove, X. Geng, M. Freyman**

9:20 PHYS 631. Tailoring the biological identity of nanomaterials. **K. Mohr, F. Wurm, V. Mailaender, K. Landfester**

9:40 PHYS 632. Robust surface plasmon resonance (SPR)-based protocol to study biomolecules-nanoparticles interactions. **A. Patra, D. Tao, G. Engudara, C.L. Drum, T.V. Venkatesan, J. Kah**

10:00 PHYS 633. Protein-gold cluster gates for autonomous drug delivery, nuclear staining, and in vivo NIR tumor imaging. **N.M. Khashab**

Section G

Boston Convention & Exhibition Center
Room 256

Physical Chemistry of Clusters & Nanoparticles

Magnetic Properties and Applications

D. Jiang, G. E. Johnson, *Organizers, Presiding*

8:00 PHYS 634. Finite-size effects on phase stability in magnetofunctional materials. **L.H. Lewis**

8:30 PHYS 635. Raspberry-like metamolecules exhibiting strong magnetic resonances. **Z. Qian, S. Park, Z. Fakhraai**

8:50 PHYS 636. State-resolved electronic relaxation dynamics of structurally precise metal nanoclusters studied using femtosecond and magneto-optical spectroscopy. **K.L. Knappenberger**

9:20 Intermission.

9:40 PHYS 637. Withdrawn.

10:10 PHYS 638. Magnetic superatoms as a source of new electronic and magnetic materials. **A.C. Reber**

10:40 PHYS 639. Transition metal oxide clusters: Accounting for spin contamination. **L.M. Thompson, H.P. Hratchian**

Section H

Boston Convention & Exhibition Center
Room 257A

Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability, & Spectroscopic Signatures Charged Species

M. S. El-Shall, R. C. Fortenberry, *Organizers*

R. L. Hudson, *Presiding*

8:00 PHYS 640. Withdrawn.

8:35 PHYS 641. Reactions of negative ions of astrochemical relevance. **Z. Wang, C. Cole, T. Snow, V.M. Bierbaum**

9:10 PHYS 642. Photodestruction and reactive processes of interstellar carbon chain anions. **R. Wester**

9:45 Intermission.

10:15 PHYS 643. Computational study of possible ion-molecule reactions leading to precursors of biomolecules in the interstellar medium. **A. Largo, C. Barrientos, P. Redondo, H. Martinez**

10:50 PHYS 644. Role of low-energy (< 20 eV) electrons in astrochemistry. **C.R. Arumainayagam**

11:15 PHYS 645. Growth of computational chemistry from the needs of astrochemistry. **R.C. Fortenberry, T. Russell, W. Morgan**

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Designs: From Molecules to Functional Materials

Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

POLY

Division of Polymer Chemistry

T. White, D. Boday and M. Jeffries-EI, Program Chairs

SOCIAL EVENTS:

Lunch, 12:00 PM: Sunday, Monday

Reception, 6:00 PM: Tuesday, Wednesday

BUSINESS MEETINGS:

Business Meeting, 6:00 PM: Sunday

SUNDAY MORNING

Section A

Westin Boston Waterfront
Grand Blrm C

Protein-Like Structure & Activity in Synthetic Systems

J. Foster, Y. C. Simon, *Organizers*

E. B. Berda, *Organizer, Presiding*

A. Prasher, *Presiding*

8:00 Introductory Remarks.

8:05 POLY 1. Modular approach to single chain nanoparticles using alternating radical copolymerization. **C. Lyon, E.B. Berda**

8:35 POLY 2. Supramolecular polymerization from synthetic polypeptide-grafted subunits. **J. Wang, H. Xia, H. Lu, J. Cheng, Y. Lin**

9:05 POLY 3. Accessing polyolefins with novel architectures. **H. Li, C. Roland, G. Rojas, A.S. Veige, K.B. Wagener**

9:35 Intermission.

9:50 POLY 4. Synthesis of conjugated polymers and biomimetic approach for the control of the secondary structures. **F. Sanda**

10:20 POLY 5. Radical polymerization ketenes. **Y. Xiang, R. Drout, T. Densmore, E. Pentzer**

10:50 POLY 6. Rational design of macromolecular superstructures. **K. Zhang**

11:20 Concluding Remarks.

Section B

Westin Boston Waterfront
Grand Blrm D

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
F. Horkay, J. A. Johnson, *Presiding*

8:00 POLY 7. From laboratory to human clinical trials: A successful investigational new drug application for detecting early stage cardiovascular disease. **A. McGrath**, E.D. Pressly, Y. Liu, R. Laforest, H. Luehmann, S. Schwarz, D. Sultan, R. Gropler, P. Woodard, C.J. Hawker

8:20 POLY 8. A single nanoparticle for pancreatic cancer combination therapy. **J. Liu**, L. Liao, K. Erazo, L. Terrab, J.A. Johnson

8:40 POLY 9. Polymeric nanoparticles: From fundamental properties to potential applications. **S. Bonetti**, **M. Farina**, A. Colombo, M. Kappel, I. Lieberwirth, M. Mauri, R. Simonutti

9:00 POLY 10. Dissolvable hydrogel-based wound sealant for trauma care. **M. Konieczynska**, J.C. Villa-Camacho, C. Ghobril, A. Nazarian, E.K. Rodriguez, M.W. Grinstaff

9:20 POLY 11. Star-like amphiphilic γ -substituted ϵ -caprolactone block copolymers for drug delivery applications. **K.E. Washington**, R.N. Kularatne, N.C. Doan, J.C. Webb, M.J. Gillings, M.C. Biewer, M.C. Stefan

9:40 POLY 12. Biological function and osmotic properties of cartilage polymers. **F. Horkay**, P.J. Bassler

10:00 POLY 13. Suprametallogels: Controlling gel properties through programmed metallo-supramolecular assembly of nanocage junctions. **A.V. Zhukhovitskiy**, M. Zhong, E.G. Keeler, V.K. Michaelis, R.G. Griffin, A.P. Willard, J.A. Johnson

10:20 POLY 14. Nucleobase-functionalized acrylics with enhanced mechanical strength and processability: From DNA to supramolecular adhesives. **K. Zhang**, G.B. Fahs, M. Alba, W. Chiang, Y. Rhee, R.B. Moore, T.E. Long

10:40 POLY 15. Withdrawn.

11:00 POLY 16. PolyKojic acid: From meat to makeup. **J. Faig**, K. Smith, K.E. Uhrich

11:20 POLY 17. Preparation of antibacterial polyimide composite. **F. Zhang**, **H. Zhang**, Y. Jiang, **W. Zhang**

Section C

Westin Boston Waterfront
Grand Blrm E

Surface Modification of Polymeric Materials

C. Wohl, *Organizer*

K. J. Wynne, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 POLY 18. High throughput, high resolution enzymatic lithography process. **R.A. Gross**, Z. Mao, M. Ganesh, A. Lyons

8:25 POLY 19. Superoleophobic issues. **L. Wang**, T.J. McCarthy

8:45 POLY 20. Preparation of superhydrophobic polymer surfaces using hydrophobic fumed silica. **C. Kosak**, E. Yilgor, I. Yilgor

9:05 POLY 21. Photocured surface modified nanodiamond hybrid composites. **A. Beyler Cigil**, M.V. Kahraman

9:25 POLY 22. Synthesis of iminodi-acetate grafted polypropylene film using chlorinated methacrylate for active packaging application. **J.Z. Lin**, E.A. Decker, J.M. Goddard

9:45 POLY 23. Signal-induced conversion of a poly(phthalaldehyde)-based gel into an adhesive. **S. Chatterjee**, S.T. Phillips

10:05 Intermission.

10:20 POLY 24. Surface grafting of conjugated polymers. **K.L. Martin**, K.R. Carter

10:40 POLY 25. Adhesion of ice to polymer surfaces: Insights on physical and mechanical properties favoring easy release from a new laboratory test. **K.J. Wynne**, C. Wang

11:00 POLY 26. Facile approach for the fabrication of multifunctional nanorods via postpolymerization modification. **H. Jo**, P. Theato

11:20 POLY 27. Surface modification of silk fibroin inverse opals for application as versatile immunosensors. **K.A. Burke**, M.A. Brenckle, D.L. Kaplan, F. Omenetto

11:40 POLY 28. Nucleophilic nanoparticles for CWA threat reduction. **S. Kim**, K.R. Carter

Section D

Westin Boston Waterfront
Commonwealth B

Silicones

S. J. Clarson, *Organizer*

J. M. Mabry, *Organizer, Presiding*

M. J. Owen, *Presiding*

8:00 Introductory Remarks.

8:05 POLY 29. Polydimethylsiloxane-based diblock copolymer nano-objects prepared in non-polar media via RAFT-mediated polymerization-induced self-assembly. **S.P. Armes**

8:35 POLY 30. Multiscale approaches to quantifying aging in filled siloxane polymers. **R.S. Maxwell**, J.P. Lewicki, W. Small, T.S. Wilson, A. Maiti, T. Weisgraber

9:05 POLY 31. Silicon, silica, and silicones in music. **S.J. Clarson**, L. Ianni

9:35 Intermission.

9:50 POLY 32. Synthesis, properties, and applications of polycaprolactone-polydimethylsiloxane-poly-caprolactone triblock copolymers. **C. Kosak**, E. Yilgor, I. Yilgor

10:15 POLY 33. Synthesis of controlled diameter hollow silicone nanoparticles and their incorporation in silicone hydrogels. **S.E. Morgan**, Q. Wu

10:40 POLY 34. Biodegradable, thermoplastic elastomers utilizing POSS as a hard segment. **E. McMullin**, H.T. Rebar, P.T. Mather

11:05 POLY 35. Sustainable polysiloxanes via siloxane metathesis. **E. Sahmetliolu**, E. Göktürk, O. Nsengiyumva, **S.A. Miller**

Section E

Westin Boston Waterfront
Commonwealth C

Herman Mark Scholars Award Symposium in Honor of Stuart Rowan

J. Pyun, *Organizer*

L. Korley, *Presiding*

8:00 Introductory Remarks.

8:05 POLY 36. Spatially controlled surface modification of continuously processed polymer nanofibers. **J.K. Pokorski**

8:35 POLY 37. Bioinspired materials for neural electrodes. **J. Capadona**

9:05 POLY 38. Harnessing the power of phase interactions — tailoring mechanics via supramolecular motifs. **L. Korley**, S. Monemian, K. Jang

9:35 POLY 39. Shape memory thermoplastic elastomers via dual electrospinning. **J.M. Robertson**, H. Birjandi Nejad, **P.T. Mather**

10:05 Intermission.

10:20 POLY 40. Polymer blending vs. precision synthesis in self-assembly. **R.K. O'Reilly**

10:50 POLY 41. Structure-property relationships in metallopolymers containing excess metal-ligand complex. **F.L. Beyer**, A. Jackson, S.D. Walck, K. Strawhecker, B. Butler, R. Lambeth

SUNDAY AFTERNOON**Section A**

Westin Boston Waterfront
Grand Blrm C

Protein-Like Structure & Activity in Synthetic Systems

E. B. Berda, J. Foster, *Organizers*

Y. C. Simon, *Organizer, Presiding*

C. Lyon, *Presiding*

1:00 Introductory Remarks.

1:05 POLY 42. Folding single-chain peptid polymers into protein-mimetic structures. **R.N. Zuckermann**, L. Guo, K. Dill

1:35 POLY 43. Single-chain folding and multichain aggregating polymers via living radical polymerization: Synthetic macromolecules with protein-like structure, spaces, and functions. **T. Terashima**, M. Sawamoto

2:05 POLY 44. Foldable supramolecular block copolymers. **M. Weck**, A. Croom, E. Elacqua, K. Manning

2:35 Intermission.

2:50 POLY 45. Single-chain nanoparticles via sonogashira cross-linking of linear polymer chains. **A. Prasher**, E.B. Berda

3:10 POLY 46. Dynamic single chain polymeric nanoparticles: From structure to function. **M. Artar**, A. Palmans, E.W. Meijer

3:30 POLY 47. Supramolecular materials from self-assembly of bioinspired macromolecular building blocks. **W.S. Horne**

4:00 POLY 48. Self-regulating dynamic materials via precision programming of the time domain of self-assemblies. **A. Walther**, T. Heuser, L. Heinen

4:30 POLY 49. Hierarchical structure and properties of polymer hybrid materials. **R. Kasi**

5:00 Concluding Remarks.

Section B

Westin Boston Waterfront
Grand Blrm D

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

C. Hager, S. Percec, *Presiding*

1:00 POLY 50. Characterization of diblock copolymer order-order transitions in aqueous solution using fluorescence correlation spectroscopy. **J. Lovett**, C.G. Clarkson, J. Madsen, S.P. Armes, M. Geoghegan

1:20 POLY 51. In situ SAXS studies of polymerization-induced self-assembly during non-aqueous RAFT dispersion polymerization. **M. Derry**, L.A. Fielding, O.O. Mykhaylyk, S.P. Armes

1:40 POLY 52. Potential of ion mobility spectrometry-mass spectrometry (IMS-MS) for elucidating polymer architecture. **S.M. Grayson**, B. Zhang, C.D. Foley, J.N. Hoskins, S. Trimpin

2:00 POLY 53. Hierarchical structure details of a series of crystalline-crystalline miktoarm star polymers in thin films. **M. Ree**, Y. Kim, H. Lee, T. Isono, T. Kakuchi, T. Satoh

2:20 POLY 54. Mechanically coupled internal coordinates: Adding color to infrared spectroscopy. **J.H. Doan**, T. Mion, I.M. Kendrick, A. Vong, N. Dimakis, E.S. Smotkin

2:40 POLY 55. Fluorescent conjugated polymer nanoparticles for the sensitive detection of aromatic analytes. **M. Levine**, W. Talbert, P. Marks

3:00 POLY 56. Sensing capabilities and optical properties of thiol and sulfur based polymers. **D.A. Boyd**, F. Bezares, J. Naciri, D.B. Pacardo, F.S. Ligler

3:20 POLY 57. Thermal properties of high melting point copolyesters. **H.E. Edling**, S.R. Turner

3:40 POLY 58. Origin and detection of impurities in ring-opened poly(carbonate) block copolymers for self-assembly. **R. Wojtecki**, A. Vora, J. Cheng, A. Chunder, D.P. Sanders, A. Nelson

4:00 POLY 59. Poly(ethylene glycol)-poly(lactic acid) co-block polymer with acidic difluoroboron β -diketone dyes. **C.A. DeRosa**, Z. Fan, C. Kerr, A.S. Mathew, C. Fraser

4:20 POLY 60. Tuning the properties of poly(2-oxazoline)s by side chain modification via isocyanide-based multicomponent reaction. **B. Verbracken**, A. Sehlinger, M. Meier, R. Hoogenboom

4:40 POLY 61. Withdrawn.

Section C

Westin Boston Waterfront
Grand Blrm E

Surface Modification of Polymeric Materials

K. J. Wynne, *Organizer*

C. Wohl, *Organizer, Presiding*

1:00 POLY 62. Sulfolane as a surface functional group. **S. Fujii**, T.J. McCarthy

1:20 POLY 63. Urethane coatings containing surface modifying co-oligomers. **J. Doss**, C. Wohl, M.H. Shanahan, J.W. Connell

1:40 POLY 64. Direct functionalization of Kevlar® with copolymers containing sulfonyl nitrenes. **J. Yatvin**, S.A. Sherman, S. Filocamo, J.J. Locklin

2:00 POLY 65. Diffusion of di(2-ethylhexyl)phthalate in poly(vinyl chloride) (PVC). **K.J. Wynne**, M. Suleman, M. Suleman, **D. Johnson**, P. Ramsinghani, R. Wickham, W. Zhang, C. Wang, D. Pestov

2:20 POLY 66. Copolyimides containing surface modifying agents: Competition between silicone and fluorine-containing oligomers. **C. Wohl**, A.M. Crow, W.T. Kim, M.H. Shanahan, J.R. Doss, Y. Lin, J.W. Connell

2:40 Intermission.

2:55 POLY 67. Fabrication and functionalization of thiol-reactive polymer brushes. **T. Gevrek**, T. Bilgic, H.A. Klok, A. Sanyal

- 3:15 POLY 68.** Novel surface modification using poly(methyl methacrylate) brush with well-controlled stereoregularity. T. Hirai, M. Sato, N. Ohta, Y. Higaki, K. Kojo, A. Takahara
- 3:35 POLY 69.** Postpolymerization modification of polymer surfaces using thiol-mediated reactions. W. Guo, E.A. Hoff, D. Amato, D. Amato, D.L. Patton
- 3:55 POLY 70.** Fouling release performance of silicone oil modified siloxane-polyurethane coatings. T.P. Galhenage, D.C. Webster, S. Stafslien, J. Daniels, J. Finlay
- 4:15 POLY 71.** Improving interfilament interfaces in large area 3D printing of polymers. E. Duranty, D. Erdman, V. Kunc, C. Duty, M.D. Dadmun
- 4:35 POLY 72.** Surface Properties of Cross-linked Lipophilic Polymer Brushes on Diamond-Like Carbon Films. A. Takahara, M. Kobayashi

Section D

Westin Boston Waterfront

Commonwealth B

Silicones

S. J. Clarson, J. M. Mabry, *Organizers, Presiding*

1:00 POLY 73. Silicon-based hyperbranched polymers. P.R. Dvornic

1:30 POLY 74. Silicone polymers in Australia. S.R. Clarke, E. Markovic, K. Nguyen, T. Aitchison, N.A. Trout, C.A. Williams

2:00 POLY 75. Water soluble polysiloxanes and their use in Interpenetrating Polymer Networks (IPN). D. Graiver, K.W. Farmer, S. Dewasthale, R. Narayan

2:30 Intermission.

2:45 POLY 76. Manufacture and characterization of multifunctional silicone architectures. J.P. Lewicki, R.S. Maxwell, M. Worsley, E. Duoss

3:10 POLY 77. Controlled synthesis of MQ silicone resins. D. Flagg, T.J. McCarthy

3:35 POLY 78. Self-healing interpenetrating networks from ionic silicones and commercial silicone elastomers. L. Yu, F.B. Madsen, S. Hvilsted, A. Skov

4:00 POLY 79. Silsesquioxane-based thermosetting oligoimides: Chemistry and delivered properties. T.S. Haddad, G.R. Yandek, J. Lamb, M.D. Ford, J.M. Mabry

Section E

Westin Boston Waterfront

Commonwealth C

Herman Mark Scholars Award Symposium in Honor of Stuart Rowan

J. Pyun, *Organizer*

L. Korley, *Presiding*

1:00 POLY 80. Making molecules into materials. R.B. Grubbs

1:30 POLY 81. Dynamic covalent polymers from elemental sulfur. J. Pyun

2:00 POLY 82. Noncovalent interactions as a design tool for stimuli-responsive polymers. C. Weder

2:30 POLY 83. Stimuli responsive block polymer micelles in ionic liquids. T.P. Lodge

3:00 Intermission.

3:15 POLY 84. New approach to well-defined polymer building blocks. C.J. Hawker

3:45 POLY 85. New approach for the construction of 2D monolayers. J.F. Stoddart, X. Hou, C. Ke

4:15 POLY 86. Structurally dynamic polymers as a route to stimuli-responsive materials. S.J. Rowan

Innovation from Discovery To Application Plenary Session

Sponsored by MPPG, Cosponsored by BIOT, MEDI, PMSE and POLY

Professional Legacy of Henry Hill

Sponsored by PROF, Cosponsored by CEPA, CMA, ETHC, HIST†, ORGN, PMSE, POLY†, PRES and SCHB†

MONDAY MORNING

Section A

Westin Boston Waterfront

Grand Blrm C

Protein-Like Structure & Activity in Synthetic Systems

Y. C. Simon, *Organizer*

E. B. Berda, J. Foster, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 POLY 87. Structure in nanoparticle containing responsive layer-by-layer films. N. Zacharia

8:35 POLY 88. The art of polymeric networks: Printing, templating, and solution crosslinking for precise sizing in nano-and microscale for adaptation and release. E. Harth, B.R. Spears, M. Marin, D. Stevens

9:05 POLY 89. Response and function in peptide-based block copolymers. G. Strange, I. Smith, C. Machado, D.A. Savin

9:35 Intermission.

9:50 POLY 90. Toward polymer-based artificial metalloenzymes: Modeling second-sphere interactions in synthetic systems. S. Pazicni, E.B. Berda

10:20 POLY 91. Endowing soft nano-objects with enzyme-mimetic activity via single-chain technology. J. Pomposo

10:50 POLY 92. Plastic antibodies, adaptable synthetic polymers as protein and peptide affinity ligands: An alternative to the lock and key paradigm. K.J. Shea

11:20 POLY 93. Virus-mimicking polymer molecular brushes are potent antibiotics with double selectivity. H. Liang, Y. Jiang, W. Zheng, H. Ma

11:40 Concluding Remarks.

Section B

Westin Boston Waterfront

Grand Blrm D

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

K. T. Wacker, K. L. Wooley, *Presiding*

8:00 POLY 94. Tuning the thermo-mechanical properties of shape memory polymer foams for endovascular embolic applications. S.M. Hasan

8:20 POLY 95. Facile synthesis and application of block copolymers based on P3HT for organic solar cells. H. Erothu, J. Kolomanska, R. Hiorns, P. Topham

8:40 POLY 96. Novel polyurethane dispersions containing nanoparticles: Synthesis, characterization, and applications. B. Sevinis, N.A. Dogan, Y.Z. Menceoğlu, S. Unal

9:00 POLY 97. Synthesis and characterization of thermoreversible hydrogels based on ABC triblock copolypeptides and their potential application toward protein and stem cell. S. Xuan, C. Lee, C. Chen, D. Hayes, D. Zhang

9:20 POLY 98. Decahydronaphthalene containing polyesters as potential BPA replacements. J.M. Dennis, N.A. Fazekas, J.S. Enokida, T.E. Long

9:40 POLY 99. Synthesis and characterization of a biobased polycarbonate derived from the neolignan honokiol. K.T. Wacker, S.L. Kristufek, K.L. Wooley

10:00 POLY 100. Non-catalytic hydrogenation of liquid natural rubber using diimide. S. M. Yusoff, N. Jamaluddin, I. Abdullah

10:20 POLY 101. Hierarchical relaxation processes in polymeric hydrogels based on histidine-metal coordination bonds. S. Tang, B.D. Olsen

10:40 POLY 102. The development of optically healable supramolecular metallopolymer. T. Spilker, J.R. Romulus, C. Plunkett, A. Savage, F.L. Beyer, S.J. Rowan

11:00 POLY 103. Novel and versatile synthetic strategy for asymmetric perylene diimide derivatives. C. Sample, N.V. Handa, C.J. Hawker

11:20 POLY 104. Synthesis, characterization, and structure-property analysis of aminated polyphenylsulfone-tetramethyl polysulfone (PPSU-TMPS) block copolymer. D. Wang, C.J. Cornelius

11:40 POLY 105. Synthesis and characterization of novel phosphonium ionenes as a new family of polyelectrolytes. R.J. Mondschein, A. Abdulahad, Q. Chen, R.H. Colby, T.E. Long

Section C

Westin Boston Waterfront

Grand Blrm E

Surface Modification of Polymeric Materials

K. J. Wynne, *Organizer*

C. Wohl, *Organizer, Presiding*

8:00 POLY 106. Surface-attached polymer layers via C,H insertion reactions. O. Prucker, J. Ruehe

8:20 POLY 107. Bioactive and anti-fouling poly(oxanorbornene) nanofiber meshes. J.S. Hersey, M.W. Grinstaff

8:40 POLY 108. Self-organization of α -cyclodextrin/poly(ϵ -caprolactone) pseudo-polyrotaxanes for nanofibrous scaffolds with enhanced surface reactivity. M. Oster, A. Hébraud, A. Lapp, E. Pollet, L. Avérous, G. Schlatter

9:00 POLY 109. Non-protein fouling polyisobutylene-based biomaterials via modular surface functionalization. A. Alvarez Albarran, E.Q. Rosenthal-Kim, L. Liu, Z. Nikolov, J.E. Puskas

9:20 POLY 110. Biofilm-disrupting antimicrobial coatings derived from natural resin acids. M.S. Ganewatta, C. Tang

9:40 POLY 111. Developing *N*-heterocyclic carbene functionalized polymers as stabilizing ligands for nanoparticles: Exploring new reactivity in aqueous media. M. Macleod, J.A. Johnson

10:00 Intermission.

10:20 POLY 112. Liposome decorated polyelectrolyte multilayer films for local and sustained therapeutic delivery. S.L. Hayward, S. Kidambi

10:40 POLY 113. Dual cyclodextrin polyelectrolytes multilayer coatings on textile for controlled drug delivery. J. Junthip, N. Tabary, B. Martel

11:00 POLY 114. Temperature controlled fluorescence resonance energy transfer on poly(propargyl acrylate) nanoparticles modified with oxadiazole and naphthalimide derivatives. O. Klep, S.H. Foulger

11:20 POLY 115. Covalent modification of synthetic hydrogels with bioactive proteins via sortase-mediated ligation. K. Renggli, E. Cambria, C. Chopko Ahrens, C.D. Cook, B. Imperiali, L. Griffith

11:40 POLY 116. Clickable nanofibers designed for reagent-free functionalization. O.I. Kalaoglu Altan, R. Sanyal, A. Sanyal

Section D

Westin Boston Waterfront

Commonwealth B

Silicones

S. J. Clarson, *Organizer*

J. M. Mabry, *Organizer, Presiding*

M. A. Brook, *Presiding*

8:00 POLY 117. Antifouling silicones prepared with PEO-silane amphiphiles: Impact of structure and concentration. M. Grunlan

8:30 POLY 118. Introducing mixed polarity into silsesquioxane and siloxane structures: Hydrophilic or oleophilic behavior? B. Arkles, Y. Pan, F. Gonzaga

9:00 POLY 119. Designing durable ice-phobic surfaces. K. Golovin, A. Tuteja

9:30 Intermission.

9:45 POLY 120. Fluorinated silsesquioxanes: Structure, solubility, and wetting. J.M. Mabry, A. Guenther, S.T. Iacono, R. Campos, S.M. Ramirez, T.S. Haddad, R. Stone, Y.J. Diaz

10:10 POLY 121. Surface tension of poly-methyltrifluoropropylsiloxane. M.J. Owen

10:35 POLY 122. One-way street for water droplet movement on a poly(dimethylsiloxane) nanocomposite (Sylgard 184). C. Wang, K.J. Wynne, S. Nair, V. Sharon, T. Shrestha

11:00 POLY 123. Wetting properties of polysiloxane networks modified in situ with fluoroalkyl-substituted linear and POSS cage structures. R. Campos, S.M. Ramirez, J.M. Mabry

Section E

Westin Boston Waterfront

Commonwealth C

Ring Opening Polymerization

D. Boday, M. Jeffries-El, *Organizers, Presiding*

8:00 POLY 124. Ring-opening polymerization of a 5-membered ring glucose carbonate, toward biocompatible degradable polymeric materials. S. Felder, A. Noel, K.L. Wooley

8:25 POLY 125. Bulk ring-opening polymerizations of hexahydrotriazines using dithiols: Structurally dynamic poly(thioaminals) for therapeutic delivery. R. Wojtecki, G.O. Jones, A.Y. Yuen, D. Boday, A. Nelson, J.M. Garcia, J. Hedrick, Y. Yang

8:50 POLY 126. Rapid synthesis of a lipocationic polyester library via ring-opening polymerization of amine and alkyl functionalized valerolactones as potent formulated siRNA delivery nanoparticles. D.J. Siegwart, J. Hao, P. Kos, K. Zhou, J.B. Miller

9:15 POLY 127. Organocatalytic ring-opening polymerization of cyclic carbonates: A versatile platform for biomedicine including drug delivery vehicles and macromolecular therapeutics. **Y. Yang, J. Hedrick**

9:40 POLY 128. General approach to sequence-controlled polymers using macrocyclic ROMP. **W.R. Gutekunst, C.J. Hawker**

10:05 POLY 129. Synthesis of polypeptides through atom efficient ring-opening polymerization of *N*-carboxyanhydrides. **S.K. Raman, E. Brulé, M. J.-L. Tschan, C. M. Thomas**

10:30 POLY 130. Water soluble, biodegradable amphiphilic polymeric nanoparticles by ROP and the molecular environment for hydrophobic encapsulants: Consistency between simulation and experiment. **R.D. Miller, R. Yusoff, W.C. Swope, J.E. Rice, A. Parker, A. Carr, J. Sly, E. Appel, T. Nguyen, V. Piuonova**

10:55 POLY 131. Synthesis of biodegradable polyesters by ring opening polymerization of functional lactide monomers to facilitate facile attachment of biomolecules. **P. Kallelkar, D.M. Collard**

11:20 POLY 132. Synthesis and characterization of phosphonium-containing polyelectrolytes and investigation of their antibacterial activity. **T. Eren, C. Suer, C. Demir, T. Kocagoz, N. Aytelkin Unubol**

11:45 POLY 133. Carbene catalyzed ring opening polymerization of trimethylene carbonate. **A. Reitz, R. Wilhelm, D. Kuckling**

Memories of Henry Hill: His Legacy in Science and in Professional Service

Sponsored by HIST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES†, PROF and SCHB

MONDAY AFTERNOON

Section A

Westin Boston Waterfront
Grand Blrm C

Industrial Innovations in Polymer Chemistry

C. Lipscomb, L. M. Stratton, *Organizers, Presiding*

1:00 POLY 134. Enhancing the properties of recycled polypropylene: Upgrading rPP for more demanding applications. **J.D. Sprinkle, J.J. Peterson, S.R. Trenor**

1:30 POLY 135. Industrial innovation in case of flame retardant thermoplastic polyurethane. **G. Scholz, O. Henze, O. Muehren**

2:00 POLY 136. Alternative light diffusion materials for LED lighting. **J. Ge, F. Mehlmann, M.T. Burchill, G.E. Moeller**

2:30 POLY 137. Inter-polymer complex hydrogels formed by thermal and/or pH triggered gelation. **P. Sullivan, J. Godoy, B. Busby**

3:00 POLY 138. Innovation in medical adhesives. **K. Tse**

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

3:30 POLY 139. Polymeric excipients for Accurins™: Design and development of polymers that enable targeted nanoparticle based cancer therapy. **M.M. Ali**

4:00 POLY 305. Industrial chemist's challenge: Making sense of financial jargon. **C. Smith**

Section B

Westin Boston Waterfront
Grand Blrm D

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

M. Buchmeiser, C. E. Hobbs, *Presiding*

1:00 POLY 140. Effect of low initiator concentration on RAFT emulsion polymerization of styrene. **K. Yan, Y. Luo, X. Gao**

1:20 POLY 141. Size and shape changes of polymer aggregates and monomer droplets during air-immune polymerization under an optical microscope. **J.K. Szymanski, J. Perez-Mercader**

1:40 POLY 142. Synthesis and characterization of amino acid-based poly(ester ureas) with different diol chain length and different branch density. **J. Yu, M. Becker**

2:00 POLY 143. Green(er) routes toward the synthesis, functionalization, and use of polymers. **C.E. Hobbs**

2:20 POLY 144. Synthesis of a series of naphthalene-bisimide based polymers by direct arylation. **K. Nakabayashi**

2:40 POLY 145. Stereo- and regioselective ring opening metathesis polymerization and cyclopolymerization of cyclic olefins and diynes containing protic functional groups by functional group-tolerant Mo- and W-based metathesis catalysts. **M. Buchmeiser, R. Schowner, S. Sen**

3:00 POLY 146. Hyperbranched-polydendrons: A new branched linear-dendritic hybrid polymer architecture. **F. Hatton, H. Rogers, A. Dwyer, P. Chambon, S. Rannard**

3:20 POLY 147. Functional polymer particles prepared by "click" thiol-ene and thiol-yne suspension polymerizations. **O.Z. Durham, D.A. Shipp**

3:40 POLY 148. Water free emulsion polymerization of co-polyacrylamides. **Z. Chen, T.P. Schuman, B. Bai**

4:00 POLY 149. Accelerated synthesis of end-functional polymers and oligomers via microwave heated catalytic chain transfer polymerization using cobalt and iron catalysts. **A. Stimpson, K. Adlington, A.R. Whittington, A. Goldstein, D.J. Irvine**

4:20 POLY 150. Living anionic polymerization of diphenylphosphino styrene for high temperature thermoplastic elastomers. **A. Schultz, M. Chen, C. Jangu, T.E. Long**

4:40 POLY 151. Solution polymerization method for polybenzimidazoles. **K. Fishel, A. Gulledege, J. Hoffman, W. Steckle, B. Benicewicz**

Section C

Westin Boston Waterfront
Grand Blrm E

Protein-Like Structure & Activity in Synthetic Systems

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*
A. M. Hanlon, B. Tuten, *Presiding*

1:00 Introductory Remarks.

1:05 POLY 175. Tuning multimeric display of peptide antigens on nanoparticles in vaccine design. **T. Moyer, C. Ke, D.J. Irvine**

1:25 POLY 176. Synthetic polymers which reproduce antifreeze (glyco) protein function; control of ice growth, and cryopreservation of donor cells. **T. Congdon, R. Deller, D. Mitchell, M. Vatsish, D. Mitchell, M. Gibson**

1:45 POLY 177. From synthetic mimics of antimicrobial peptides to new delivery reagents inspired by cell penetrating peptides. **G.N. Tew**

2:15 POLY 178. Effects of hydrophobic content and density on transduction efficiency of polymer protein mimics. **C.M. Backlund, G.N. Tew, F. Sgolastra, R. Otter**

2:35 Intermission.

2:50 POLY 179. OGP-functionalized phenylalanine-based poly(ester ureas) for enhancing osteoinductive potential of human mesenchymal stem cells. **G.M. Policastro, F. Lin, M. Becker**

3:10 POLY 180. Hydrophilic and cationic polymers as potent antimicrobial materials: Another pathway to fight tough bacterial infections. **Y. Jiang, H. Liang**

3:30 POLY 181. Sugar-based amphiphilic nanoassemblies reduce smooth muscle cell proliferation in restenosis. **J.W. Chan, L.K. Petersen, D.R. Lewis, P. Moghe, K.E. Uhrich**

3:50 POLY 182. Green routes to peptides that enable their use in a broader range of applications. **R.A. Gross**

4:10 Concluding Remarks.

Section D

Westin Boston Waterfront
Commonwealth B

Silicones

S. J. Clarson, *Organizer*

J. M. Mabry, *Organizer, Presiding*

1:00 POLY 159. Rapid prototyping of silicones using the Piers Rubinsztajn reaction. **M.A. Brook, Y. Chen, A. Schneider, L. Zepeda, X. Li, V. Rajendra, E. Lovinger**

1:30 POLY 160. Effect of silicon substitution on the crystal properties of cyanate ester monomers. **A.J. Guenther, S.M. Ramirez, D. Soto, M.D. Ford, J.A. Boatz, J.M. Mabry**

2:00 POLY 161. Selective-assemblies of Si-based giant tetrahedra and surfactants via precisely controlled positional interactions. **S.Z. Cheng, M. Huang, K. Yue, C. Hsu, W. Zhang**

2:30 Intermission.

2:45 POLY 162. Mesoscale simulations on silicon containing polymer composites. **L. Subramanian, A. Bick**

3:10 POLY 163. Development of new siloxane modified particles as stabilized active ingredients for sunscreens. **D.A. Loy, S. Tolbert**

3:35 POLY 164. Synthesis of well-defined dual functional siloxanes. **S. Sulaiman, J.D. Goff, B. Arkles**

4:00 POLY 165. Partially fluorinated organically modified silicas possessing latent reactivity for post-functionalization. **A.R. Jennings, C. Thrasher, S. Budy, S.T. Iacono**

Section E

Westin Boston Waterfront
Commonwealth C

Biomacromolecules/Macromolecules Young Investigator Award

P. Majumder, *Organizer*

T. P. Lodge, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 POLY 166. Tough materials using thiol-yne click chemistry. **A.P. Dove**

1:30 POLY 167. 3D patterning for guided cell growth. **M.S. Shoichet, R.Y. Tam, S. Fisher, A.E. Baker, R. Wylie, Y. Aizawa, C.M. Morshead, K. Maxwell**

1:55 POLY 168. Programming polymers and polymeric nanomaterials with biomolecules. **N.C. Gianneschi**

2:20 POLY 169. Translationally relevant strategies for functional biomaterials. **M. Becker**

2:50 Intermission.

3:05 POLY 170. Strategies toward functional polymer materials and nanoscopic devices derived from natural products. **K.L. Wooley**

3:30 POLY 171. Tunable pH- and CO₂-responsive sulfonamide-containing polymers by RAFT polymerization. **C.L. McCormick, B. Abel, M.B. Sims**

3:55 POLY 172. ATRP in water — challenges and opportunities. **K. Matyjaszewski**

4:20 POLY 173. Probing mechanisms and creating materials through dynamic-covalent chemistry. **B.S. Sumerlin, H. Sun, C. Deng, J. Cash, W. Brooks, T. Kubo, C. Kabb**

4:50 Concluding Remarks.

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector

Sponsored by SCHB, Cosponsored by CMA, COLL, HIST, I&EC, POLY, PRES and PROF

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

D. Boday, *Organizer*

8:00 - 10:00

POLY 174. Wrap n' Sense: Di- and trifluoromethylated single-walled carbon nanotubes wrapped with derivatized PEDOT polymers for nerve agent detection. **J.F. Fennell, T.M. Swager**
246, 255, 274, 279, 282, 284, 287, 309-311, 318-319, 324-326, 335, 350, 360, 364. See Subsequent Listings.

From Raw to Varoom: The Science Behind Getting a Car on the Road

Sponsored by CHED, Cosponsored by PMSE, POLY, RUBB and SCC†

TUESDAY MORNING

Section A

Westin Boston Waterfront
Grand Blrm C

Herman Mark Award Symposium in Honor of Timothy Lodge

F. S. Bates, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 **POLY 152.** New methods for controlling polymer sequence and stereochemistry. G.W. Coates

8:35 **POLY 153.** Glycopolymers for stabilization of therapeutic proteins. H.D. Maynard, E. Pelegri-O'Day, Y. Liu, J. Ko, J. Lee

9:05 **POLY 154.** Precision functional polymers by precision polymerizations: A bridge from polymer chemistry to polymer physics. M. Sawamoto

9:35 **POLY 155.** Thermoplastic elastomers with semicrystalline, glassy, and rubbery blocks. A. Burns, W. Mulhearn, R.A. Register

10:05 Intermission.

10:20 **POLY 156.** Synthesis, morphology, and ion transport properties of block copolymer electrolytes. M. Park

10:50 **POLY 157.** Remarkable role of molecular architecture in chain exchange in block copolymer micelles. F.S. Bates, J. Lu, T.P. Lodge

11:20 **POLY 158.** New insights into the thermoreversible gelation of methylcellulose. T.P. Lodge

Section B

Westin Boston Waterfront
Grand Blrm D

Value of Basic Research in Solving Industrial Polymer Problems

R. S. Moore, C. P. Radano, *Organizers*

S. A. Eastman, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 **POLY 183.** Innovations and applications of new hybrid adhesives. J. Liu

8:35 **POLY 184.** Existing and advanced rheological measurements of polymers and rubber compounds. M. Namani

9:05 **POLY 185.** Free volume and water vapor transport properties of non-chromated primer films. W. Zhang, M. Jaworowski, G.S. Zafiris

9:35 **POLY 186.** Enhance resource efficiency through innovative polymer design. J. Wang

10:05 **POLY 187.** Beyond poly(hexahydrotriazines)s: From high strength materials to self-healing polymerizable organogels and the development of new polymer-forming reactions. J.M. Garcia

10:35 **POLY 188.** Reactive compatibilization of polylactide-polypropylene blends: From discovery to application opportunities. V. Topolkaev, R. McEneaney, Y. Xu, J. Loi, P. Delgado, C.W. Macosko, M.A. Hillmyer

Section C

Westin Boston Waterfront
Grand Blrm E

Henkel Award for Outstanding Graduate Research in Polymer Chemistry

W. T. Ford, *Organizer, Presiding*

8:00 **POLY 189.** Targeted drug nanocarriers via self-assembling synthetic peptide copolymers. P.T. Hammond

8:30 **POLY 190.** Self-assembly and properties of glycopolymer biohybrid materials. S. Lecommandoux

9:00 **POLY 191.** Engineering energy dissipation in protein gels. L. Dooling, D.A. Tirrell

9:30 Intermission.

9:45 **POLY 192.** Hypersialylation via Glycocalyx Engineering Confers Resistance to Immune Surveillance. C.R. Bertozzi

10:15 **POLY 193.** Functional polypeptides and thermoresponsive responsive hydrogels. T.J. Deming

10:45 Award Presentation.

10:50 **POLY 194.** Synthetic glycopolymer peptides for biomedical applications. J. Kramer, T.J. Deming, C.R. Bertozzi

Section D

Westin Boston Waterfront
Commonwealth B

Silicones

S. J. Clarson, J. M. Mabry, *Organizers, Presiding*

8:00 **POLY 195.** Making alternating siloxane copolymers. J.G. Matison

8:30 **POLY 196.** Functional silicone copolymers and elastomers with high dielectric permittivity. F.B. Madsen, A. Daugaard, S. Hvilsted, A. Skov

9:00 **POLY 197.** High elongation silicone elastomers derived from dual functional siloxane macromonomers. J.D. Goff, S. Sulaiman, B. Arkles

9:30 Intermission.

9:45 **POLY 198.** Self-healing of polydimethylsiloxane-polyurethane (PDMS-PUR) Cu-catalyzed networks. Z. Wang, R. Burtovyi, I. Luzinov, M.W. Urban

10:10 **POLY 199.** Stabilization to UV of polysiloxane resins in geostationary environment. M. Planes, S. Carloti, S. Lewandowski, S. Remaury

10:35 **POLY 200.** Conformal polysiloxane thin-film electrolytes for lithium ion batteries. N. Chen, B. Rejja-Jayan, J. Lau, P. Moni, A. Liu, B. Dunn, K. Gleason

11:00 **POLY 201.** Minimization of hydrophobic recovery of commercial silicone substrates after oxygen plasma treatment. L. Nguyen, M. Hang, W. Wang, Y. Tian, L. Wang, T.J. McCarthy, W. Chen

Section E

Westin Boston Waterfront
Commonwealth C

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Cosponsored by HIST, PMSE†, PRES and PROF†

G. N. Tew, *Organizer*

M. Jeffries-El, L. Korley, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 **POLY 202.** Advanced materials for regenerative engineering. R. James, C. Laurencin

8:35 **POLY 203.** Soft multifaced colloids by constrained volume self-assembly. R.D. Priestley

9:05 **POLY 204.** Printed electronics revolution: Conducting polymers, transistor paints, and printed metals. R.D. McCullough

9:35 **POLY 205.** Energy migration in conjugated polymers: Physics, applications, and opportunities. T.M. Swager

10:05 **POLY 206.** Innovation in polymer science: Imprint lithography and 3D additive fabrication. J. Desimone

10:35 **POLY 207.** Thiol-ene enabled functional film formation strategies for polymeric semiconductors. K.R. Carter, A.R. Davis, K.L. Martin

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

Sponsored by CHED, Cosponsored by ANYL†, BIOL†, BIOT†, BMGT†, CORP†, DAC†, ENFL†, PHYS† and POLY†

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES†, PROF and SCHB

TUESDAY AFTERNOON

Section A

Westin Boston Waterfront
Grand Blrm C

Multi-component & Sequential Reactions in Polymer Science: Efficient Synthesis of Structural Diverse Polymers

M. Meier, P. Theato, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 **POLY 208.** Facile multistep synthesis of liquid crystalline elastomers. T.J. White, T. Ware, M. McConney, J. Wie, V. Tondiglia

1:30 **POLY 209.** Signal amplification in polymeric materials using self-propagating responses and continuous head-to-tail depolymerization. H. Kim, M.S. Baker, S.T. Phillips

1:55 **POLY 210.** Dual networks incorporating both reversible and irreversible polymers. G. Berg, T. Gong, C. Fenoli, A.D. Baranek, C. Bowman

2:20 **POLY 211.** Bioinspired mucin-mimetic brush polymers with selective antiviral properties to influenza A. S. Tang, B. Seifried, X. Dong, W. Puryear, J. Runstadler, B.D. Olsen, R. Katharina

2:45 **POLY 212.** Facile synthesis of novel HTPBs and EHTPBs with high *cis*-1,4 content and extremely low glass transition temperature. Q. Zhou, S. Jie, B. Li

3:10 Intermission.

3:25 **POLY 213.** Redox-switchable block copolymerization of lactide and epoxides catalyzed by bis(imino)pyridine iron(II/III) alkoxide complexes. A.B. Biernesser, K.R. Delle Chiaie, J.B. Curley, J.A. Byers

3:50 **POLY 214.** Poly(propargyl L-glutamate)-based block copolymers for smart drug delivery applications. M. Quadir, S. Morton, L.B. Mensah, K. Shopsowitz, P.T. Hammond

4:15 **POLY 215.** Semicrystalline diblock copolymer nano-objects prepared via RAFT alcoholic dispersion polymerisation of stearyl methacrylate. M. Semsarilar, N.J. Penfold, E. Jones, S.P. Armes

4:40 **POLY 216.** RAFT polymerization of hydroxy-functional methacrylic monomers under heterogeneous conditions: Effect of varying the core-forming block. L.P. Ratcliffe, A. Blanzas, C.N. Williams, S.L. Brown, S.P. Armes

Section B

Westin Boston Waterfront
Grand Blrm D

Value of Basic Research to Industrial Polymer Science – A Senior Chemist's Perspective

S. A. Eastman, R. S. Moore, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 **POLY 217.** Taking advantage of the academia-industry partnership: From molecules to manufacturing. T.E. Long

1:35 **POLY 218.** New look at an old monomer for renewable materials. D. Boday

2:05 **POLY 219.** Biorefinery technology: Basic research catalyzes new product development. K.O. Havelka

2:35 **POLY 220.** Inorganic chemistry and polymers – synthesizing everything but the polymer. A.M. Mazany

3:05 **POLY 221.** Convergence of computational and experimental chemistries driving the new era of accelerated materials discovery. J. Hedrick

3:35 **POLY 222.** The value proposition for industrial research: What it was and what it is? T.W. Smith

Section C

Westin Boston Waterfront
Grand Blrm E

Ionic Liquids in Polymer Design: From Energy to Health

Y. A. Elabd, T. E. Long, J. Yuan, *Organizers, Presiding*

1:00 Introduction.

1:05 **POLY 223.** Innovative poly(ionic liquids) for energy and environment. D. Mecerreyes, M. Isik, A. Fernandes, A. Aboudzadeh

1:45 **POLY 224.** New materials from polymerized ionic liquids. J. Texter

2:10 **POLY 225.** Reactive poly(ionic liquid)s (PILs) and precision synthesis of PIL-based nanostructures. D. Taton, P. Coupillaud, J. Vignolle, M. Weiss-Maurin, D. Mecerreyes, C. Detrembleur

2:35 Intermission.

2:50 **POLY 226.** Polymerized ionic liquids: From ion conductive materials to water pump. H. Ohno

3:15 **POLY 227.** 3D printing phosphonium ionic liquid networks with mask projection microstereolithography. A. Schultz, P. Lambert, N. Chartrain, D. Ruohoniemi, Z. Zhang, C. Jangu, M. Zhang, C. Williams, T.E. Long

3:40 **POLY 228.** Organometallic-mediated radical polymerization for the precision design of novel poly(ionic liquid) copolymers in water. D. Cordella, A. Kermagoret, A. Debuigne, D. Taton, D. Mecerreyes, C. Jérôme, C. Detrembleur

Section D

Westin Boston Waterfront
Commonwealth B

Silicones

S. J. Clarson, J. M. Mabry, *Organizers, Presiding*

1:00 **POLY 229.** Alternate mechanism for nucleophilic attack at Si(OR)₄. R.M. Laine, J.C. Furgal, T.G. Goodson

1:30 **POLY 230.** Modifying properties of catalysts derived from POSS-Sn-POSS. E.V. Beletskiy, M. Kung, H. Kung

2:00 POLY 231. Hybrid porous materials derived from octavinylsilsesquioxane. H. Liu

2:30 Intermission.

2:45 POLY 232. Synthesizing new hybrid architectures of natural rubber and silicon based polymers. T. Aitchison, G. Leveque, P. Pasetto, S. Clarke

3:10 POLY 233. POSS polymers. E. Markovic, S.R. Clarke, J.G. Matison

3:35 POLY 234. High Surface Area Methylsilsesquioxane Polymer Gels Made by Fluoride Catalyzed Rearrangement of Methyltriethoxysilane and Bistriethoxysilylthane and Other Inorganic Hybrid Microporous Materials. R.M. Laine, H.C. Yamane, Y. Chujo

Section E

Westin Boston Waterfront
Commonwealth C

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Cosponsored by HIST, PMSE†, PRES and PROF†

M. Jeffries-Ei, Organizer

L. Korley, G. N. Tew, Organizers, Presiding

1:00 POLY 235. Click synthetic polypeptides for structural biomimetic molecules and networks. P.T. Hammond

1:30 POLY 236. Manipulating solution-assembled and stimuli-responsive copolymer nanostructures for nucleic acid delivery and gene silencing. T.H. Epps, M.O. Sullivan, M. Green, A. Foster

2:00 POLY 237. New fabrication strategy toward functional fiber mats and composites. L. Korley, A.M. Jordan, J.K. Pokorski, E. Baer

2:30 POLY 238. Thermal properties of polymers derived from 2-substituted ionic liquid imidazolium monomers. T.W. Smith

3:00 POLY 239. Teaching polymers to act like proteins. G.N. Tew

Academic Innovations for Tomorrow's Industries: GSSPC Symposium

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Innovation in Materials for Emerging Uses

Sponsored by MPPG, Cosponsored by PHYS, PMSE and POLY

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

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Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

TUESDAY EVENING

Section F

Boston Convention & Exhibition Center
Ballroom West

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, Organizer

6:00 - 8:00

POLY 240. Polymer characterization using multidetector gel permeation chromatography at temperatures ranging from 40 °C to 220 °C. A.K. Brewer, I. Koliq

POLY 241. Use of high speed/high resolution size based chromatographic separation of surfactants and oligomeric materials with single quadrupole mass spectrometry detection. M.J. O'Leary

POLY 242. Molecular weight and particle size determination of polyvinylpyrrolidone (PVP) using macrolMS macroion mobility spectrometer. A. Huang, R. Cavallera, A. Zerrath, P. Hutchins, E. Willis

POLY 243. KnowItAll® ATR/IR ID Expert™ polymer analysis applications. D. Garcia, F. Borden, M. Scandone

POLY 244. Structure-property relationships for polycyanurate networks derived from renewable resources. M.D. Ford, A.J. Guenther, B.G. Harvey, M.C. Davis, H. Meylemans, M. Wright, A. Chafin, J.M. Mabry

POLY 245. Facile synthesis of fluorescent conjugated polyelectrolytes as metal ion chemosensors. W. Wu, A. Chen, R. Dolma, W.E. Bernier, W.E. Jones

POLY 246. Partially crystalline epoxy resins: Investigations on dynamics, morphology, and mechanical behavior. A. Arnebold, S. Wellmann, A. Hartwig

POLY 247. Structure-property-morphology relationships of high-performance segmented liquid crystalline copolyesters. A.M. Nelson, G.B. Fahs, J.M. Dennis, R.B. Moore, T.E. Long

POLY 248. Double hydrophilic, schizophrenic diblock copolymers. A. Parthiban, V. Vasantha

POLY 249. Systematic approach for identifying and confirming extractables from common packaging materials. B. Cabovska, M. O'Leary, P.G. Alden

POLY 250. Supramolecular aggregates of π -acidic coinage metal pyrazolates and π -basic aromatic hydrocarbons. R. Dias, N. Jayaratna

POLY 251. Blending modification of epoxy resin by reactive POSS or its block copolymer. Y. Xu, J. Chen, Q. Li, X. Chen, Y. Cao, L. Dai

POLY 252. Mechanistic study of polysulfone-based model compounds for application in anion exchange membrane fuel cells. S. Tignor, A. Mohanty, C. Bae

POLY 253. Environmentally benign thiol-ene cure systems as replacements for isocyanates in polybutadienes. J.C. Marcischak, A. Guenther, T.S. Haddad, J.M. Mabry

POLY 254. High temperature molding compound from renewably sourced cyanate ester resins. K. Lamison, A. Chafin, M.C. Davis, B.G. Harvey, A. Guenther, G.R. Yandek, J.M. Mabry

POLY 255. Doubly-charged DABCO salt-containing building blocks for synthesis of ion-containing polymers. K.J. Drumme, K. Zhang, G.B. Fahs, M. Aiba, W. Chiang, Y. Rhee, R.B. Moore, T.E. Long

POLY 256. Morphology and thermal properties of poly (alkyl methacrylate)/bentonite nanocomposites prepared via in situ polymerization initiated by Ni (II) α -Benzoinoxime (NBO) complex. K. Ouad, S. Djadoun, N. Sbirrazzuoli

POLY 257. Poly(amino acid)/ and polyamide/SiO₂ composites by (coupled) twin polymerization. K. Nagel, L. Kassner, R. Grütner, M. Korb, H. Lang, S. Spange

POLY 258. Grafting of polyimide onto chemically-functionalized graphene nanosheets for mechanically-strong barrier membranes. H. Yeo, J. Lim, M. Goh, B. Ku, S. Kim, H. Lee, N. You

POLY 259. Highly adaptive poly(urea-amide) that display solvent, light, and heat modulated chiroptical behavior. G.D. Jaycox

POLY 260. Tailoring polyester structure for structure-property-performance relationships: From high impact to solvent resistance. J.M. Dennis, G.B. Fahs, R.B. Moore, S.R. Turner, T.E. Long

POLY 261. Covalent organic frameworks as photovoltaic materials. E. Chant, S. Duhovic

POLY 262. Characterization of phenolated sodium lignosulfonate prepared from lignin depolymerization at mild conditions. H. Fang, P. Cui, Q. Wu

POLY 263. Hypercrosslinked phenolic polymers with well developed mesoporous frameworks. J. Zhang, S.M. Mahurin, S. Dai

POLY 264. Computational study of the Horner-Wadsworth-Emmons reactions for their reactivity and selectivity. S.V. Sambasivarao, K.H. DuBay

POLY 265. Transparent, high-performance biopolyimides derived from functional trioxalates. T. Kaneko

POLY 266. Synthesis and characterization of novel amide tethered polymers. R. Priefer

POLY 267. Synthesis and characterization of high refractive index polyimides derived from 2,5-bis(4-aminophenylene-sulfanyl)-3,4-ethylenedithiophene and aromatic dianhydrides. H. Yeo, J. Lee, M. Goh, B. Ku, N. You

POLY 268. Preparation of mono-disperse emulsion polymer. Y. Ren, X. Sun, Y. Jiang, H. Zhang

POLY 269. Semi-fluorinated thioether polymers via step growth polymerization. B.R. Donovan, D.L. Patton

POLY 270. Poly(2-hydroxyethyl methacrylate): A new star polymer. A. Machado, A.S. Abreu, I. Moura

POLY 271. Synthesis of tris(propargyloxymethyl)phosphine oxide and the corresponding crosslinked polymers by click chemistry. G. Gang, D. Ya-Qing, Q. Jin-Jun, Z. Tu, C. Liu

POLY 272. Main chain and chain end functional polyacetals: pH degradable water soluble polymers with extraordinary lower critical solution temperature behavior. R. Balaj, S. Samanta, J.T. Koberstein

POLY 273. Precision synthesis of telechelic PNIPAAm for design of homogeneous gels via end-crosslinking by thiol-ene reaction. Y. Hirokawa, S. Ida, M. Yamawaki, S. Tanimoto

POLY 274. Synthesis of branched poly-amido-saccharides by ring-opening polymerization of a lactosyl- β -lactam. R. Xiao, W. Blessing, M.W. Grinstaff

POLY 275. High sulfur content polymer nanoparticles obtained from interfacial polymerization in water. J. Lim, U. Jung, W. Joe, E. Kim, J. Pyun, K. Char

POLY 276. Approaches to the design and synthesis of soluble 9,10-anthracene containing conjugated polymers. C. Kulkarni, D.M. Collard

POLY 277. Withdrawn.

POLY 278. Microwave assisted chemical synthesis using polydimethylsiloxane polymer. O. Alomainy

POLY 279. Synthesis and characterization of ionically crosslinked elastomers. G. Deng, K.A. Cavicchi

POLY 280. Peroxalate ester-containing ferulic acid-based poly(anhydride-esters) for hydrogen peroxide scavenging. J. Faig, S. Klein, M.A. Morano, W. Yu, K.E. Uhrich

POLY 281. Synthesis of hyperbranched glyco-polydendrons via methanolic ATRP of *n*-butyl methacrylate. A. Dwyer, P. Chambon, S. Rannard

POLY 282. Synthesis of planar polycyclic aromatics based on 2,5-di(thiophen-2-yl)-1H-pyrrole (SNS). T.N. Truong, T.M. Swager

POLY 283. Synthesis of biodegradable glycopolymers and their uses in antibiotic formulation. X. Chen, M. King, B. Wu, E.A. Kurt-Jones, J. Wang, R. Finberg, M. Yan

POLY 284. Effects of alkyl substitution in oligomers of the pBTTT family. B.P. Cherniawski, E. Burnett, S. Lopez, K.N. Houk, A.L. Brisenio, I. Yavuz

POLY 285. Prop-2-yn-1-yl 2-brom-2-methylpropanoate: Identification and suppression of side reactions of a commonly used terminal alkyne-functional ATRP initiator. W.K. Storms-Miller, C.R. Pugh

POLY 286. Novel functional copolymers of styrene and ring-substituted butyl 2-cyano-3-phenyl-2-propenoates. G.B. Kharas, T. Spann

POLY 287. Reversible polymerization of core-substituted naphthalene diimide-bispyridine. H. Shokouhi Mehr, D.A. Modarelli

POLY 288. Hydrogel forming brine soluble polysulfobetaines. A. Parthiban, V. Vasantha

POLY 289. Swelling behavior of thermoresponsive gels prepared by post-polymerization crosslinking of triblock prepolymers with hydrophilic blocks. S. Ida, H. Kitanaka, T. Ishikawa, S. Tanimoto, Y. Hirokawa

POLY 290. Shape memory biomaterials prepared from polyurethane/ureas containing sulfated glucose. Q. Chai, Y. Huang, X. Yu, N. Ayres

POLY 291. Polypinosylvin: A novel biocompatible and biodegradable poly(anhydride-ester) for extended release of antioxidant and antibacterial pinosylvin. S. Bien-Aime, W. Yu

POLY 292. Biodegradable polymeric crosslinked micelle for DNA and drug delivery. D. Wu

POLY 293. Polyether-based lipids with targeting functions for biomedical applications. A. Danner, S. Mueller, K. Ruzitzka, J. Markl, H. Frey

POLY 294. pH-Responsive hyperbranched-polydendrons for drug delivery applications. H. Rogers, L. Tatham, P. Chambon, A. Owen, S. Rannard

POLY 295. Impact of static spatial heterogeneity on the swelling of sensitive microgels. A. Habicht, W. Schmolke, S. Seiffert

POLY 296. Novel liquid crystalline brush block copolymers for drug delivery. D. Ndayan, L.H. Mahajan, C. Nguyen, P.B. Deshmukh, L. Gonzalez-Fajardo, D. Hargrove, L. Lai, X. Lu, R. Kasi

POLY 297. Hydroxypropyl methylcellulose esters of substituted succinates for hydrophobic drug dissolution enhancement. **L.M. Johnson, L. Yin, M.A. Hillmyer**

POLY 298. Thio-urethane oligomers improve mechanical properties and reduce polymerization stress in dental composites. **C. Pfeifer, A. Bacchi, A. Dobson**

POLY 300. Branched polymerisation systems as stable emulsifiers for nanoemulsion drug delivery. **S. Edwards, F.Y. Hern, S. Auty, S. Rannard**

POLY 299. Catalytic chain transfer controlled continuous flow microwave polymerisation. **K. Adlington, S. Kingman, C. Dodds, D.J. Irvine**

POLY 301. Finding the right nanofiber for making highly graphitic carbon nanofibers. What to know about templating mechanism? **A. Furmanchuk, B. Saha, Y.A. Dzenis, G.C. Schatz**

POLY 302. Linear, mannitol-based poly(anhydride-esters) with high tunability: Biodegradability with sustained anti-inflammatory activity. **N.D. Stebbins, W. Yu, K.E. Uhrich**

POLY 303. Modifying the electronic properties of graphene by plasma treatment: Beyond defect formation. **J.S. Wallace, A. Quinn, J. Hu, E. Kong, H. Joh, J.A. Gardella**

POLY 304. Withdrawn.

Section F

Boston Convention & Exhibition Center Ballroom West

Ionic Liquids in Polymer Design: From Liquids to Health

Y. A. Elabd, T. E. Long, J. Yuan, *Organizers*

6:00 - 8:00

POLY 306. Novel polyvinylimidazolium nanoparticles as high-performance binders for lithium-ion batteries. **J. Yuan, S. Prescher, K. Sakaushi, H. Lin, M. Antonietti**

POLY 307. Ionic liquid-derived thermoresponsive polyelectrolyte gels that show reversible water pumping. **Y. Kohno, Y. Deguchi, H. Ohno**

POLY 308. Controlling actuation of porous poly(ionic liquid) membranes by aligned carbon nanotubes. **H. Lin, J. Dunlop, J. Yuan**

POLY 309. Ionic liquid containing sulfonated block copolymer membranes. **E. Margareta, M. Chen, R.M. Abrahamson, T.E. Long**

POLY 310. Imidazolium-containing (co) polyesters as a platform for biodegradable nonviral gene delivery vehicles. **A.M. Nelson, A. Pekkanen, N.L. Forsythe, J.H. Herlihy, M. Zhang, M.N. Rylander, T.E. Long**

POLY 311. Development of an ammonium-based step-growth poly(RTIL)/RTIL coating system for containment and adsorption. **D.I. Mori, R.M. Martin, D.L. Gin, B.J. Elliott**

Section F

Boston Convention & Exhibition Center Ballroom West

Multi-component & Sequential Reactions in Polymer Science: Efficient Synthesis of Structural Diverse Polymers

M. Meier, P. Theato, *Organizers*

6:00 - 8:00

POLY 312. Regioselective synthesis of semi-fluorinated aryl ethers and poly(arylene ether)s. **A. Parthiban, R. Krishnan**

POLY 313. Use of a thio-bromo click approach toward the functionalization of polynorbornenes. **V. Kothapalli, M. Shetty, C.E. Hobbs**

POLY 314. Convergent synthesis of dendrimers via the Passerini three-component reaction. **J. Jee, J.G. Rudick**

POLY 315. Chondroitin sulfate-*g*-poly(ϵ -caprolactone) for CD44-targeting delivery. **L. Wang**

POLY 316. Efficient synthesis of diverse core photolabile dendrimers via combination of Passerini reaction and thiol-yne reaction. **Y. Wu, Z. Li**

POLY 317. Synthesis of complex amphiphilic polymers by aziotropic distillation techniques. **G.M. Kraft, J. Bento, D. Madugula, D.H. Adamson**

POLY 318. Assembling multiple mesogenic components in a Passerini reaction. **S. Song, J.G. Rudick**

Section F

Boston Convention & Exhibition Center Ballroom West

Protein-Like Structure & Activity in Synthetic Systems

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

6:00 - 8:00

POLY 319. High molecular weight, post-translationally modified protein brushes through tyrosine modification chemistry. **B. Seifried, B.D. Olsen**

POLY 320. High stability graphene-enzyme-hydrogel electrodes for "sugar-to-power" conversion in a microbiofuel cell. **A. Ghimire, A. Pattammattel, R. Kasi, Y. Lei, T. Fan, X. Lu, C.V. Kumar**

POLY 321. Tuning assembly and enzymatic degradation of silk fibroin/poly(N-vinylcaprolactam) multilayers via molecular weight and hydrophobicity. **V.A. Kozlovskaya, A. Espinosa-Dzib, E.P. Kharlampieva**

POLY 322. Elucidating the intrachain radical mechanism in poly(norbornene imide) single-chain nanoparticle formation. **J.P. Cole, J. Lessard, C. Lyon, B. Tuten, E.B. Berda**

POLY 323. Promoting cell-matrix interaction through multivalent presentation of bioactive peptides. **Y. Hao, T. Ozdemir, M. Martinez, S. Pradhan-Bhatt, D. Harrington, R. Witt, M.C. Farach-Carson, X. Jia**

POLY 324. Toward well-defined single-chain nanoparticles via multiple intrachain reactions. **A.M. Hanlon, E.B. Berda**

POLY 325. Supramolecular dendrimers with a folded, protein-like core. **J. Marine, J.G. Rudick**

POLY 326. Modular approach to creating single-chain polymer nanoparticles. **B. Tuten, J.P. Cole, C. Lyon, E.B. Berda**

POLY 327. Application of anthracene toward the synthesis and manipulation of single-chain polymer nanoparticles. **P. Frank, E.B. Berda**

Section F

Boston Convention & Exhibition Center Ballroom West

Ring Opening Polymerization

D. Boday, M. Jeffries-El, *Organizers*

6:00 - 8:00

POLY 328. Design of stable block copolymer micelle-based drug formulations using AB copolymers synthesized by living anionic polymerization: Effect of pendant functional groups on aggregation behavior and drug retention. **F. Le Devedec, A. Wong, L. Houadaheid, C. Yip, C. Bohne, C. Allen**

POLY 329. Novel biodegradable copolymers via chemical vapor deposition. **F. Xie, X. Deng, C. Friedmann, D. Kratzer, L. Solorio, S. Qi, J. Lahann**

POLY 330. Toward the reduction of solvent waste in ring opening metathesis polymerization reactions. **M. Shetty, V. Kothapalli, C.E. Hobbs**

POLY 331. Ring-opening polymerizations of epoxide (GPTS) and lactide with the catalysts of silyliminophenolate based zirconium compounds. **O. Mert, A. Kayan**

POLY 332. Organocatalytic ring-opening polymerization of a cyclic thioester from thiol initiators. **T.J. Bannin**

POLY 333. Ring-opening polymerization of thionolactone. **P. Datta, M. Kiesewetter**

POLY 334. Divergent mechanistic avenues to an aliphatic polyesteracetal or polyester from a single cyclic esteracetal. **A. Neitzel, M. Petersen, E. Kokkoli, M.A. Hillmyer**

POLY 335. Sequenced copolymers with controlled molecular weight prepared via entropy-driven ring-opening metathesis polymerization. **A.L. Short, R.M. Weiss, T.Y. Meyer**

POLY 336. Redox-switchable crosslinking polymerization. **K.R. Delle Chiaie, L. Yablon, A.B. Biernesser, J.A. Byers**

POLY 337. Sulfur-rich nanoparticles from in situ nanoparticulation of sulfur-containing norbornene derivatives and their optical applications. **J. Lim, Y. Cho, K. Char**

POLY 338. Withdrawn.

POLY 339. Metal-free polymerization of poly(trimethylene carbonate). **J.P. Chesterman, B.G. Amsden**

POLY 340. Stereoselectivity in the ring-opening polymerization of β -butyrolactone. **A. Kronast, B. Rieger**

POLY 341. Facile synthesis of cyclic poly(lactic acid) via ring opening polymerization of lactide using tin octoate and furfuryl alcohol. **K. Walton, F. Hild, S.M. Howdle, M. Gimeno-Fabra, D.J. Irvine, H. Liedtke**

POLY 342. Synthesis of cinnamoyl and coumarin functionalized polycarbonates. **J.P. Chesterman, B.G. Amsden**

Section F

Boston Convention & Exhibition Center Ballroom West

Silicones

S. J. Clarson, J. M. Mabry, *Organizers*

6:00 - 8:00

POLY 343. Separation performance of hydrophobic membranes for fuel treatment operations. **A.J. Guenther, J. Reams, K. Greeson, J.R. Alston, K. Lamison, A. Vam, C. Lee, A.K. Kota, G. Kwon, A. Tuteja, J.M. Mabry**

POLY 344. Comparison of the behavior of PEG-POSS stars with unlinked POSS in PEO films and fibers. **Y. Caydamli, J. Shen, X. Fang, R.J. Spontak, A.E. Tonelli**

POLY 345. Copolymerization of fluoroalkyl-substituted polyhedral oligomeric silsesquioxane (fluoroPOSS) macromers via ring-opening metathesis polymerization (ROMP). **S.M. Ramirez, Y.J. Diaz, T.S. Haddad, R. Campos, J.M. Mabry**

POLY 346. Silylation of Dantocol in the elucidation of bonding agent interaction, within polymer bonded explosives. **C.A. Williams, S. Walker, I. Lochert, S. Clarke**

POLY 347. Improved curing of sodium silicate solutions for soil stabilization. **S.R. Clarke, N.A. Trout, A. Keough**

POLY 348. Polydimethylsiloxane-based materials formed by nanoscale ordering of monodisperse supramolecular building blocks. **R.H. Zha, B.F. de Waal, E.W. Meijer**

POLY 349. Study of the polymer-solvent interactions for polysiloxanes with different functional groups using dissipative particle dynamics. **J. Vallejo, A. Gama Goicochea, J.A. Cervantes, E. Pérez, A. Villegas Gasca**

POLY 350. Controlling block copolymer composition and architecture in functionalized siloxane-based antifouling coatings. **B. Wenning, J. Finlay, N. Aldred, A. Clare, C.K. Ober**

POLY 351. Silsesquioxane-based aminated monomers as building blocks in thermosetting oligoimides: Chemistry and delivered properties. **J. Lamb**

Section F

Boston Convention & Exhibition Center Ballroom West

Surface Modification of Polymeric Materials

C. Wohl, K. J. Wynne, *Organizers*

6:00 - 8:00

POLY 352. Effect of cross-linking agent on the grafting modification from silicone rubber. **Y. Jiang, P. Qu, S. Tu, X. Ren**

POLY 353. Xanthate mediated sequential thiol-acrylate Michael addition. **F.Y. Hern, S. Auty, S. Rannard**

POLY 354. Grafting of poly(N-isopropylacrylamide) brushes on the surface of cylindrical mesopores of periodic mesoporous organosilica via atom transfer radical polymerization. **A.S. Manchanda, M. Kruk**

POLY 355. Tailoring of PVA cryogel porosity using ionic liquids. **A.S. Papancea**

POLY 356. Hybrid polymer-peptide hydrogels for cell therapy. **A. C. Kumar, H. Erothu, G. Battaglia, P. Topham**

POLY 357. Functionalization of nanoparticles with pH sensitive copolymers for smart self-assembly. **J. Tinklepaugh, O. Sheppard, M.M. Maye**

POLY 358. Development of antimicrobial fibers using biologically-derived peptide-nucleic acids (PNAs): Attachment, efficacy, and release. **R.J. Mondschein, A. Pekkanen, D. Guenette, N. Mohapatra, T.E. Long**

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POLY 359. Nutraceuticals loaded poly(lactic-co-glycolic acid) nanofibers by solution blow spinning for the treatment of cervical cancer. **K. Punia**, K. Chatterjee, A. Mancuso, V. Rajendra, M.R. Castellanos, J.E. Fata, K.S. Raja

POLY 360. Surface and interfacial modification of polyethersulfone films via POSS modified chain ends. **K.M. Knauer**, L. Moore, S.E. Morgan

POLY 361. Ligand clustered nanoparticles to target ErbB3 in high grade serous ovarian cancer. **L. Gu**, C. Kroll, K. Renggli, L.B. Mensah, B. Imperiali, L. Griffith, P.T. Hammond

POLY 362. Fouling release performance of siloxane-polyurethane marine coatings: Comparison of laboratory biological assays and field immersion studies in the marine environment. **T.P. Galhenage**, D.C. Webster, D. Hoffman, S. Silbert, S. Stafslin, L. Vanderwal, J. Finlay, S. Franco

POLY 363. Surface attached hydrogel films via novel diazo-ester cross-linkers. **P. Kotrade**, O. Prucker, J. Ruehe

POLY 364. Development and modification of crosslinked, electro-spun poly(ethylene oxide) for soft tissue engineering. **L.J. Anderson**, A. Pekkanen, T.E. Long, R.B. Moore

POLY 365. Preparation of silicon-containing porous carbon microspheres for Li-ion secondary battery. **K. Onozuka**, M. Ota, T. Ishibashi, K. Arai, O. Tanaika, K. Imoto, N. Yoshizawa

Joint PMSE/POLY Poster Session

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WEDNESDAY MORNING

Section A

Westin Boston Waterfront
Grand Blrm C

Multi-component & Sequential Reactions in Polymer Science: Efficient Synthesis of Structural Diverse Polymers

M. Meier, P. Theato, *Organizers, Presiding*

8:00 POLY 366. Polyimidazolium salts — novel versatile cationic polymers. **J. Lindner**

8:25 POLY 367. Novel isocyanate-free polyurethanes from biobased resources. **K. Zhang**, S.J. Talley, A.M. Nelson, R.B. Moore, T.E. Long

8:50 POLY 368. Synthesis and characterization of polyacrylates with different pendant groups for thermoplastic elastomers. **W. Lu**, N. Kang, K. Hong, J.W. Mays

9:15 POLY 369. Polymerization of segmented semifluorinated poly(aryl ether)s (Co)polymers via formation of fluorinated arylene/vinylene ether (FAVE). **D. Brown**, S.T. Iacono, K.A. Christensen, D.W. Smith

9:40 Intermission.

9:55 POLY 370. Ugi and Passerini multicomponent reaction in macromolecular chemistry: Novel and efficient approaches toward highly diverse polymers. **A. Sehlinger**, M. Meier

10:20 POLY 371. Multifunctionality in branched monodisperse macromolecules. **J.G. Rudick**

10:45 POLY 372. Withdrawn.

11:10 POLY 373. Synthesis of alkyne macromolecules with structural diversity through multicomponent polymerization. **B. Tang**

11:35 POLY 374. Sequence-defined polymers via multicomponent reactions. **S.C. Solleder**, M. Meier

Section B

Westin Boston Waterfront
Grand Blrm D

Charles Overberger Award Symposium in Honor of Krzysztof Matyjaszewski

R. M. Laine, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 POLY 375. Efficient one-pot synthesis of hyperbranched polymers with well-controlled structures using unprotected AB₂ monomers. **H. Gao**

8:35 POLY 376. Soft surface science and engineering: Serendipitous discoveries (easy) and targeted design and outcomes (tough). **K.J. Wynne**

9:05 POLY 377. Polymers with redox-active functional groups: Synthetic methodologies, properties, and applications. **N.V. Tsarevsky**

9:35 Intermission.

10:05 POLY 378. Catenated and knotty living polymerizations. **R.C. Advincula**

10:35 POLY 379. Sensing the surface: What can polymer brushes tell us about surface interactions? **K. Beers**, C. Deodhar, R.J. Sheridan, S.V. Orski

Section C

Westin Boston Waterfront
Grand Blrm E

Ionic Liquids in Polymer Design: From Energy to Health

Y. A. Elabd, T. E. Long, J. Yuan, *Organizers, Presiding*

8:00 POLY 380. Functional ion gels. **T.P. Lodge**

8:40 POLY 381. Protein dissolution and properties in neat ionic liquids. **S. Strassburg**, H. Bermudez, D.A. Hoagland

9:05 POLY 382. Synthesis of poly(ionic liquids) by RAFT polymerization and poly(ionic liquid)/guar/ionic liquid ionogels thereof. **B. Zhang**, A. Serghel, G. Sudre, A. Charlot, J. Bernard, E. Fleury

9:30 Intermission.

9:45 POLY 383. Reprocessing and recycling of highly cross-linked ion-conducting networks through transalkylation exchanges of C-N bonds. **M. Obadia**, E. Drockenmuller, L. Montarnal

10:10 POLY 384. Ionic liquid microemulsions for directing the assembly and morphology of cellulose nanoparticles. **J.R. Alston**, A. Guenther, J.M. Mabry

10:35 POLY 385. Ionic liquids as nonvolatile media for the study of soft matter dynamics by in situ electron microscopy. **D.A. Hoagland**, P.Y. Kim, T.P. Russell, A. Ribbe

Section D

Westin Boston Waterfront
Commonwealth B

Herman Mark Young Scholars Award Symposium in Honor of Bradley Olsen

P. T. Hammond, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 POLY 386. Associative protein hydrogels. **D.A. Tirrell**, P.B. Rapp

8:35 POLY 387. Sequence specific polypeptides for exploring the role of shape and sequence on polymer self-assembly. **R.A. Segalman**, R.N. Zuckermann, H. Buss, A. Patterson, G. Rizis

9:05 POLY 388. Using chemistry to characterize and control connectivity in 3D polymers. **M. Zhong**, K. Kawamoto, B.D. Olsen, J.A. Johnson

9:35 Intermission.

9:50 POLY 389. Seeing clearly: Using protein nanofibers to promote orderly corneal wound healing. **J.A. Kornfield**

10:20 POLY 390. Polymer-peptide hybrids: Tuning mechanics via nature's building blocks. **L. Korley**, J. Johnson, M. Tsige

Section E

Westin Boston Waterfront
Commonwealth C

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

R. Smith, *Presiding*

8:00 POLY 391. Synthesis and properties of polyamide aerogels from *p*-phenylenediamine and terephthaloyl chloride. **J. Williams**, M. Meador, L. Mccorkle

8:20 POLY 392. Synthesis and characterization of poly(maleic anhydride)s cross-linked polyimide aerogels. **H. Guo**, M. Meador

8:40 POLY 393. Withdrawn.

9:00 POLY 394. Ferulic acid and *p*-coumaric acid-based copolymers as biorenewable polyethylene terephthalate and polystyrene mimics. **H. Nguyen**, S.A. Miller

9:20 POLY 395. Small structural changes in monomer structure yield divergent properties in a class of sustainable polyesters synthesized from glucose and castor oil derivatives. **L.M. Lillie**, W.C. Shearouse, T.M. Reineke, W.B. Tolman

9:40 POLY 396. Vulcanization of silicone conformal coatings for anti-corrosion applications. **J. Wertz**, B.M. Kobilka, J. Kuczynski, J. Zhang, D. Boday

10:00 POLY 397. Sulfur-rich polymer nanoparticles through interfacial polymerization: Synthesis, size control, and sulfur content variation. **J. Lim**, U. Jung, J. Pyun, K. Char

10:20 POLY 398. Preparation and properties of phosphonium polyelectrolytes: Synthesis, film characterization, and supramolecular assembly with conjugated polyelectrolytes. **R. Smith**, C.A. Conrad, X. Yang, W. Wan, M.S. Bedford

10:40 POLY 399. Degradation of thermoset shape memory polyurethanes and foams. **A.C. Weems**, D.J. Maitland

11:00 POLY 400. Studying of supercritical carbon dioxide effect on physicochemical properties of cassava-based cellulose. **P. Nanta**, W. Skolpap, **K. Kasemwong**

11:20 POLY 401. Correlating cyclic defects with mechanical properties in trifunctional and tetrafunctional poly(ethylene glycol) networks. **K. Kawamoto**, M. Zhong, B.D. Olsen, J.A. Johnson

11:40 POLY 402. Dynamic metallo-supramolecular rubber. **Y. Wang**, M. Zhong, A.V. Zhukhovitskiy, J.A. Johnson

WEDNESDAY AFTERNOON

Section A

Westin Boston Waterfront
Grand Blrm C

Multi-component & Sequential Reactions in Polymer Science: Efficient Synthesis of Structural Diverse Polymers

M. Meier, P. Theato, *Organizers, Presiding*

1:00 POLY 403. Cu-catalyzed two-component polymerization. **T. Choi**

1:25 POLY 404. Catalyst-free multicomponent polymerizations of alkynes, elemental sulfur, and amine. **R. Hu**, W. Li, B. Tang

1:50 POLY 405. Passerini multicomponent polymerization for new polymers with a range of diversity in both structure and function. **Z. Li**

2:15 POLY 406. Isocyanide-free multicomponent reactions for postpolymerization modifications. **R. Kakuchi**, P. Theato

2:40 POLY 407. Multicomponent coupling approaches to conjugated poly(1,3-dipoles) and polyheterocycles. **L.V. Kayser**, B. Arndtsen

3:05 Intermission.

3:20 POLY 408. Functionalized ABC triblock copolymers: Multicompartment micelles as a scaffold for advanced nanoreactors. **A. Cohen**, M. Weck

3:45 POLY 409. Chemoselective polymerization: From multicomponent feedstocks to sequence controlled block copolymers. **Y. Zhu**, C. Romain, C.K. Williams

4:10 POLY 410. Oxidized sulfur polyolefin functionalization via ADMET. **T.W. Gaines**, E.B. Trigg, K.I. Winey, **K.B. Wagener**

4:35 POLY 411. Tandem living radical polymerization with transesterification as modular synthetic approaches to gradient, telechelic, and pinpoint-functionalized polymers. **T. Terashima**, Y. Ogura, M. Sawamoto

5:00 POLY 412. Novel preparation of hybrid thiol-acrylate/thiol-epoxy materials synthesized using a single base-catalyzed cure. **E.A. Dhulst**, J.M. Torkelson, W. Heath, N. Wilmot

Section B

Westin Boston Waterfront
Grand Blrm D

Charles Overberger Award Symposium in Honor of Krzysztof Matyjaszewski

R. M. Laine, *Organizer, Presiding*

1:00 POLY 413. Particle brush materials: Building blocks for multifunctional nanocomposites with engineered properties. **M.R. Bockstaller**

1:30 POLY 414. Polymerizations with elemental sulfur. **J. Pyun**

2:00 POLY 415. Mimicking fibrous biological tissues and beyond. **E. Kumacheva**

2:30 Intermission.

3:00 POLY 416. Polymer-protein conjugates for the treatment of disease. **B.S. Tucker**, C.A. Figg, **B.S. Sumerlin**

3:30 POLY 417. Methods for diversifying protein structure. **D.A. Tirrell**

4:00 POLY 418. From new catalytic and initiating systems for ATRP to new materials. **K. Matyjaszewski**

Section C

Westin Boston Waterfront
Grand Blrm E

Ionic Liquids in Polymer Design: From Energy to Health

Y. A. Elabd, T. E. Long, J. Yuan, *Organizers, Presiding*

- 1:00 POLY 419.** Mesoscale-structuring of polymeric ionic liquids. F. Makafui, C. Applah, P. Zare, A. Stojanovic-Marinow, F. Kremer, **W.H. Binder**
- 1:40 POLY 420.** Molecular weight effects on ionic conductivity in diblock copolymer/ionic liquid mixtures. **K.I. Winey**
- 2:05 POLY 421.** Conductivity scaling relationships in nanostructured membranes based on protic polymerized ionic liquids. **R.A. Segalman**, G. Sanoja, C.M. Evans, B. Beckingham, Y. Schneider
- 2:30** Intermission.
- 2:45 POLY 422.** Dynamics of polymerized ionic liquids and their monomers. U. Choi, A. Mittal, T. Price, H.W. Gibson, J.P. Runt, **R.H. Colby**
- 3:10 POLY 423.** Multiresponsive porous polymer actuators: A matter of speed and sensitivity. H. Lin, Q. Zhao, J. Yuan
- 3:35 POLY 424.** Cholinium based ion gels: Preparation, characterization, and application as electrolyte for long-term cutaneous recordings. **M. Isik**, E. Ismailova, T. Lonjaret, R. Marcilla, G. Malliaras, D. Mecerreyes

Section D

Westin Boston Waterfront
Commonwealth B

Herman Mark Young Scholars Award Symposium in Honor of Bradley Olsen

P. T. Hammond, *Organizer, Presiding*

- 1:00** Introductory Remarks.
- 1:05 POLY 425.** Shear localization in associating polymer gels. Z. Wang, A. Omar
- 1:35 POLY 426.** Hypervelocity projectile impact of layered materials: Lamellar block copolymers and multilayer graphene. **E.L. Thomas**, J. Lee
- 2:05 POLY 427.** Self-assembly and ion transport in sequence-defined block copolypeptides. **N.P. Balsara**, J. Sun, R.N. Zuckermann
- 2:35** Intermission.
- 2:50 POLY 428.** Charge and energy transfer in conjugated block copolymers. **E. Gomez**
- 3:20 POLY 429.** Controlling micro-phase separation in globular protein polymer diblock copolymers. **B.D. Olsen**, C. Lam, A. Huang, M. Kim

Section E

Westin Boston Waterfront
Commonwealth C

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
S. Ahn, J. Barnes, *Presiding*

- 1:00 POLY 430.** Microwave-assisted synthesis and characterization of polyurethanes from carbohydrates and diisocyanates. **H.N. Cheng**, A. Biswas
- 1:20 POLY 431.** Preparation and characterization of solid state fluorescent conjugated polymer chemosensors for metal testing. **A. Chen**, W. Wu, W.E. Bernier, W.E. Jones

- 1:40 POLY 432.** Synthesis and self-assembly of amphiphilic hybrid nano building blocks via self-collapse of polymer single chains. W. Li, C. Kuo, I. Kanyo, S. Thanneeru, **J. He**
- 2:00 POLY 433.** Shape programmable materials from photoresponsive liquid crystalline elastomers. **S. Ahn**, T. Ware, K. Lee, V. Tondiglia, T.J. White
- 2:20 POLY 434.** Power of automation in controlled radical polymerization. **L. Voorhaar**, R. Hoogenboom
- 2:40 POLY 435.** Radiopaque, iodine functionalized phenylalanine-based poly(ester urea)s. S. Li, J. Yu, M.B. Wade, G.M. Policastro, M. Becker
- 3:00 POLY 436.** Efficient synthesis of unimolecular polymers with absolute control over mass, monomer sequence, and stereochemistry. **J.C. Barnes**, D. Ehrlich, A. Gao, F.A. Leibfarth, Y. Jiang, E. Zhou, T.F. Jamison, J.A. Johnson
- 3:20 POLY 437.** Synthesis of poly(butylene succinate) and its copolymers for coating applications. **B. Tan**, K. Emery, M.J. Sobkowicz
- 3:40 POLY 438.** Host-guest systems for supramolecular polymers. **H.R. Wessels**, T. Price, F. Mazzini, H.W. Gibson
- 4:00 POLY 439.** Withdrawn.
- 4:20 POLY 440.** Well-defined poly(ε-silicon-caprolactone) for X-ray imaging materials via oxime click reactions. S.E. Nicolau, L.L. Davis, C.C. Duncan, T.R. Olsen, F. Alexis, D.C. Whitehead, **B.A. Van Horn**
- 4:40 POLY 441.** Polyacetals: A new family of water-soluble, pH-degradable polymers with remarkable lower critical solution temperature behavior. **J.T. Koberstein**, S. Samanta

Polymer Concepts in Inorganic Chemistry Courses

Sponsored by CHED, Cosponsored by INOR, PMSE and POLY

WEDNESDAY EVENING

Joint PMSE/POLY Awards Reception and Plenary Lecture

Sponsored by PMSE, Cosponsored by POLY†

THURSDAY MORNING

Section A

Westin Boston Waterfront
Grand Blrm C

Multi-component & Sequential Reactions in Polymer Science: Efficient Synthesis of Structural Diverse Polymers

M. Meier, P. Theato, *Organizers, Presiding*

- 8:00 POLY 442.** Creating complex interfaces using orthogonal click reactions. **J.J. Locklin**
- 8:25 POLY 443.** Functional polymer surfaces via (sequential) post-polymerization modification reactions. **H.A. Klok**
- 8:50 POLY 444.** Use of hemiaminal organogels as processable templates for subsequent polymerization. **M. Fevre**, G.O. Jones, M. Zhang, J.M. Garcia, J. Hedrick
- 9:15 POLY 445.** Widening the bicontinuous compositional window. **G.N. Tew**
- 9:40** Intermission.
- 9:55 POLY 446.** Thiolactone chemistry in macromolecular science. **F.E. Du Prez**, P. Espeel

- 10:20 POLY 447.** Sequential post-polymerization modifications. **P. Theato**, F. Moldenhauer
- 10:45 POLY 448.** Tandem post-polymerization modification: Routes to effective glycopolymer inhibitors of bacterial toxins. **S. Richards**, D.M. Haddleton, M. Gibson
- 11:10 POLY 449.** Polymer scaffolds with pendent blocked isocyanates for sequential postpolymerization modification. E.A. Hoff, B. Abel, C. Tretbar, C.L. McCormick, **D.L. Patton**
- 11:35 POLY 450.** Postmodification of polymers with borane functional groups and their applications. **F. Jaekle**
- 12:00** Concluding Remarks.

Section B

Westin Boston Waterfront
Grand Blrm D

Ring Opening Polymerization

D. Boday, M. Jeffries-El, *Organizers, Presiding*

- 8:00 POLY 451.** Fabrication of semiconductor block copolymers via ring-opening metathesis polymerization. E. Elacqua, M. Weck
- 8:25 POLY 452.** Ring-opening metathesis polymerization as a strategy to prepare organic electronic materials via backbone-driven molecular self-assembly. S. Moench, M. Nguyen, J.D. Biberdorf, **B.J. Holliday**
- 8:50 POLY 453.** Renewable furan-based epoxy systems for self-healing applications. F. Hu, G. Palmese
- 9:15 POLY 454.** Controlling NCA ring opening polymerisation to achieve well-defined hydrogels. C.D. Vacogne, H. Schlaad
- 9:40 POLY 455.** Linear and branched polyesters with a high affinity to polyolefins: Synthesis, characterization, and their application. L. Jasinska-Walc, M. Bouyahyi, R. Duchateau
- 10:05 POLY 456.** Tailoring hyperbranched polyether polyols with adjustable degree of branching and hydrophilicity by random anionic copolymerization of alkylene oxides and glycidol. **J. Seiwert**, M. Schoemer, M. Bauer, H. Frey
- 10:30 POLY 457.** Poly[caprolactone-ran-cinnamoyl modified caprolactone]-b-PCL block copolymer with light-actuated shape memory properties. **H. Xu**, B.M. Budhllal
- 10:55 POLY 458.** Grignard-based anionic ring-opening polymerization of propylene oxide activated by triisobutylaluminum. **K. Roos**, S. Carlotti
- 11:20 POLY 459.** Understanding organocatalytic ring opening polymerization. **O.I. Kazakov**, M.K. Kiesewetter

Section C

Westin Boston Waterfront
Grand Blrm E

Ionic Liquids in Polymer Design: From Energy to Health

Y. A. Elabd, T. E. Long, J. Yuan, *Organizers, Presiding*

- 8:00 POLY 460.** Ionic liquids inspiring the design of phosphonium-containing polymers: From 3D printed objects to block copolymer elastomers. S. Hemp, R.J. Mondschein, C. Jangu, A. Schultz, N. Chartrain, C. Williams, T.E. Long
- 8:40 POLY 461.** Evolution of cyclopropenium cations into functional polyelectrolytes. **J. Freyer**

- 9:05 POLY 462.** 1,2,3-Triazolium-based poly(ionic liquids): A new class of functional ion conducting materials. **E. Drockenmuller**

9:30 Intermission.

- 9:45 POLY 463.** Imidazolium-containing ABA triblock copolymers for electroactive devices. **E. Margareta**, G.B. Fahs, D. Ingfield, C. Jangu, Z. Zhang, D. Wang, J. Hellin, R.B. Moore, T.E. Long
- 10:10 POLY 464.** Polymeric ionic networks: Synthesis and application in catalysis. **P. Zhang**, X. Jiang, S. Dai
- 10:35 POLY 465.** Cation-containing polymers with co-continuous micro-phase-separated morphologies for rapid transport membranes. **F.L. Beyer**, S. Price, A. Savage, X. Ren, N. Pomerantz, W.X. Zukas

Section E

Westin Boston Waterfront
Commonwealth C

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

M. von Czapiewski, J. Zhang, *Presiding*

- 8:00 POLY 466.** Dodecagonal quasicrystalline morphology in a poly(styrene-*b*-isoprene-*b*-styrene-*b*-ethylene oxide) tetrablock terpolymer. **J. Zhang**, F.S. Bates
- 8:20 POLY 467.** Cycloaddition strategies to polyhalogenated carbon-rich architectures: *Ortho*-arylene foldamers, polycyclic aromatics, and graphene nanoribbons. **D. Lehnher**, J.M. Alzola, W. Dichtel
- 8:40 POLY 468.** Fragmentable oligocatic materials assembled through anchimeric-assisted nucleophilic substitution of thiabicyclo[3.3.1]nonane derivatives and their application in transesterification. **Z. Geng**, M.G. Finn
- 9:00 POLY 469.** Accessing block copolymers containing conductive and insulating segments through multitasking catalysts. **K. Souther**, E. Palermo, A.J. McNeil
- 9:20 POLY 470.** Urea-containing ABA triblock copolymers from RAFT polymerization: High glass transition segments for thermoplastic elastomers. **M. Chen**, D. Ingfield, A. Hudson, R.B. Moore, T.E. Long
- 9:40 POLY 471.** Living anionic polymerization of 4-vinylbenzyl piperidine ABC triblock copolymer thermoplastic elastomers. **M. Chen**, A. Schultz, C. Jangu, T.E. Long
- 10:00 POLY 472.** Synthesis of novel ketal functional ε-caprolactone (KCL) monomer and its polymerization to obtain poly(ε-caprolactone) with variable biodegradation rates. **A.L. Garle**, B.M. Budhllal

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.

10:20 POLY 473. Novel polynorbornenes: Synthetic flexibility before and after polymerization. **B.J. Sundell**, J.A. Lawrence, T. Pilyugina

10:40 POLY 474. Comparison of an oligomer mixture to pentafluorophenyl-terminated hyperbranched polyfluorinated poly(benzyl ether) by NMR and MS. **F.J. Wyzgoski**, M.J. Quast, A. Mueller, C. Gao, L. Cool, C. Wesdemiotis, P.L. Rinaldi

11:00 POLY 475. ROMPing in and out: Synthesis and self-assembly of conjugated H-shaped polymers. **J.A. Kalow**, T.M. Swager

11:20 POLY 476. Novel architecture for stimuli-responsive liquid crystalline brush block copolymers and its phase behavior. **L.H. Mahajan**, D. Ndaya, P.B. Deshmukh, Y. Choo, M. Gopinadhan, C.O. Osuji, R. Kasi

11:40 POLY 477. Regioselective acetoxylation of limonene: Access to renewable building blocks via catalysis and the Passerini three-component reaction. **M. von Czapiewski**, M. Meier

THURSDAY AFTERNOON

Section B

Westin Boston Waterfront
Grand Blrm D

Ring Opening Polymerization

D. Boday, M. Jeffries-El, *Organizers, Presiding*

1:00 POLY 478. Trichloroethanol functions as a bifunctional initiator for the synthesis of functionalized block copolymers utilizing orthogonal, sequential ring opening and atom transfer radical polymerization: Simulation and experiment. **R.D. Miller**, H.W. Horn, G.O. Jones, J.E. Rice, V. Pionova

1:25 POLY 479. Synthesis, modeling, and micellization behavior of gradient and block copoly(2-oxazoline)s. **B. Verbraken**, P.H. Van Steenberge, M. Reyniers, D.R. D'hooge, S.K. Filippov, R. Hoogenboom

1:50 POLY 480. Controlled ROMP of cyclobutenes by tuning the steric bulk of the monomer pendant chains: An efficient route towards well-defined cyclobutene-based diblock copolymers. **J. Wei**, S. Granados Focil

2:15 POLY 481. Cationic ring-opening polymerization of an epoxide: Effect of oxetane additives on dark cure and physical properties. **S. Kaalberg**, J.L. Jessop

2:40 POLY 482. Thermoresponsiveness and mechanical properties of highly concentrated aqueous poly(L-proline) solutions. **M. Gkikas**, R.K. Avery, B.D. Olsen

3:05 POLY 483. Cooperative hydrogen-bond pairing in organocatalytic ring-opening polymerization. **M.K. Kiesewetter**, E. Kiesewetter, O. Kazakov, P. Datta

3:30 POLY 484. Enzymatic ring-opening polymerization of ω -pentadecalactone by reactive extrusion. **S. Spinella**, G.L. Re, J. Raquez, P. Dubois, M. Ganesh, **R.A. Gross**

3:55 POLY 485. Mechanistic investigation of lactide polymerization with cyclopropanimine catalysts. **T.S. Stukenbroeker**, J. Bandar, T.H. Lambert, R.M. Waymouth

4:20 POLY 486. Combining ring opening polymerisation and ring opening copolymerisation to synthesise block copolymers. **S. Paul**, C. Romain, C.K. Williams

4:45 POLY 487. Improved rate and selectivity in the synthesis of and ring opening polymerisation with initiators derived from sorbitol by application of microwave selective heating. **F. Hild**, K. Walton, G. Dimitrakis, S. Kingman, E. Lester, H. Liedtke, **D.J. Irvine**

Section C

Westin Boston Waterfront
Grand Blrm E

Ionic Liquids in Polymer Design: From Energy to Health

Y. A. Elabd, T. E. Long, J. Yuan, *Organizers, Presiding*

1:00 POLY 488. Polymerized ionic liquid block copolymers as anion exchange membranes. **Y.A. Elabd**

1:40 POLY 489. Ionic liquid-based polyelectrolyte membranes: Synthesis and applications. **F. Yan**

2:05 POLY 490. Polymer design of sterically-protected anion exchange membrane. **A. Wright**, S. Holdcroft

2:30 Intermission.

2:45 POLY 491. Efficient removal of toxic cationic dyes from wastewater using disulfide-linked porous polymer networks. **M. Atas**, H. Cavusoglu, A. Ozkaya, M. Yavuz

3:10 POLY 492. Imidazolium- and triazolium-containing polyester networks as ion-selective electrode membranes. **R.D. Johnson**, K.M. Miller

3:35 POLY 493. Synthesis of nanoporous asymmetric poly(ionic liquid) membranes. **Q. Zhao**, K. Tauerer, J. Yuan

4:00 Conclusion.

Section E

Westin Boston Waterfront
Commonwealth C

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers, Presiding*

1:00 POLY 494. Probing spin-exciton and spin-charge interactions in open-shell organic semiconductors. **T.L. Andrew**

1:20 POLY 495. Photoredox catalysts, an efficient tool for living polymerization and post-modification. **C. Boyer**

1:40 POLY 496. Initiatorless photopolymerization of liquid crystal monomers. **K. Lee**, W. Taylor, V. Tondiglia, T.J. White, M. McBride, X. Zhang, C. Bowman

2:00 POLY 497. Photoinitiated cationic polymerization of 4-methoxystyrene in the presence of methanol: Kinetic and mechanistic studies. **A. Perkowski**, W. You, D.A. Nicewicz

2:20 POLY 498. Design and synthesis of conjugated metallopolymers consisting of repeating main-chain tetradentate redox-active binding sites. **S. Lin**, T.M. Swager

2:40 POLY 499. Milling toward polymers: Solvent-free, Ru-catalyzed mechanochemical olefin metathesis polymerizations. **L. Do**, T. Frisic

3:00 POLY 500. Isocyanate-free elastomers as replacements for isocyanate-cured polyurethanes. **J. Reams**, A.J. Guenther, J.C. Marcischak, M.D. Ford, T.S. Haddad, J.M. Mabry

3:20 POLY 501. Improvement in photocontrolled radical polymerization with trithiocarbonate: Facilitated by flow techniques and photoredox catalysis. **M. Chen**, J.A. Johnson

3:40 POLY 502. Cooperative capture in polymer synthesis. **C. Ke**, X. Hou, J.F. Stoddart

PMSE

Division of Polymeric Materials Science and Engineering

C. Soles, **C. Stafford** and **A. Tsou**, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Innovation from Discovery to Application
Plenary Session (see MPPG, Sunday)

Accelerated Discovery of Chemical Compounds: Design New Polymers & Inorganic Materials from Integration of Polymer Science, Materials Science, & Informatics (see COMP, Sunday, Monday)

The Fred Kavli Innovations in Chemistry Lecture (see MPPG, Monday)

The Kavli Foundation Emerging Leader in Chemistry Lecture (see MPPG, Monday)

Innovation in Materials for Emerging Uses (see MPPG, Tuesday)

Polymer Concepts in Inorganic Chemistry Courses (see CHED, Wednesday)

SOCIAL EVENTS:

Reception, 5:30 PM: Wednesday

BUSINESS MEETINGS:

Executive Committee, 4:30 PM: Sunday

Business Meeting, 5:00 PM: Tuesday

SUNDAY MORNING

Section A

Westin Boston Waterfront
Harbor Blrm III

Eastman Chemical Student Award in Applied Polymer Science

Financially supported by Eastman Chemical Company

J. W. Gilmer, *Organizer*

J. C. Jenkins, *Presiding*

8:30 PMSE 1. Probing percolation pathways in binary polymer nanoparticle films. **L. Renna**, M. Bag, T. Gehan, X. Han, P.M. Lahti, D. Maroudas, D. Venkataraman

9:00 PMSE 2. Ternary blend polymer solar cells with enhanced power conversion efficiency. **L. Lu**

9:30 PMSE 3. Improving therapeutic delivery for lung diseases: In vitro and in vivo characterization of PEGylated polyphosphoester-based nanocarrier. **F. Zhang**, S. Zhang, J.A. Smolen, S.F. Pollack, M. Elsbahy, R. Li, A.M. Gonzalez, S. Cho, P.N. Shah, J.E. Raymond, T. Gustafson, C.L. Cannon, K.L. Wooley

10:00 PMSE 4. Bicomponent nanofibers produced by GJF process. **S. Rajgarhia**, S.C. Jana

10:30 PMSE 5. Solid-state self-assembly: For advanced electronic and optical materials/devices. **Y. Kim**, N. Kotov

11:00 PMSE 6. Thermosetting resin compositions based on bioderived phenols and sugars. **K.S. Ogueri**

Section B

Westin Boston Waterfront
Lewis

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Tutorial

Cosponsored by INOR†

R. F. Jordan, *Organizer*

G. A. Vaughan, *Organizer, Presiding*

9:00 PMSE 7. Development and mechanisms of Ziegler and single-site olefin polymerization catalysts. **R.F. Jordan**

9:30 PMSE 8. Tutorial: Process and product considerations in producing polyolefins. **G.A. Vaughan**

10:00 PMSE 9. Polyolefin structure-property relationships: Precisely tailored polyolefin structures deliver innovations for sustainable performance. **P. Brant**

10:30 PMSE 10. Tutorial: A history of Ziegler-Natta polypropylene catalysts. **V. Busico**

11:00 PMSE 11. Ring opening metathesis polymerization (ROMP) in the synthesis of precise polymer structures and commercial applications. **R.H. Grubbs**

Section C

Westin Boston Waterfront
Douglas

Patterning Materials for Bio-Interface

Financially supported by Nature Chemistry
J. Hedrick, A. Nelson, *Organizers, Presiding*

8:00 PMSE 12. Direct write of proteins by electron beam lithography using a new water-soluble resist. **H.D. Maynard**, U. Lau, J. Lee, E. Bat

8:30 PMSE 13. Cells touching polymers. **L.M. Campos**

9:00 PMSE 14. 3D printing tailored interfaces with mask projection microsteerolithography. **J. Sirrine**, N. Chartrain, A. Schultz, C. Williams, **T.E. Long**

9:30 PMSE 15. Printing degradable polymers in 3D. **A.P. Dove**, I. Barker, E. Cant, S. Leigh

10:00 Intermission.

10:10 PMSE 16. Stimuli-responsive hydrogels for 3D printable ink. **M. Zhang**, A. Vora, W. Han, H. Maune, R. Wojtecki, A. Nelson

10:30 PMSE 17. 3D-printed biodegradable polyester tissue scaffolds for cell adhesion. **J. Sirrine**, A.M. Nelson, A. Pekkanen, A. Schultz, N. Chartrain, P.M. Lambert, C. Williams, **T.E. Long**

10:50 PMSE 18. Design and comprehensive evaluation of 3D printable initiator-free polyesters with modular functionality and tunable degradation. **S.R. Govindarajan**, J. Jain, I.S. Isayeva, K. Vorvolakos, J. Choi, A. Joy

11:10 PMSE 19. Design and fabrication of a biomimetic superhydrophobic biocompatible surface using 3D printing. **B. Mondal**, Q. Xu, M. Barahman, A.M. Lyons

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:
www.acs.org/boston2015

Section D

Westin Boston Waterfront
Alcott

Advanced Materials for High Performance Formulations

Financially supported by The Dow Chemical Company

M. Johnson, J. S. Katz, B. McCulloch, Organizers

J. Wilbur, Organizer, Presiding

8:30 PMSE 20. Solving humanity's future challenges through fundamental science. **D.S. Bem**

9:00 PMSE 21. New phenomena in the diffusion of complex polymer systems. **B.D. Olsen, M. Wang, S. Tang**

9:30 PMSE 22. Passive cooling with UV-resistant siloxane coatings in direct sunlight. **J.J. Benkoski, C.M. Hoffman, K.S. Caruso**

9:50 PMSE 23. Polyurea coatings for cavitation erosion resistance. **V. Shahi, S. Patil, J. Morris, A. Amirkhizi**

10:10 Intermission.

10:25 PMSE 24. Crystallization-driven assembly of conducting organic nanostructures. **R.C. Hayward**

10:55 PMSE 25. Controlling crystallization and polymorphism to enhance charge mobilities in conjugated polymers. **E. Gomez**

11:25 PMSE 26. Micro vs. macrofluidics. Encapsulation of hydrochloric acid in porous polymer beads. **J. Ferrer, A. Menner, A. Bismarck**

11:45 PMSE 27. High power factor, completely organic, thermoelectric polymer nanocomposite thin film multilayer assemblies. **J.C. Grunlan, C. Yu, C. Cho**

Section E

Westin Boston Waterfront
Faneuil

Phase Separation and Morphology Development in Polymers

Block Copolymers and Polymer Blends

Financially supported by ExxonMobil Chemical Company

M. L. Robertson, S. Tallury, Organizers

C. R. Lopez-Barron, Organizer, Presiding

8:30 PMSE 28. Composition-dependent phase behavior of broad dispersity poly(methyl methacrylate)/poly(styrene) triblock copolymers. **M. Mahanthappa**

9:10 PMSE 29. Morphology of block ionomer regulates the electromechanical performance as applied in ionic polymer-metal composites. **W. Zheng, C.J. Cornelius, D. Wang**

9:30 Intermission.

9:45 PMSE 30. Dynamics of phase separation, morphology development, and surface energy in mixtures of fluorinated silsesquioxanes and acrylate polymers. **A.J. Guenther, J.R. Alston, Y.J. Diaz, M.A. Khan, R. Campos, G.R. Yandek, J.M. Mabry**

10:05 PMSE 31. Influence of poly(acrylic acid) content on phase separation and water uptake in polyisobutylene based miktoarm star polymers. **K.M. Knauer, Y. Zhu, R.F. Storey, S.E. Morgan**

10:25 PMSE 32. Synthesis and characterization of poly(L-lactide)-based semicrystalline-rubbery multiblock copolymers. **T. Panthani, F.S. Bates**

10:45 PMSE 33. Effects of high speed extrusion on catalyzed interchange reaction in biobased polyester/polyamide blends. **J. Gug, M.J. Sobkowicz, A. Farahanchi, M. Palacios, J. Barrington**

SUNDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Blrm III

Journal of Polymer Science Award Symposium

Financially supported by John Wiley and Sons
V. Cleave, Organizer

C. J. Hawker, Organizer, Presiding

1:00 PMSE 34. Engineering surfaces using block copolymer assembly. **B. Wenning, J. Jiang, C.K. Ober**

1:30 PMSE 35. Radical polymers in solid-state organic electronic devices. **B.W. Boudouris**

2:00 PMSE 36. Directed self-assembly of block copolymers for high resolution lithographic applications: From materials design to pattern transfer. **G. Hadziioannou**

2:30 PMSE 37. Close look at the surface orientation of semiconducting polymers with X-rays. **M.L. Chabinyk**

3:00 PMSE 38. Self-assembly and ion transport in single-ion-conducting block copolymers for lithium batteries. **N.P. Balsara, A. Rojas, J. Thelen, S. Inceoglu**

3:30 PMSE 39. Polymer melts inside nanoscale cylindrical pores: Chain conformations, polymer diffusion, and local dynamics. **K.I. Winey**

4:00 PMSE 40. Design, synthesis, and assembly of sequence-defined peptid polymers. **R.N. Zuckermann**

4:30 PMSE 41. Consequences of ideality in ionic copolymerization. **N.A. Lynd**

5:00 PMSE 42. Controlling thermal and electrical transport in polymers. **R.A. Segalman**

Section B

Westin Boston Waterfront
Lewis

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Technical Session

Cosponsored by INOR \ddagger

G. A. Vaughan, Organizer

R. F. Jordan, Organizer, Presiding

L. R. Sita, Presiding

1:00 PMSE 43. Linear low density polyethylenes using well defined tandem catalysts and a single monomer feed. **J.E. Bercaw, J.A. Labinger, A. Sattler**

1:30 PMSE 44. Isoselective polymerization of propylene by group 4 complexes of [ONNO] ligands. **M. Kol, K. Press, V. Venditto, I. Goldberg**

2:00 PMSE 45. Advances in alkene polymerization. **G.W. Coates**

2:30 PMSE 46. Development of group IV molecular catalysts for high temperature Ethylene- α -olefin copolymerization reactions. **J. Klosin, P. Fontaine, R. Figueroa**

3:00 Intermission.

3:10 PMSE 47. Electronically unsymmetrical Pd catalysts for the copolymerization of olefins with polar vinyl monomers. **R.F. Jordan, N. Contrella**

3:40 PMSE 48. Molecular kinetics of catalytic olefin polymerization: Back to the start and then a bit forward. **V. Busico**

4:10 PMSE 49. Precision polymerization with sterically congested hafnocenes: The search for the perfect iPP helix. **B. Rieger**

4:40 PMSE 50. Coordination copolymerization of olefins with polar monomers catalyzed Pd complexes of unsymmetrical bidentate ligands. **K. Nozaki**

Section C

Westin Boston Waterfront
Douglas

Patterning Materials for Bio-Interface

Financially supported by Nature Chemistry

J. Hedrick, A. Nelson, Organizers, Presiding

1:00 PMSE 51. Nano- and microfabricated hydrogels for regenerative engineering. **A. Khademhosseini**

1:30 PMSE 52. Tunable micro and nanostructures for the modulation of fibrosis and wound healing. **T. Desai**

2:00 PMSE 53. Printing living tissues. **J. Lewis**

2:30 PMSE 54. Advanced technologies in bioprinting and biofabrication for on-chip tissue models. **U. Demirci**

3:00 Intermission.

3:10 PMSE 55. Free-form microfabrication of biopolymers into structures capable of guiding cell morphology and alignment. **J. Jaworski**

3:30 PMSE 56. Surface-attached polymer layers for the control of surface-cell interactions. **O. Prucker, M. Eichhorn, K. Anselm, J. Ruehe**

3:50 PMSE 57. Decreased bacterial activity on nanopatterned PDMS replica for catheter-associated infection prevention. **L. Liu, B. Ercan, L. Sun, T. Webster**

4:10 PMSE 58. Interfacial bioorthogonal crosslinking for the fabrication and patterning of functional hydrogels. **K.T. Dicker, H. Zhang, J.M. Fox, X. Jia**

4:30 PMSE 59. Surface patterning of ionically cross-linked alginate hydrogels. **M. Bruchet, A. Melman**

Section D

Westin Boston Waterfront
Alcott

Advanced Materials for High Performance Formulations

Financially supported by The Dow Chemical Company

M. Johnson, J. S. Katz, J. Wilbur, Organizers

B. McCulloch, Organizer, Presiding

1:30 PMSE 60. Advantages of precision in functional copolymers: Mechanical properties and chain dynamics. **K.I. Winey**

2:00 PMSE 61. High performance waterborne coatings with improved eco-footprint through the use of self assembled polymer pigment composites. **J. Bohling**

2:30 PMSE 62. Modified graphitic interfaces for effective load transfer in polymer composites. **A. Fumanchuk, M.R. Roenbeck, Z. An, J.T. Paci, X. Wei, S.T. Nguyen, G.C. Schatz, H.D. Espinosa**

2:50 PMSE 63. Carbon fiber reinforced polymer (CFRP) with an optimized discrete self-healing function: Toward design and application. **P. Jarzynka, D. Wass, I. Bond**

3:10 Intermission.

3:25 PMSE 64. Direct integration of polymers and colloidal nanocrystals for electrochromic materials. **D.J. Milliron, E.L. Runnerstrom, J. Kim, G.K. Ong, B. Helms**

3:55 PMSE 65. Experimental approach to direct characterization of the Z-mer in gradual addition emulsion polymerization. **R. Even, W. Gao, D.A. Kline, T. Zhang**

4:25 PMSE 66. Tailor-made compositional gradient copolymer by many-shot RAFT emulsion polymerization method and its application on multishape memory polymers. **Y. Guo, Y. Luo, X. Gao**

Section E

Westin Boston Waterfront
Faneuil

Phase Separation and Morphology Development in Polymers

Block Copolymers and Polymer Blends

Financially supported by ExxonMobil Chemical Company

C. R. Lopez-Barron, M. L. Robertson, S. Tallury, Organizers

Z. Bai, J. Zhang, Presiding

1:30 PMSE 67. Self-assembly of block copolymers with bottle-brush architecture. **J. Rzaev**

2:10 PMSE 68. Tunability of phase behavior in thermoplastic polyhydroxyurethane: Interplay of soft segment and hydrogen bonding. **G. Beniah, E. Leitsch, K. Liu, K. Scheidt, J.M. Torkelson**

2:30 PMSE 69. Chemical and morphological changes of sulfonated poly(styrene-2-phenoxylethyl methacrylate): Effect of block composition. **M. Perez Perez, D. Suleiman Rosado**

2:50 Intermission.

3:05 PMSE 70. Double-stage phase separation in dynamically asymmetric ternary polymer blends. **C. Kuang, S. Qavi, R. Foudazi**

3:25 PMSE 71. Viscoelasticity and interfacial dynamics in a polymeric bicontinuous microemulsion. **R. Hickey, T. Gillard, T.P. Lodge, F.S. Bates**

3:45 PMSE 72. Shape memory polymer blends. **K.A. Cavicchi, H. Fairbairn, J. Lee, M. Pantoja**

4:05 PMSE 73. Polyhydroxyurethanes: The critical role of hydroxyl groups on morphology when formulating thermoplastic elastomers. **E. Leitsch, G. Beniah, K. Liu, K. Scheidt, J.M. Torkelson**

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Innovation from Discovery To Application Plenary Session

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Professional Legacy of Henry Hill

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MONDAY MORNING

Section A

Westin Boston Waterfront
Burroughs

New Advances in Nanostructured Polymeric Membranes for Filtration

Nanostructured Membranes for Gas Separation

B. T. Chu, B. S. Hsiao, *Organizers*

W. Koros, G. C. Rutledge, *Presiding*

8:30 PMSE 74. Membrane-based hydrocarbon separations using ZIF mixed-matrix membranes. W. Koros, C. Zhang

9:00 PMSE 75. Electrospun polymeric fibers for particle and gas filtration. S. Chattopadhyay, E.S. Sterner, T.M. Swager, G.C. Rutledge

9:30 Intermission.

9:45 PMSE 76. Carbon nanotube immobilized composite hollow fiber membranes for extraction of volatile organics from air. S. Ragunath, S. Mitra

10:15 PMSE 77. Hybrid silica-titanium-polyimide block copolymer composite membranes: Gas transport properties. F. Huang, C.J. Cornelius

10:45 PMSE 78. Size-selective ionically crosslinked polymer multilayer films for light gas separation. J.C. Grunlan, B.A. Wilhite

Section B

Westin Boston Waterfront
Lewis

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Technical Session

Cosponsored by INOR

R. F. Jordan, G. A. Vaughan, *Organizers*

G. W. Coates, J. Klosin, *Presiding*

8:00 PMSE 79. Synthesis of functionalized oligomers by ROMP and their hydrogenation. S.E. Klein, C. Dumrath, M. Beller, R. Kadyrov

8:30 PMSE 80. Stereospecific polymerization of cyclic olefins through ROMP. R.R. Schrock

9:00 PMSE 81. Design and applications of olefin metathesis catalysts for precise structural control. R.H. Grubbs

9:30 PMSE 82. (Imido)vanadium(V) complex catalysts for olefin insertion/metathesis polymerization. K. Nomura

10:00 Intermission.

10:10 PMSE 83. New opportunities for precision polyolefins. L.R. Sita

10:40 PMSE 84. Effect of aluminum alkyls on a homogeneous and silica-supported ethylene oligomerization catalyst. R. Duchateau, F. Karbach, S. Vadake Kulangara

11:10 PMSE 85. Homogeneous meets heterogeneous catalysis: Cooperative properties of electrophilic organometallic ensembles. T.J. Marks

11:40 PMSE 86. Multicenter olefin polymerization processes. Where homogeneous and heterogeneous catalysis meet. T.J. Marks

Section C

Westin Boston Waterfront
Douglas

Materials for Printed Electronics

Big Picture

Financially supported by The Dow Chemical Company

C. Gilmore, J. J. Watkins, *Organizers*

D. DeLongchamp, Y. Rao, *Organizers, Presiding*

8:00 PMSE 87. Strategic approach to flexible and printed electronic materials research and development. C. Markham

8:30 PMSE 88. High-performance printed organic transistors: Materials, processes, and devices. V. Subramanian, G. Grau, H. Kang, R. Kitsomboonloha

9:00 PMSE 89. Solution processing and device integration at the 2D limit. M. Hersam

9:30 Intermission.

10:00 PMSE 90. Withdrawn.

10:30 PMSE 91. Development of flexible hybrid electronics materials and processes for Air Force applications. B.J. Leever, M.F. Durstock, C.E. Tabor, J.D. Berrigan, A.T. Juhl

11:00 PMSE 92. New materials and printing processes for flexible electronics. C.D. Frisbie

Section D

Westin Boston Waterfront
Alcott

Advanced Materials for High Performance Formulations

Financially supported by The Dow Chemical Company

M. Johnson, B. McCulloch, J. Wilbur, *Organizers*

J. S. Katz, *Organizer, Presiding*

8:25 PMSE 93. New surfactants from recombinant proteins. D.A. Hammer, K. Vargo, R. Parthasarathy, G. Chen, E. Wang, A. Al Zaki, P. Heiney, A. Tsourkas, D. Lee

8:55 PMSE 94. Functionalized cellulose derivatives for enhanced nasal drug delivery. S.L. Jordan, J.S. Katz, R. Jemison, J.L. Curtis-Fisk

9:25 PMSE 95. Porous polymers in situ with RT-IL and their possible application as separator membranes in Li-ion batteries. W. Paschinger, A. Bismarck

9:45 PMSE 96. Magnetically responsive silicon carbide whiskers for nanocomposite materials. J. Townsend, R. Burtovy, P. Aprelev, K. Kornev, I.A. Luzinov

10:05 Intermission.

10:20 PMSE 97. Control of stimuli-responsive polymers by new methods. Y. Zhao

10:50 PMSE 98. Delivery of industrial antimicrobials. I.A. Tomlinson, F. Zeng, D. Laganella, T. Ghosh, R.W. Stephens

11:20 PMSE 99. Overcoming the critical micelle concentration: Exploring nanoparticles with amphiphilic grafts as concentration-independent "unimolecular micelle" nanodispersants for oil spill remediation. S.M. Grayson, M. Ejaz, A.M. Alb, K.C. Bentz, D.A. Savin

11:40 PMSE 100. Nonlaminated graphene oxide membrane with underwater superoleophobic property: Preparation and effective oil/water separation. T. Huang, L. Zhang, C. Gao

Section E

Westin Boston Waterfront
Faneuil

Phase Separation and Morphology Development in Polymers

Solution Assemblies and Thin Films

Financially supported by ExxonMobil Chemical Company

C. R. Lopez-Barron, S. Tallury, *Organizers*

M. L. Robertson, *Organizer, Presiding*

M. A. Pasquini, *Presiding*

8:00 PMSE 101. Interfacial layers with photoswitching surface energy for block copolymer alignment and directed self-assembly. M. Maher, C. Bates, W. Durand, G. Blachut, D. Janes, J. Cheng, D.P. Sanders, C.G. Willson, C.J. Ellison

8:40 PMSE 102. Phase behavior and micellar packing of impurity-free pluronic block copolymers in water. C.Y. Ryu, H. Park

9:00 PMSE 103. Industrially-relevant polymerization-induced self-assembly formulations in nonpolar solvents: RAFT dispersion polymerization of benzyl methacrylate. M. Derry, L.A. Fielding, S.P. Armes

9:20 Intermission.

9:35 PMSE 104. Effects of polydispersity in thin films of diblock copolymers: theories, simulations and experiments. R. Kumar, B.S. Lokitz, S. Sides, J. Chen, W. Heller, J. Ankner, J. Browning, M. Kilbey, B. Sumpter

9:55 PMSE 105. Additive-based approach for perpendicularly oriented polycarbonate-containing high- χ block copolymer domains for directed self-assembly. A. Vora, A. Chunder, M. Tjio, T. Magbitang, N. Arellano, E. Lofano, K. Nguyen, J. Cheng, D.P. Sanders

10:15 PMSE 106. Testing the vesicular morphology to destruction: Birth and death of diblock copolymer vesicles prepared via polymerization-induced self-assembly. N. Warren, O.O. Mykhaylyk, S.P. Armes, M. Williams, T. Doussineau, A. Ryan

10:35 Intermission.

10:50 PMSE 107. Synthesis and characterization of random and block copolymers for surface-patterning applications. D. Yi, C. Black, R.B. Grubbs

11:10 PMSE 108. Determination of the contribution of polymer chain configuration to solvent quality within confined thin films. S.V. Orski, R. Sheridan, E. Chan, K. Beers

11:30 PMSE 109. Cationic and reactive primary amine-stabilized nanoparticles by RAFT aqueous dispersion polymerization. M. Williams, N.J. Penfold, S.P. Armes

MONDAY AFTERNOON

Section A

Westin Boston Waterfront
Burroughs

New Advances in Nanostructured Polymeric Membranes for Filtration

Nanostructured Membranes for Biomedical and Industrial Applications

B. T. Chu, B. S. Hsiao, *Organizers*

V. Chen, Y. Na, *Presiding*

1:00 PMSE 110. High productive systems of nanofibers for filtration, separation, and purification. A. Tanioka, M. Takahashi

1:30 PMSE 111. Ionomeric block polymer membranes for filtration applications. M. Green, P. Singh, Y. Yang

2:00 PMSE 112. Separation of water from ultra-low sulphur diesel using polymer nanofibers with interpenetrating network morphology. S. Rajgarhia, S.C. Jana, G. Chase

2:30 Intermission.

2:45 PMSE 113. Nanostructured TiO₂ functionalized polymeric membranes: Platform for enzymatic membrane reactors. V. Chen, J. Hou, C. Ji

3:15 PMSE 114. Self-assembly of zwitterionic copolymers for fouling resistant, high flux membranes with ~1 nm effective pore size. P. Bengani, Y. Kou, A. Asatekin

3:45 PMSE 115. Study of molecular adsorption of cationic surfactant on membrane fibres with atomic force microscopy. I. Sokolov, G. Zorn, J.M. Nichols

Section B

Westin Boston Waterfront
Lewis

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Technical Session

Cosponsored by INOR

R. F. Jordan, G. A. Vaughan, *Organizers*

C. Chen, *Presiding*

1:30 PMSE 116. Structure control in olefin polymerization by organo rare-Earth catalysts. Z. Hou

2:00 PMSE 117. Catalytic polymerization of norbornenes via the rectification-insertion mechanism. B. Commaieu, J. Potier, J.P. Claverie

2:30 PMSE 118. Catalysts for olefin (co)polymerization and for controlled waste plastics conversion. C. Chen, M. Chen, S. Dai

3:00 Intermission.

3:10 PMSE 119. Precise synthesis of cyclic olefin copolymers by *ansa*-dimethylsilylene(fluorenyl)(amido)dimethyltitanium-based catalysts. T. Shiono

3:40 PMSE 120. Withdrawn.

Section C

Westin Boston Waterfront
Douglas

Materials for Printed Electronics

Materials

Financially supported by The Dow Chemical

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at:

www.acs.org/boston2015

Company

C. Gilmore, J. J. Watkins, *Organizers*

D. DeLongchamp, Y. Rao, *Organizers, Presiding*

1:00 PMSE 121. PEALD ZnO TFTs for flexible and large area applications. T. Jackson

1:30 PMSE 122. iXsenic S, a solution-processed metal oxide for future displays. R. Anselmann, K. Su, D. Pham, M. Marincovic, A. Merkulov

2:00 PMSE 123. NDI electron-transport agents incorporated into polyesters. W.T. Ferrar, D.S. Weiss, M. Molaire, L. Sorriero, X. Jin

2:20 PMSE 124. Poly(3, 4-ethylenedioxythiophene) as a conductor for flexible, stretchable, and wearable electronics. Y. Guo, M. Otley, M. Li, G. Sotzing

2:40 Intermission.

3:10 PMSE 125. Bottom-up solution synthesis of atomically precise pristine and nitrogen-doped graphene nanoribbons. A. Sinitskii

3:30 PMSE 126. One pot synthesis of electrophoretic inks in non-polar media for e-paper applications. D. Mirbel, C. Brochon, E. Cloutet, C. Navarro, G. Hadziioannou

3:50 PMSE 127. Enhanced stability and reduced operating voltage in ZnPc nanostructured based organic thin film transistor. A. Dey

4:10 PMSE 128. New form of an old natural dye — indigo-derived novel electron acceptors for high performance organic electronic materials. Y. Liu

Section D

Westin Boston Waterfront

Alcott

Advanced Materials for High Performance Formulations

Financially supported by The Dow Chemical Company

J. S. Katz, B. McCulloch, J. Wilbur, *Organizers*

M. Johnson, *Organizer, Presiding*

1:30 PMSE 129. What goes in, must come out: Designing biodegradable polymers from bioactives. K.E. Uhrich

2:00 PMSE 130. Design of AFFINISOL™ cellulosic polymers for increased processing efficiency in solubilizing pharmaceutical actives. S. Khot, K. O'Donnell, W. Porter, R. Schmitt

2:30 PMSE 131. Integrated experimental-modeling approach on the role of the N-terminus of spider silk protein: Water soluble silk to macroscopic fibers. O.S. Tokareva, M. Jacobsen, D. Ebrahimi, W. Huang, M. Simon, C. Staii, K. Quinn, I. Georgakoudi, M. Buehler, J.Y. Wong, D.L. Kaplan

2:50 PMSE 132. Developing electrospinning for oral solid dosage forms. I. Bhattacharyya, G.C. Rutledge

3:10 Intermission.

3:25 PMSE 133. Delivering convenience in a complex world: The challenge and opportunity for novel formulations in pesticide delivery. R. Boucher

3:55 PMSE 134. Zwitterionic nanocomposite gels with high mechanical toughness, controlled UCST type thermosensitivities, and unique swelling and self-healing behaviors. K. Haraguchi

4:15 PMSE 135. Broadening the scope of mechanical and morphological characteristics of poly(1,3,5-hexahydro-1,3,5-triazine) networks by the introduction of an engineering thermoplastic. M. Fevre, K. Virwani, J.M. Garcia, J. Hedrick

Section E

Westin Boston Waterfront
Faneuil

Phase Separation and Morphology Development in Polymers**Energy Relevant Materials and Conducting Polymers**

Financially supported by ExxonMobil Chemical Company

C. R. Lopez-Barron, M. L. Robertson, S. Tallury, *Organizers*

S. Lee, *Presiding*

1:30 PMSE 136. Block copolymer compatibilizers for controlled morphology and interfacial properties in polymer-fullerene blend. D. Kipp, J. Mok, S.B. Darling, V. Ganesan, R. Verduzco

2:10 PMSE 137. Synthesis of sulfonimide-containing triblock copolymers for improved conductivity and mechanical performance. C. Jangu, A.M. Savage, Z. Zhang, L.A. Madsen, F.L. Beyer, T.E. Long

2:30 PMSE 138. Liquid crystalline assembly and alignment of perylene diimide nanocrystals with poly(3-hexyl thiophene). W. Huang, R.C. Hayward

2:50 Intermission.

3:05 PMSE 139. Preparation and characterization of photolabile block copolymers for control of morphology in organic photovoltaics. D. Choi, P.W. Majewski, K.G. Yager, R.B. Grubbs

3:25 PMSE 140. Phase behavior and Li⁺ ion conductivity of styrene-Ethylene oxide multiblock copolymer electrolytes. J.M. Sarapas, K. Saijo, Y. Zhao, M. Takenaka, G.N. Tew

3:45 PMSE 141. Controlling polyelectrolyte complex morphology: Applications in drug delivery and adhesives. J. Serrine, T.E. Long

4:05 PMSE 142. Control of crystallization to promote microphase separation in fully conjugated block copolymers. Y. Lee, T.P. Le, Q. Wang, E. Gomez

4:25 PMSE 143. Diblock and triblock lithium conducting polymers from strongly incompatible PEGMA and PAAMPSA segments, effect of interdomain surface area on morphology and ionic transport. X. Chen, D. Luong, L. Smith, S. Granados Focil

4:45 PMSE 144. Concave-porosity PDMS beads by addition of metal-ion catalysts. M.J. Nee

Undergraduate Research Posters**Polymer Chemistry**

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

C. L. Soles, *Organizer*

8:00 - 10:00

204, 208-209, 214-215, 222, 224, 229, 232-233, 238, 242-243, 248, 250-251, 253, 256, 258-262, 264-265, 267, 269, 273, 275-276, 281-283, 285-286, 288, 290-291, 294-297, 299, 304, 309, 313, 318, 322, 324, 327-328. See subsequent listings.

From Raw to Varoom: The Science Behind Getting a Car on the Road

Sponsored by CHED, Cosponsored by PMSE, POLY, RUBB and SCC

Chemical Innovation and Design (CID) Talks: The Future of Innovation Now

Sponsored by MPPG, Cosponsored by AGFD, AGRO, BIOT, MEDI, PMSE and SCHB

TUESDAY MORNING

Section A

Westin Boston Waterfront
Lewis

New Advances in Nanostructured Polymeric Membranes for Filtration**Nanostructured Membranes for Water Purification**

B. T. Chu, B. S. Hsiao, *Organizers*

V. Freger, A. Tanioka, *Presiding*

8:00 PMSE 145. Highly permeable nanofibrous membranes for water purification. B.S. Hsiao, B.T. Chu

8:30 PMSE 146. Reusable bacteria immobilized electrospun nanofibrous webs for wastewater treatment. N.O. San, O.F. Sarioglu, A. Celebioglu, T. Tekinay, T. Uyar

9:00 PMSE 147. Novel PES/amphiphilic gradient copolymers blend ultrafiltration membrane using for potential water and wastewater treatment applications. G. Zhang, Q. Zhang, X. Zhan, F. Chen

9:30 Intermission.

9:45 PMSE 148. Separation of oil-in-water emulsions using electrospun fiber membranes and modeling of the fouling mechanism. Y. Lin, L. Choong, G.C. Rutledge

10:15 PMSE 149. Ultrafiltration membranes by reversible assembly of polymer brush nanoparticles. I. Zharov

10:45 PMSE 150. Bottom up self-assembly strategies for the fabrication of nanostructured polymeric membranes. M. Mahanthappa, G. Sorenson, J. Jennings

11:15 PMSE 151. Adsorption of bacteria into electrospun cellulose nanofiber mats: Effect of surface functionality. J.D. Schiffman, K. Rieger

Section B

Westin Boston Waterfront
Adams

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control**Technical Session**

Cosponsored by INOR#

R. F. Jordan, G. A. Vaughan, *Organizers*

G. E. Alliger, *Presiding*

8:30 PMSE 152. Living vinyl addition polymerization of substituted norbornenes by a *t*-Bu₃P-ligated methylpalladium complex. D. Kim, A. Bell, R.A. Register

9:00 PMSE 153. Organometallic chromium catalysts in olefin polymerization. G.E. Alliger

9:30 PMSE 154. Kinetic modeling of 1-hexene polymerization using group IV amine bis-phenolate catalysts. P. Pletcher, J.M. Switzer, D. Steelman, G.A. Medvedev, J.M. Caruthers, W. Delgass, M.M. Abu-Omar
10:00 Intermission.

10:10 PMSE 155. Morphology control in polyolefin synthesis via self-assembled hybrid supports. M. Klapper, S. Nietzel, D. Joe, K. Muellen, A.A. Alsaygh

10:40 PMSE 156. Metallocene-catalyzed olefin polymerization studied by dissolution dynamic nuclear polarization (DNP) NMR. C. Chen, W. Shin, C.B. Hilty

Section C

Westin Boston Waterfront
Douglas

Materials for Printed Electronics**Materials**

Financially supported by The Dow Chemical Company

D. DeLongchamp, Y. Rao, *Organizers*

C. Gilmore, J. J. Watkins, *Organizers, Presiding*

8:00 PMSE 157. Functionalization and deposition of carbon nanomaterials for chemical sensing. T.M. Swager

8:30 PMSE 158. Development of novel polymer thick film materials for diverse printed electronics applications. J.R. Dorfman

9:00 PMSE 159. Linear and hyperbranched polymers for printed electronic applications. B. Voit, A. Kiry, T. Erdmann, R. Poetzsch

9:20 PMSE 160. Functionally graded order in liquid crystal elastomers: Anisotropic substrates for stretchable electronics. T. Ware, T.J. White

9:40 Intermission.

10:10 PMSE 161. Facile formation of P3HT organogels via spin-coating. C. Lee, W. Yin, A. Hoyt, J. Sangoro, A.P. Sokolov, M.D. Dadmun

10:30 PMSE 162. Printed macroporous polymers with complex structures and shapes. Q. Jiang, A. Menner, A. Bismarck

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Section D

Westin Boston Waterfront
Alcott

Roy W. Tess Award: Symposium in Honor of Jamil Baghdachi

K. Matyjaszewski, C. K. Ober, *Organizers*
B. D. Freeman, D. C. Webster, *Organizers, Presiding*

9:00 PMSE 163. Synthesis and characterization of omniconjugated compounds and their applications as polymer coatings. **P. Zarras**

9:30 PMSE 164. In search of smart polymers: Asking nature for help. **K. Zhang, M. Tamami, S. Cheng, S. Hemp, R. Gao, A.E. Smith, T.E. Long**

10:00 PMSE 165. Concepts for the understanding and structure of films — graphene nanocomposites and enzyme triggered deposition of casein and melanine. **W. Bremser**

10:30 Intermission.

11:00 PMSE 166. Block copolymer coatings: From advanced semiconductor patterning to antimicrobials. **R. Allen**

11:30 PMSE 167. Glycidyl carbamate functional resins: Polyurethanes through epoxy chemistry. **D.C. Webster**

Section E

Westin Boston Waterfront
Faneuil

Celebrating 50 Years of Polymer Science and Engineering

K. Carter, E. B. Coughlin, T. Emrick, *Organizers*
A. Misra, G. N. Tew, *Presiding*

8:00 PMSE 168. Polymer science and engineering at UMASS: The early years. **W.J. MacKnight**

8:20 PMSE 169. Characterizing a novel polysaccharide/DNA complex and application to targeting delivery of therapeutic oligonucleotides. **K. Sakurai**

8:50 PMSE 170. Tough supramolecular hydrogels and the effect of molecular architecture on properties. **R.A. Weiss, F. Wang, H. Niu**

9:20 Intermission.

9:50 PMSE 171. Polyelectrolytes in multi-valent ionic media. **M.V. Tirrell**

10:20 PMSE 172. Polymeric immunonano-micelles for targeted delivery in cancer. **M.S. Shoichet, J. Logie, C. McLaughlin, R.Y. Tam, S.C. Owen, D. Chan, J. Lu**

10:50 PMSE 173. Polymer science and Moore's Law: The essential role of polymers in photolithography. **K. Camera, J. Jiang, C.K. Ober**

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Sponsored by POLY, Cosponsored by HIST, PMSE†, PRES and PROF‡

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

TUESDAY AFTERNOON

Section A

Westin Boston Waterfront
Lewis

New Advances in Nanostructured Polymeric Membranes for Filtration

Nanostructured Membranes for Desalination

B. T. Chu, B. S. Hsiao, *Organizers*

B. D. Freeman, A. Roy, *Presiding*

1:00 PMSE 174. Ion sorption, diffusion, and transport in polymer membranes. **B.D. Freeman**

1:30 PMSE 175. Molecular mechanisms of membrane desalination. **V. Freger**

2:00 PMSE 176. Quest for understanding fundamental structure-transport relationships for RO membranes.

A. Roy, S. Rosenberg, R.C. Cieslinski, M. Paul, I. Tomlinson, M. Peery, S. Jons

2:30 Intermission.

2:45 PMSE 177. Surface modification of water purification membranes by using self-assembly of nanogel star polymers. **Y. Na, R. Wang, J. Diep, S. Yahyazadeh, A. Tek, V. Pitunova, J. Sly**

3:15 PMSE 178. Using neutron radiography to verify the film model for permeation through forward osmosis membranes.

D. Shaffer, E. Chan, D. Hussey, M. Elimelech

3:45 PMSE 179. Model thin film composite membranes based on molecular layer-by-layer assembly of aromatic polyamides. **C.M. Stafford, K.E. Feldman, S.C. Lee, N.K. Nadermann, E. Chan**

Section B

Westin Boston Waterfront
Adams

Adhesion Science and Adhesive Materials

Mechanism of Adhesion

Financially supported by 3M Company, ExxonMobil Chemical Company

R. Tripathy, *Organizer*

A. Crosby, A. R. Fornof, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 PMSE 180. Adhesion aspects of polymeric materials. **J. Baghdachi**

2:00 PMSE 181. Surface tension and its effect on the mechanics of contact and fracture of soft material. **C. Hui, T. Liu, X. Xu, A. Jagota**

2:45 Intermission.

3:00 PMSE 182. Adhesion enhanced by octopus-inspired miniaturized suction cups. **N. Lu**

3:35 PMSE 183. Exploring nanoshape of 1D tapered nanorods: Effect on dry adhesion. **Y. Cho, G. Kim, Y. Cho, S. Lee, H. Minsky, K. Turner, D. Gianola, S. Yang**

3:55 PMSE 184. Rolling wrinkles on elastic substrates. **M.J. Imburgia, A. Crosby**

4:15 Concluding Remarks.

Section C

Westin Boston Waterfront
Douglas

Materials for Printed Electronics

Processing Techniques and Device Construction

Financially supported by The Dow Chemical

Company

D. DeLongchamp, Y. Rao, *Organizers*

C. Gilmore, J. J. Watkins, *Organizers, Presiding*

1:00 PMSE 185. Advanced micro- and nanomanufacturing of large-area functional surfaces. **B. Stadlober, D. Nees, U. Palfinger, S. Rutloff, M. Beleggratis**

1:30 PMSE 186. Roll-to-roll manufacturing of flexible hybrid electronics: From silicon wafers to thin flexible glass. **M.D. Poliks**

2:00 PMSE 187. Roll-to-roll nanofabrication using 1D nanomaterials. **J. John, K.R. Carter**

2:30 Intermission.

3:00 PMSE 188. Scale-up of oCVD: Large-area conductive polymer thin films for next-generation electronics. **P. Kovacic, K. Gleason**

3:20 PMSE 189. Semiconducting SWCNT: Materials, inks, and printed thin film transistors. **R.R. Malenfant, Z. Li, J. Ding, J. Lefebvre, F. Cheng, N. Du, C.M. Homenick, J. Dunford, G. Lopinski, R. James, C.T. Kingston, B. Simard, J. Humes, J. Kroeger**

3:40 PMSE 190. Highly conductive PEDOT:PSS nanofibrils induced by solution-processed crystalline formation and its application as flexible and transparent electrodes. **S. Kee, N. Kim, K. Lee**

4:00 PMSE 191. Design of dimeric sandwich compounds as n-dopants for organic electronics. **K. Moudgil, J.H. Delcamp, S.K. Mohapatra, M. Damm, L. Bottomley, S. Barlow, S.R. Marder**

Section D

Westin Boston Waterfront
Alcott

Roy W. Tess Award: Symposium in Honor of Jamil Baghdachi

B. D. Freeman, D. C. Webster, *Organizers*
K. Matyjaszewski, C. K. Ober, *Organizers, Presiding*

1:30 PMSE 192. Controlled crosslinking in ATRP. **K. Matyjaszewski**

2:00 PMSE 193. Nanofabrication for detecting and controlling single biopolymer. **Q. Lin**

2:30 PMSE 194. Surface modification of porous polymer membranes to reduce fouling. **B.D. Freeman**

3:00 Intermission.

3:30 PMSE 195. Polymer brush films: "grown from" block copolymer and mixed brushes. **D. Calabrese, M. Welch, C.K. Ober**

4:00 PMSE 196. Smart and functional materials. **J. Baghdachi**

Section E

Westin Boston Waterfront
Faneuil

Celebrating 50 Years of Polymer Science and Engineering

E. B. Coughlin, T. Emrick, *Organizers*

K. R. Carter, *Organizer, Presiding*

G. N. Tew, *Presiding*

1:00 PMSE 197. Synthesis and assembly of hydrophilic organic nanotubes. **J. Rzyayev**

1:30 PMSE 198. Polymer chemist's perspective on protein science and engineering. **D.A. Tirrell**

2:00 PMSE 199. Modular and orthogonal approaches for the construction of functional biomaterials. **K.T. Dicker, H. Zhang, S. Liu, J.M. Fox, X. Jia**

2:30 Intermission.

3:00 PMSE 200. Toward functional hybrid materials. **T. Xu**

3:30 PMSE 201. From rational design and synthesis of nonlinear block copolymers to functional hairy nanoparticles, nanorods, and shish-kebabs. **Z. Lin, X. Pang**

4:00 PMSE 202. Three decades of polymer calorimetry in less than a microcentury. **R.E. Lyon**

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Sponsored by POLY, Cosponsored by HIST, PMSE†, PRES and PROF‡

Innovation in Materials for Emerging Uses

Sponsored by MPPG, Cosponsored by PHYS, PMSE and POLY

TUESDAY EVENING

Section A

Boston Convention & Exhibition Center
Ballroom West

Joint PMSE/POLY Poster Session

Cosponsored by POLY†

C. L. Soles, *Organizer*

6:00 - 8:00

PMSE 203. Carbazole-assisted electrodeposition of graphene oxide: Synthesis, characterization, and directed deposition. **P. Advincula, J.D. Mangadiao, R.C. Advincula**

PMSE 204. Polymer grafted graphene oxide (GO) nanoparticle dispersions. **A. Advincula, J. Mangadiao, R.C. Advincula**

PMSE 205. Post-synthetic modification of a bis(imino)pyridine-linked porous polymer with inorganic fluorinated ions for highly selective CO₂ capture. **P. Arab, H.M. El-Kaderi**

PMSE 206. New polyurethane-like material based on proteins. **A. Araujo, A. Machado, B.D. Olsen**

PMSE 207. Preparation and adhesion performance of transparent acrylic pressure sensitive adhesives with biomass-based acrylic monomer. **S. Baek, Y. Cho, S. Hwang**

PMSE 208. Controlled release of ClO₂ gas from polymeric films. **Z. Bai, D.E. Cristancho, A.A. Rachford, A.L. Reder, A. Williamson, A.L. Grzesiak**

PMSE 209. Infusion of polyamide into polymer/graphene composite foams. **J. Bento, S.J. Woltonist, D.H. Adamson**

PMSE 210. Removal of heavy metal ions by a polymer matrix containing dithiocarbamate as a chelating group. **F. Damkaci, N. Boke Sarikahya, H. Sarikahya, V. Niri, A. Alawaed**

PMSE 211. Sensing nanoscale polymer films under gamma radiation: Damage mitigation study. **N. Borodinov, J.M. Giammarco, N. Patel, A. Agarwal, K.R. O'Donnell, C.J. Kucera, L.G. Jacobssohn, I.A. Luzinov**

PMSE 212. Hydrogel based protein microarray for SIRS detection. **A. Buderer, T. Brandstetter, O. Prucker, J. Ruehe**

PMSE 213. Emission tuning of boron coordinated β-diketonate poly(lactic-acid) materials through methoxy substitution. **T.P. Butler, C.A. DeRosa, C. Fraser**

PMSE 214. Hydrophilic yet non-water soluble electrospun nanofibers for specific contamination detection using microfluidics. **L. Buttaro, E. Druva, M.W. Frey**

- PMSE 215.** Evaluating cytocompatibility of bone cells on glycosaminoglycan (GAG) containing biomimetic scaffolds. **J. Cardenas Turner, E.A. Blaber, G. Collins, E.A. Almeida, T.L. Arinzech**
- PMSE 216.** Synthesis of group VA polyesters containing 3,5-pyridinedicarboxylic acid. **C.E. Carraher, M. Roner, K. Black**
- PMSE 217.** Synthesis of group IVB metallocene polyamine esters from reaction of 6-aminopenicillanic acid with group IVB metallocene dichlorides employing interfacial polycondensation. **C.E. Carraher, D. Patel, N. Sookedo, M. Roner**
- PMSE 218.** Synthesis of organotin polyether esters from reaction of salicylic acid and organotin dihalides. **C.E. Carraher, M. Lynch, N. Sookedo, M. Roner**
- PMSE 219.** MALDI MS results of the products from the salt of D-camphoric acid and organotin dihalides. **C.E. Carraher, A. Campbell, M. Roner**
- PMSE 220.** Ability of organotin polyamines synthesized from the reaction of 3-amino-1,2,4-triazole and organotin dichlorides to inhibit cancer cell lines. **C.E. Carraher, M. Roner, A. Moric-Johnson, L. Miller, R. Crichton**
- PMSE 221.** Ability of group VA organoethers derived from the anticoagulant dicumarol to inhibit cancer cells. **C.E. Carraher, M. Roner, N. Sookedo, A. Moric-Johnson, L. Miller**
- PMSE 222.** New method for measuring the temperature change of photothermal Au nanostructures using smart polymers. **H. Cavusoglu, H. Sakalak, B. Buyukbekar, G. Demirel, M. Citir, M. Yavuz**
- PMSE 223.** Bioinspired intermolecular and intramolecular metal-coordinating polymers for use as mechanical and structural soft materials. **S. Cazzelli, N. Holten-Andersen**
- PMSE 224.** Preparation and characterization of polymethacrylate derivatives having self-healing properties via reversible covalent bonding formation and dissociation. **S. Cha, K. Lee**
- PMSE 225.** Optically responsive luminescent metallogels based on lanthanide coordination polymers. **P. Chen, N. Holten-Andersen, S.C. Grindy, Q. Li**
- PMSE 226.** Ink-jet printing multilayer for controlling bioactive materials and cell-based high-throughput immunological drug screening. **M. Choi, S. Hwangbo, D. Choi, J. Hong, J. Choi**
- PMSE 227.** Electrospinning silk with selenium nanoparticles for antibacterial skin applications. **S. Chung, M. Stolzoff, B. Ercan, T. Webster**
- PMSE 228.** Mechanical characterization of soft materials with AFM: Procedures for tip shape variation, adhesive, viscoelastic, and layered substrate models. **M. Chyasnachyus, S.L. Young, A. Hoffman, V.V. Tsukruk**
- PMSE 229.** Design and functional evaluation of zwitterionic polymer networks as cartilage lubricants. **B.G. Cooper, B.D. Snyder, M.W. Grinstaff**
- PMSE 230.** Preparation and characterization of a nanocomposite constrained high temperature drilling fluid with water soluble AM-SAS-SSS copolymers by inverse microemulsion polymerization. **Q. Deng, Y. Ke**
- PMSE 231.** Oxygen sensing difluoroboron dinaphthoylethane polylactide. **C.A. DeRosa, J. Samonina-Kosicka, Z. Fan, H.C. Hendargo, D. Weitzel, G.M. Palmer, C. Fraser**
- PMSE 232.** Low-cost photolithographic fabrication of nanowires and microfilters for advanced bioassay devices. **N. Doan, L. Qiang, Z. Li, S. Vaddiraju, G.W. Bishop, J. Rusling, F. Papadimitrakopoulos**
- PMSE 233.** Morphological studies on polymer electrolyte membranes (PEMs) used in fuel cells: The effects of environmental conditions on structural changes as determined by FTIR spectroscopy. **K.J. Dye, K.W. Kittredge**
- PMSE 234.** Design and synthesis of Janus-type dendrimers as efficient therapeutic carriers. **L. Ezell, D. Williams, D. Watkins**
- PMSE 235.** Selective dye uptake from aqueous industrial waste mixtures by novel covalent organic frameworks. **S. Filicki, M. Ulasan, M. Citir, M.S. Yavuz**
- PMSE 236.** Application of nanoparticles of titanium dioxide for mass-coloration of polyimide fibers. **N. Fjodorova, T. Diankova, M. Novic, A. Ostanan**
- PMSE 237.** Synthesis and characterization of magnetic molecularly imprinted polymer (magnetic MIP) for penicillin G. **R.R. Pupin, M.V. Foguel, M.T. Sotomayor**
- PMSE 238.** Novel sustained release strategy of protein drugs from biodegradable electrospun nanofibers for controlled protein delivery. **Y. Gao, A. Land, J. Bundy, G.M. Policastro, T. Ritzman, M. Becker**
- PMSE 239.** Silk-on-silk self-(un)rolling microconstructs: Rings, tubes, and helical tubes. **C. Ye, S. Nikolov, R. Geryak, M. Chyasnachyus, R. Calabrese, A. Alexeev, D.L. Kaplan, V.V. Tsukruk**
- PMSE 240.** Spontaneously formatted triazole gels as tissue adhesives. **M. Gkikas, R.K. Avery, A. Khademhosseini, B.D. Olsen**
- PMSE 241.** Functional electrospun nanofibers for biosensor applications. **E. Gonzalez, L. Buttaro, M.W. Frey**
- PMSE 242.** Mussel-inspired reversible metal-coordinate bonds as a pathway towards temporal control over the mechanical hierarchy of soft materials. **S.C. Grindy, R. Learsch, J. Cheng, D.G. Barrett, P.B. Messersmith, N. Holten-Andersen**
- PMSE 243.** Water-based melanin multilayer thin films with broadband UV absorption. **T. Guin, J.C. Grunlan**
- PMSE 244.** Rheological characterization of bioinspired mineralization in hydrogels. **A. Halim, N. Holten-Andersen**
- PMSE 245.** Withdrawn.
- PMSE 246.** Inhibitor-induced combination therapy of K-RAS driven NSCLC. **B. Heckert, K. Woody, D. Thompson, S. Santra**
- PMSE 247.** Poly(methyl methacrylate) derivatives with polyhedral oligomeric silsesquioxane moiety for fouling and wettability control. **H. Hong, E. Sohn, D. Kim, K. Song, N. Kim, J. Lee**
- PMSE 248.** Hybrid silica-titanium-polyimide composite membranes for gas separation. **F. Huang, C.J. Cornelius**
- PMSE 249.** Rice straw, inorganic filler reinforced R- polyethylene composites: Morphology and surface energy analysis. **R. Huang, M. Yu, C. Zhou, Q. Wu**
- PMSE 250.** Isolation of cellulose nanocrystals from *Miscanthus x. Giganteus*. **M. Hunsen, A. Way, Z. Xue, E. Cudjoe, S.J. Rowan**
- PMSE 251.** Controllable wettability of layer-by-layer assembled nanofilm with durability and high transmittance for biomedical applications. **S. Hwangbo, J. Hong, M. Choi**
- PMSE 252.** High performance electric heating nanocomposite films composed of heterocyclic aromatic polymers and carbon nanomaterials. **Y. Jeong, Y. Kim, T. Lee, S. Yu, E. Lee, J. Park**
- PMSE 253.** Mass dependence of the activation enthalpy and entropy of unentangled N-alkanes in the melt. **C. Jeong, J. Douglas**
- PMSE 254.** Preparation of polymer-SiO₂ nanocomposite microspheres and the investigation of the plugging property in porous media. **J. Ji, Y. Ke**
- PMSE 255.** Near infrared absorbing polymers based on substituted bithiophene unit. **L. Jin, Y. Li, T. Dutta, Z. Peng**
- PMSE 256.** Statistical mechanical – spectroscopic analysis of water distribution in ion exchange membranes. **C. Johnson, E. Steele, F. Flor, N. Navarro, N. Dimakis, E.S. Smotkin**
- PMSE 257.** Synthesis and electro-phosphorescent properties of carbazole-based bipolar host materials incorporating a trifluoromethyl moiety. **J. Jun, S. Hwang, K. Lee**
- PMSE 258.** Robust transesterification reactions of cellulose in imidazolium-based ionic liquids. **R. Kakuchi, M. Yamaguchi, Y. Shibata, K. Ninomiya, T. Ikai, K. Maeda, K. Takahashi**
- PMSE 259.** Conjugation study of engineered cellulase with end-functionalized polymers. **P. Katyal, Y. Yang, H. Xia, O. Vinogradova, Y. Lin**
- PMSE 260.** Modulating oxygen sensitivity with halide substitution in BF₂dbmPLA materials. **C. Kerr, C.A. DeRosa, Z. Fan, M. Kolpaczynska, A.S. Mathew, R.E. Evans, G. Zhang, C. Fraser**
- PMSE 261.** Study of the properties and application of a difluorodiphenyl sulfone based ionomer. **W. Khan, D. Wang, C.J. Cornelius**
- PMSE 262.** Plasma modification of low bandgap polymer and its application in solar cell. **I.T. Kim, J. Kim, T. Cho**
- PMSE 263.** Organic thin-film transistors (OTFTs) based on biocompatible blends of poly(3-hexylthiophene) (P3HT) and poly(2-hydroxyethyl methacrylate) derivative for biomedical applications. **N. Kim, J. Bae, E. Sohn, H. Hong, H. Jang, B. Kim, J. Lee**
- PMSE 264.** Infusion of catalytically active polymers for templated condensation of metal oxides in foam composites. **G.M. Kraft, S.J. Woltonist, C. Hire, D.H. Adamson**
- PMSE 265.** Fractionation of graphene oxide. **H. Kumar, D.H. Adamson**
- PMSE 266.** Preparation of shape memory PCL-based blends. **S. Lai, Y. Chiu, X. Wang, J. Han**
- PMSE 267.** Determining properties of bio-inspired metal-coordinate thin films at soft interfaces. **E. Lai, M. Kolle, N. Holten-Andersen**
- PMSE 268.** Antimicrobial peptide stars: The road to discovery and development. **S. Lam, N. O'Brien-Simpson, N. Pantarat, A. Sulistio, E. Wong, A. Blencowe, E. Reynolds, G. Qiao**
- PMSE 269.** Hybrid organic-inorganic sulfonated ionomers for the application of vanadium redox flow batteries. **T. Largier, C.J. Cornelius**
- PMSE 270.** Engineering pH metal coordinated crosslinks in PEG double network hydrogels. **R. Learsch, S. Grindy, N. Holten-Andersen**
- PMSE 271.** Preparation of metal-ion containing polymers and their possible applications. **K. Lee, S. Cha, J. Bae**
- PMSE 272.** Stacking phosphorus-based multilayer thin film onto clay-based nanobrick wall to impart self-extinguishing flame retardant behavior to polyurethane. **K. Holder, M. Huff, M. Cosio, M. Leistner, J.C. Grunlan**
- PMSE 273.** Solubility and diffusivity of solvents in crosslinked polydimethylsiloxane studied by inverse gas chromatography at infinite dilution condition. **Y. Xia, X. Zhan, M. Fang, X. Li, Z. Zhang, J. Li**
- PMSE 274.** Criteria for quick and consistent synthesis of poly(glycerol sebacate) for tailored mechanical properties and biodegradability. **X. Li, H. Chung**
- PMSE 275.** Weak polyelectrolyte multilayers with controllable wet adhesive behaviors. **C. Li, Y. Gu, N. Zacharia**
- PMSE 276.** Fully-biobased poly(limonene carbonate)s as novel coating resins. **C. Li, R.J. Sablong, C.E. Koning**
- PMSE 277.** Exploring the effect of sequence on the self-assembly of ELP-mCherry fusion proteins. **C.E. Mills, G. Qin, B.D. Olsen**
- PMSE 278.** Microfluidic synthesis of uniform microparticles with structural and chemical anisotropy. **N. Min, B. Kim, T. Lee, D. Kim, D. Lee, S. Kim**
- PMSE 279.** Triptycene based poly(ether ether ketone) for proton exchange membranes. **L.C. Moh, J.B. Goods, T.M. Swager**
- PMSE 280.** Electrically conductive hydrogels containing a self-assembled percolating graphene scaffold. **R. Mohammadi Sejoubarsi, T. Xu, S.J. Woltonist, D.H. Adamson**
- PMSE 281.** New technique for preparation of uniform brush polymers using surface-initiated atom transfer radical polymerization. **R. Mohammadi Sejoubarsi, D.H. Adamson**
- PMSE 282.** Mechanoresponsive polymers for self-healing applications. **C. Nagamani, H. Liu, J. Moore**
- PMSE 283.** Preparation of thermoresponsive cationic copolymer brushes for stem cell separation. **K. Nagase, Y. Hatakeyama, T. Shimizu, K. Matsura, M. Yamato, N. Takeda, T. Okano**
- PMSE 284.** Thermoresponsive anionic copolymer brushes having strong acid group for effective separation of basic proteins. **K. Nagase, J. Kobayashi, A. Kikuchi, Y. Akiyama, H. Kanazawa, T. Okano**
- PMSE 285.** Structured membranes by nano-organized triblock copolymers. **S. Nehache, D. Quemener**
- PMSE 286.** Aggregation properties of temperature-responsive graft copolymer with poly(trimethylene carbonate) oligo segment. **K. Nitta, A. Kimoto, J. Watanabe, Y. Ikeda**
- PMSE 287.** Dynamics of cartilage extracellular matrix components. **W. Oh, J.C. White, S.R. Raghavan, P.J. Basser, F. Horkay**
- PMSE 288.** Synthesis of sulfur-pyrene copolymers as cathode materials for lithium-sulfur batteries. **J. Lim, S. Park, J. Pyun, K. Char**
- PMSE 289.** Advanced radiation-resistant elastomers. **B. Peters**
- PMSE 290.** Liposome-loaded backpacks for targeted and cell-mediated drug carriers. **R. Polak, R.M. Lim, R.E. Cohen, M.F. Rubner**
- PMSE 291.** Analysis of polymer materials by computed tomography on a laboratory diffractometer. **J.E. Quinn, A. Adilbhatla**

- PMSE 292.** Amphiphilic RAFT copolymers for biomedical applications. **M.S. Rahman**
- PMSE 293.** Thermal stability of acetylene-functional polybenzoxazine after prepolymerization. **Q. Ran, Y. Xu, Y. Gu**
- PMSE 294.** Effect of moisture on cationic polymerization of silicone epoxy monomers. **R. Ranaweera, T.P. Schuman, R. Wang, B.D. Miller, K.V. Kilway**
- PMSE 295.** Morphology and hydrogen bonding properties of model thermoplastic polyurethanes with monodisperse hard segments. **L. Ren, P. Shah, N. Kang, R. Faust**
- PMSE 296.** Layer-by-layer assembled nucleic acids microsponges for efficient packaging and delivery of nucleic acid therapeutics. **Y. Roh, P.T. Hammond**
- PMSE 297.** Amphiphilic random copolymers with charged groups as membrane selective layers. **I. Sadeghi, A. Asatekin**
- PMSE 298.** Carbon-filled thermoplastic polyurethanes as stretchable, conductive composites. **K.S. Sallah, I.A. Aksay**
- PMSE 299.** Silk fibroin/poly(ethylene glycol) bioconjugates for medical applications. **S. Saska, A. Obermeyer, B.D. Olsen**
- PMSE 300.** Fabrication of reduced graphene oxide (rGO) double layers with high conductivity. **M. Savchak, R. Burtovyy, N. Borodinov, K. Hu, R. Ma, V.V. Tsukruk, I.A. Luzinov**
- PMSE 301.** Susceptibility of biomimetic polymer networks to enzymatic degradation. **S. Sharma, B.G. Cooper, M.W. Grinstaff, B.D. Snyder**
- PMSE 302.** Tuning Magnetic Properties of Dy-containing Metal-Organic Frameworks through Coordination Geometries. **K. Liu, W. Shi, P. Cheng**
- PMSE 303.** HOMO-LUMO orbitals and band gaps of models of donor-acceptor polymers: A DFT study. **G. Singh, R.M. Peetz**
- PMSE 304.** Fungal based biopolymer composites. **L. Smith, G. Tudyln, L. Schadler, C. Hart**
- PMSE 305.** Fluorous solvent-soluble imaging materials by photodimerization using anthracene moieties. **J. Son, Y. Kim, J. Lee**
- PMSE 306.** Innovative anti-oxidant nanoceria for the early diagnosis and treatment of lung cancer. **S. Sulthana, B. Heckert, J. Kallu, S. Santra**
- PMSE 307.** Effect of carbonization time and temperature on graphitization of polyacrylonitrile interphases in nanocomposites. **N. Tajaddod, Y. Zhang, H. Li, M. Minus**
- PMSE 308.** Cationic polythiophenes for DNA detection. **Y. Takeoka, E. Yamaguchi, M. Yoshizawa-Fujita, M. Rikukawa**
- PMSE 309.** pH-responsive polymeric microspheres for micronutrients fortification of salt. **X. Xu, W. Tang, Y. Zeng, E. Rosenberg, R. Langer, A. Jaklenc**
- PMSE 310.** Multifunctional silicon carbide whiskers for nanocomposite materials. **J. Townsend, R. Burtovyy, P. Aprelev, K. Kornev, I.A. Luzinov**
- PMSE 311.** Significant and visible transparency change upon D-glucose addition on copolymers comprising boronic acids and hydrophilic/hydrophobic fine tuning "spacer" monomers: Introduction to contact lens materials. **K. Tsukamoto, S. Tanikawa, M. Lamrani**
- PMSE 312.** Electrospinning of polymer nanocomposite fibers. **R.N. Udangawa, R.J. Linhardt, T.J. Simmons, L. Hou, A. Pochiraju, V. Kumar**
- PMSE 313.** Mechanically-controlled release from elastomeric substrates with superhydrophobic coatings. **J. Wang, J. Kaplan, Y. Colson, M.W. Grinstaff**
- PMSE 314.** Preparation of hydrogenated rosin ester/acrylic hybrid latexes with core-shell structure. **D. Wang, M. Shen, K. Zhang, S. Shang, J. Song**
- PMSE 315.** Controllable antibiofouling thin films for implantable biosensors. **D. Wang, Z. Li, F. Papadimitrakopoulos**
- PMSE 316.** Study of the rates of release of methylene blue (MB) from hyperbranched poly(acrylic acid)/poly(allylamine hydrochloride) (PAA/PAH) films. **A.M. Washington, K.W. Kitzredge**
- PMSE 317.** Development of crosslinked diacetylene-containing membrane derived from feluric acid and gas permeation properties. **D. Watabe, K. Nagai**
- PMSE 318.** Highly tunable nanocomposite foams from pristine graphene stabilized emulsions. **S.J. Woltornist, A.V. Dobrynin, D.H. Adamson**
- PMSE 319.** Withdrawn.
- PMSE 320.** Effects of silica content on the properties of Poly(N-isopropylacrylamide)/silica nanocomposite hydrogels. **L. Wu, S. Tang, Y. Li, S. Feng, C. Zhang**
- PMSE 321.** Reversible adsorption of carbon dioxide in Poly(N-isopropylacrylamide)/graphene composite hydrogel. **L. Wu, Y. Li, S. Feng, C. Zhang**
- PMSE 322.** Controlled release of aspirin from Poly(N-isopropylacrylamide)/graphene composite hydrogel. **S. Feng, L. Wu, Y. Li, C. Zhang**
- PMSE 323.** Development of multifunctional bioactive polymers for wound-contact applications. **J. Lundin, B. Streifel, G. Daniels, S.L. Giles, R. Baumann, J.H. Wynne**
- PMSE 324.** Quantum dots encapsulated in block co-polymer micelles: What is the role of surfactant? **B.E. Wyslouzil, G. Nabar, B. Miller, J.O. Winter**
- PMSE 325.** Novel kafirin based electrospun fiber with improved mechanical and release profile by blending with polycaprolactone: Fabrication, encapsulation, and in vitro release profile. **J. Xiao**
- PMSE 326.** Thermoplastic polymer functional nanofibers by melt blending extrusion: Application in Cr(VI) adsorption. **D. Xu, R. Xiao**
- PMSE 327.** Withdrawn.
- PMSE 328.** Synthesis, characterization, and UV curing of (meth)acrylate end-functional polyisobutylene macromers. **B. Yang, C. Parada, R.F. Storey**
- PMSE 329.** Preparation and properties of polypropylene composites reinforced with chemically modified lignin particle. **J. Yeo, D. Seong, S. Hwang**
- PMSE 330.** Permeation properties of Ethyl acetate solution through poly(lactic acid) membrane. **T. Yonezu, K. Nagai**
- PMSE 331.** Withdrawn.
- PMSE 332.** Water vapor sorption properties in ABA-type triblock copolymer membranes composed of polyimide and polyhedral oligomeric silsesquioxane. **A. Yoshida, K. Nagai**
- PMSE 333.** Gas permeation and separation properties of polyimide modified by aromatic amine vapor. **T. Yoshioka, K. Nagai**
- PMSE 334.** Synthesis of thermo responsive polymers containing N-vinylcaprolactam and N-vinylimidazole onto polypropylene films. **E. Zavala-Lagunes, E. Bucio**
- PMSE 335.** Synthesis of atactic and isotactic Poly(1,2-glycerol carbonate)s: Degradable polycarbonates for biomedical and pharmaceutical applications. **H. Zhang, M.W. Grinstaff**
- PMSE 336.** 3D hyaluronan bifunctional hydrogels as matrices for breast spheroid formation. **A.E. Baker, R.Y. Tam, M.S. Shoichet**
- PMSE 337.** Ordered DNA fragmentation on surfaces for NGS sequencing. **N. Cho, K. Zhu, J. Budassi, J. Sokolov**
- PMSE 338.** Study on the preparation of nucleating agents for polymer by using modified heavy oil residual. **Q. Zhou, M. Qin, Y. Ke**
- PMSE 339.** Control of cell interaction from oligopeptide- and oligosaccharide-based self-assembled nanostructure. **E. Garanger, C. Drappier, C. Bonduelle, S. Lecommandoux**
- PMSE 340.** Four-component copolyesters/polypropylene nanocomposite short fibers: Preparation, characterization, and plugging performance in the fracture reservoir. **S. Lu, Y. Ke, Q. Zhou, G. Zhang, J. He, J. Ji, Q. Deng, C. Yuan**
- PMSE 341.** Surface modification for microfluidic devices fabrication of biodegradable polymeric materials via laser ablation. **Y. Hsieh, S. Chen, W. Huang, J. Wang**
- PMSE 342.** Development of protein and cell resistant functional brush polymer on stainless steel. **G. Alas, D.M. Collard, A. Garcia**
- PMSE 343.** Pressure sensors with microstructured polydimethylsiloxane dielectrics fabricated via the breath figures method. **S. Miller**
- PMSE 344.** Trifaceted gastric retention of capecitabine exploiting xanthan gum. **Y. Singh, M.K. Chourasia**
- PMSE 345.** Withdrawn.
- PMSE 346.** Controlling the oxygen vapor permeability in side-chain liquid crystalline polymers. **S. Hassan, R. Anandakathir, M.J. Sobkowicz, B.M. Budhlall**

WEDNESDAY MORNING

Section A

Westin Boston Waterfront
Lewis

General Papers/New Concepts in Polymeric Materials

Biological and Biomedical Polymers

C. L. Soles, *Organizer, Presiding*

8:00 PMSE 347. Complete biobased polymer derived from polylactic acid and starch nanocrystal: The preparation process for practical model of green disposable plastic. **K. Laohasurayotin, P. Songkhum, K. Kasemwong, W. Pinket**

8:20 PMSE 348. Construction of a versatile and functional diblock copolypeptide-based nanoparticle platform for siRNA delivery. **J. Fan, S. Khan, R. Li, X. He, K. Seetho, F. Zhang, J. Zou, M. Elsbahy, K.L. Wooley**

8:40 PMSE 349. Polyethylene glycol (PEG) polymer brushes protect nucleic acid from DNase degradation by steric hindrance. **X. Lu, F. Jia, X. Tan, K. Zhang**

9:00 PMSE 350. Efficient synthesis of multiblock copolymer microfibers via interfacial bioorthogonal polymerization. **S. Liu, H. Zhang, J.M. Fox, X. Jia**

9:20 PMSE 351. Delivery of carbon monoxide using polymeric nanoparticles for bioapplications and biofilm dispersal. **C. Boyer, D. Nguyen, K. Nguyen**

9:40 Intermission.

10:00 PMSE 352. Characteristics of polycaprolactone grafted propargyl dehydroabiatic ester (PCL-g-DAPE) by on-line differential pressure viscometer and light scattering detectors. **N. Hamidi, F. Clemons**

10:20 PMSE 353. Two-in-One polymer multilayer coatings for prosthesis-related infections. **J. Min, R.D. Braatz, M. Spector, P.T. Hammond**

10:40 PMSE 354. Novel irreversibly degradable complex coacervate system. **H. Maune, B. Lin, F. Ibrahim, J. Chan, A. Engler, J. Hedrick, A. Nelson**

11:00 PMSE 355. Novel LbL nanoparticles for ovarian cancer therapy. **L.B. Mensah**

11:20 PMSE 356. Discovery of a novel polymer for human pluripotent stem cell expansion and multi-lineage differentiation. **A. Celiz, J. Smith, A. Patel, A. Hook, D. Rajamohan, V. George, M. Patel, V. Epa, T. Singh, R. Langer, D.G. Anderson, N. Allen, D. Hay, D. Winkler, D. Barrett, M. Davies, L. Young, C. Denning, M. Alexander**

Section B

Westin Boston Waterfront
Adams

Adhesion Science and Adhesive Materials

Interfacial Wetting

Financially supported by 3M Company, ExxonMobil Chemical Company

A. R. Fornof, *Organizer*

A. Crosby, R. Tripathy, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 PMSE 357. Contact mechanics of soft solids. **E. Dufresne**

9:25 PMSE 358. Foams made of gel like materials- stability over time and under shear. **C. Monteux, R. Deleurence, F. Lequeux, T. Saison**

10:00 Intermission.

10:15 PMSE 359. Withdrawn.

10:35 PMSE 360. Direct measurement of adhesion properties of different ligands on nanoparticles via radioanalytical techniques. **K. Davis, B. Qi, M. Witmer, C.L. Kitchens, B.A. Powell, O.T. Mefford**

10:55 PMSE 361. Modulating wet adhesive properties of polyelectrolyte multilayers. **C. Li, Y. Gu, N. Zacharia**

11:15 Concluding Remarks.

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

Section C

Westin Boston Waterfront
Douglas

Materials for Printed Electronics

Device Design, Function and Fabrication

Financially supported by The Dow Chemical Company

D. DeLongchamp, J. J. Watkins, *Organizers*

C. Gilmore, Y. Rao, *Organizers, Presiding*

8:30 PMSE 362. Materials for epidermal and water-soluble forms of flexible electronics. J.A. Rogers

9:00 PMSE 363. Thin and flexible organic electronic devices for wearable or implantable electronics. P. Zalar, T. Someya

9:30 PMSE 364. 3D printing of flexible electronics and sensors. J. Lewis

10:00 Intermission.

10:30 PMSE 365. Field-effect transistors based on room-temperature processed conjugated polymer/doped carbon nanotube composites for flexible electronics. K. Yu, K. Lee

10:50 PMSE 366. Polymers for all-printable field-effect chemical sensors and biosensors. H.E. Katz, K. Besar, X. Guo, W. Huang

11:10 PMSE 367. Parasitic capacitance effect on dynamic performance of printed sub-2 volt electrolyte-gated poly(3-hexylthiophene) transistors. F. Zare Bidoky, C.D. Frisbie

11:30 PMSE 368. Flexible macroporous polymer cages as spacer/spring elements for REWOD energy harvesting devices. A. Menner, Q. Jiang, A. Bismarck

Section D

Westin Boston Waterfront
Alcott

General Papers/New Concepts in Polymeric Materials

Biological and Biomedical Polymers

C. L. Soles, *Organizer, Presiding*

8:00 PMSE 369. Enzyme-triggered self-assembly of peptide-functionalized block copolymers. L. Adamiak, A. Luthi, C. LeGuyader, M. Hahn, N.C. Gianneschi

8:20 PMSE 370. SNAPping Gram-negative bacteria with star-shaped polypeptides. S. Lam, N. O'Brien-Simpson, N. Pantarat, A. Sulistio, E. Wong, Y. Chen, A. Blencowe, E. Reynolds, G. Qiao

8:40 PMSE 371. Self-assembled peptide amphiphile nanofibers and PEG composite hydrogels for tissue engineering and regenerative medicine. G. Cinar, M. Goktas, I. Orujalipoor, S. Ide, A. Tekinay, M.O. Guler

9:00 PMSE 372. Thin-film catalysts from enzymatically active polymer bioconjugates. A. Huang, G. Qin, B.D. Olsen

9:20 PMSE 373. Nanoparticle delivery of *Vibrio cholerae* communication signals. H. Lu, N. Weissmueller, A. Spiegel, A. Hurley, L. Perez, K. Maisel, L. Ensign, J. Hanes, B. Bassler, M.F. Semmelhack, R.K. Prudhomme

9:40 PMSE 374. Supramolecular polymer gel as an enteric elastomer for safe gastric devices. S. Zhang, J. Zhu, R.S. Langer, G. Traverso

10:00 Intermission.

10:20 PMSE 375. Hybrid liposomal polymeric nanoparticle delivery of combination chemo-, immuno-, and RNAi therapy for triple negative breast cancer. C. Scandore, R. Jadia, C. Tsiros, P. Rai, F. Ekiz

10:40 PMSE 376. Development of multifunctional DNA-based nanomaterials for biomedical applications. P. Lo, M. Chan, Z. Dai, D. Tam

11:00 PMSE 377. Comparative dynamics and sequence dependence of DNA and RNA binding to single walled carbon nanotubes. M. Landry, L. Vukovic, S. Kruss, G. Bisker, A. Landry, S. Islam, R. Jain, K. Schulten, M. Strano

11:20 PMSE 378. pH and thermal dual-responsive nanoparticles for controlled drug delivery with high loading content. Y. Zheng, L. Wang, B.C. Benicewicz

11:40 PMSE 379. Phospholipid polymer interfaces reveal activation dynamics of C-reactive protein. T. Goda, Y. Miyahara

Section E

Westin Boston Waterfront
Faneuil

Celebrating 50 Years of Polymer Science and Engineering

K. Carter, E. B. Coughlin, G. N. Tew, *Organizers*

T. Emrick, T. J. McCarthy, *Presiding*

8:00 PMSE 380. Stabilizing unique multilevel hierarchical structures using synthetic polymers and polymer hybrid materials. R. Kasi

8:30 PMSE 381. TissuGlu®: The first internal tissue adhesive approved for use in the United States. E.J. Beckman

9:00 PMSE 382. Molecular brush amphiphile. M. Herrera-Alonso

9:30 Intermission.

10:00 PMSE 383. Using basic polymer science to optimize morphology and performance of organic photovoltaics. T.P. Russell

10:30 PMSE 384. Nanostructure and material construction through peptide or block copolymer solution assembly. D.J. Pochan

11:00 PMSE 385. Illumination alters the assembly and conformation of conjugated polymers in solution. B. Morgan, M.D. Dadmun

WEDNESDAY AFTERNOON

Section A

Westin Boston Waterfront
Lewis

General Papers/New Concepts in Polymeric Materials

Membranes and Ion Containing Polymers

C. L. Soles, *Organizer, Presiding*

1:00 PMSE 386. Development of scattering model for characterization of water channel in diblock copolymer lamellar structure from small angle neutron scattering(SANS) and small angle X-ray scattering(SAXS). C. Jeong, C. Soles, T. Tsai, E.B. Coughlin

1:20 PMSE 387. Withdrawn.

1:40 PMSE 388. Composite sulfonated polyether ether ketone (SPEEK) proton exchange membranes for automotive fuel cells. J.R. Romeo, J.H. Doan, A. Vong, E.S. Smotkin

2:00 PMSE 389. Unveiling the morphology-dependent mechanical properties of a midblock-sulfonated pentablock ionomer. W. Zheng, D. Wang, C.J. Cornelius

2:20 PMSE 390. Simultaneous electronic and ionic conduction in ionic liquid imbedded conjugated polymer films.

A. Sreeram, S. Krishnan, S.J. DeLuca, M.C. Turk, D. Roy, E. Honarvarfar, P. Goulet

2:40 PMSE 391. Physical and transport properties of functionalized poly(phenylene)s, and their application in vanadium redox flow batteries. T. Largier, C.J. Cornelius

3:00 Intermission.

3:20 PMSE 392. Redox active polymer nanostructures for size-exclusion based transport in nonaqueous redox flow batteries. N. Gavvalapalli, E. Montoto, E. Chenard, K. Cheng, J. Hui, J. Rodriguez Lopez, J. Moore

3:40 PMSE 393. Effect of ionic side-chain length in a sulfonated polyphenylsulfone-based proton exchange membrane for fuel cell applications. B. Motealleh, C.J. Cornelius

4:00 PMSE 394. Pristine graphene stabilized emulsions as the basis for flexible conductive foams for oil and pressure sensing. S.J. Woltonist, D. Varghese, D. Massucci, A.V. Dobrynin, D.H. Adamson

4:20 PMSE 395. Design of PAMAM-COO dendron-grafted surfaces to promote Pb(II) ion adsorption. L. Chong, M. Dutt

4:40 PMSE 396. Design and synthesis of polymeric electrolytes for the development of nonaqueous flow batteries. E. Chenard, E. Montoto, K. Cheng, N. Gavvalapalli, J. Hui, J. Rodriguez Lopez, J. Moore

Section B

Westin Boston Waterfront
Adams

Adhesion Science and Adhesive Materials

Functional Chemistry and Design for Adhesion

Financially supported by 3M Company, ExxonMobil Chemical Company

A. Crosby, *Organizer*

A. R. Fornof, R. Tripathy, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 PMSE 397. Sticking with adhesives: From nucleobase-containing ABC triblock acrylic copolymer elastomers to phosphonium- and sulfonamide-containing adhesives. K. Zhang, C. Jangu, A. Schultz, T.E. Long

2:25 PMSE 398. Form follows function: Rethinking optically clear adhesives. C. Campbell

3:00 Intermission.

3:15 PMSE 399. Using dynamic chemistry as a route to shape-memory, photoreversible adhesives. S.J. Rowan, B.T. Michal

3:50 PMSE 400. TAPE: A plant-derived medical adhesive as an effective hemostatic material as well as a pH-sensitive patch in vivo. S. Hong, K. Kim, H. Lee

4:10 PMSE 401. Functionalization of polyurethane particles for controlled interactions with different substrate. L. Breucker, K. Landfester, A. Taden

4:30 PMSE 402. Catechol-based monomers containing electron withdrawing substituents for improving interfacial adhesion. B.R. Donovan, J. Cobb, L. Kendrick, D.L. Patton

4:50 Concluding Remarks.

Section C

Westin Boston Waterfront
Douglas

General Papers/New Concepts in Polymeric Materials

Advances in Polymer Synthesis and Processing

C. L. Soles, *Organizer, Presiding*

1:00 PMSE 403. Synthesis and characterization of a supramolecular thermoplastic elastomer. L. Voorhaar, M. Diaz, F. Leroux, A. Abakumov, G. Van Assche, B. Van Mele, R. Hoogenboom

1:20 PMSE 404. Preparation and characterization of copolymer containing cadmium. Y. Jiang, L. Sha, Q. Liu, H. Zhang

1:40 PMSE 405. Preparation and characterization of amphiphilic polymer metal complexes with cadmium. H. Zhang, L. Yang, F. Zhang, J. Chang, Y. Jiang

2:00 PMSE 406. Cross-linked main-chain polybenzoxazine nanofibers by electrospinning. Y. Ertaş, T. Uyar

2:20 PMSE 407. Introducing metal-containing monomers in emulsion polymerization for the preparation of smart stimuli-responsive polymeric opal structures. D. Scheid, M. Gallei

2:40 PMSE 408. Continuous processing of polyamides with superheated water. G.C. Evans, A.J. Lesser

3:00 Intermission.

3:20 PMSE 409. Chemical vapor deposition of 2D polymeric carbon nitride. J. Therrien, D.F. Schmidt, Y. Li

3:40 PMSE 410. Utilizing electron transfer mechanism of chlorophyll A under visible light for living polymerization. C. Boyer, S. Shanmugam, J. Xu

4:00 PMSE 411. Investigation of dose rate effects in electron-beam initiated polymerization. S.M. Schissel, S.C. Lapin, J.L. Jessop

4:20 PMSE 412. Synthesis and photophysical properties of triblock copolymer-carbon nanotube hybrid materials functionalized with ruthenium complex photosensitizers. W.K. Chan, H. Shi, L. Du, D.L. Phillips

4:40 PMSE 413. Photopolymerized thiol-ene networks made from natural products. J.R. Davidson, R. Reit, B.R. Lund, W. Voit, R. Saldone

Section D

Westin Boston Waterfront
Alcott

General Papers/New Concepts in Polymeric Materials

Fundamentals of Polymers

C. L. Soles, *Organizer, Presiding*

1:00 PMSE 414. Stimuli responsive elastomer based hybrids with tunable multifunctionality. S. Zeng, W. Huang, H. Nguon, A.T. Smith, L. Sun

1:20 PMSE 415. Multiresponsive surface via wrinkling. S. Zeng, W. Huang, H. Nguon, A.T. Smith, L. Sun

1:40 PMSE 416. Withdrawn.

2:00 PMSE 417. Facile fabrication of hyperbranched polymer nanoparticles via nonemulsion polymerization. C. Hyun, H. Jeong, Y. Jiang, B. An

2:20 PMSE 418. Designing of polymeric microstructures using a dynamic reaction-diffusion process. T. Shim, S. Yang, S. Kim

2:40 **PMSE 419.** Micelle-based multifunctional catalytic systems for tandem reactions. J. Lu, J. Dimroth, M. Weck

3:00 Intermission.

3:20 **PMSE 420.** Withdrawn.

3:40 **PMSE 421.** Using sulfur as reinforcing agent in thermoplastic composites. S. Al Hassan

4:00 **PMSE 422.** Study of the properties and application of a polysulfone based diblock copolymer. W. Khan, D. Wang, C.J. Cornelius

4:20 **PMSE 423.** Engineering biorenewable source based polymeric materials for environmental remediation: Hexavalent chromium removal and mechanism study. S. Wei, B. Qiu, X. Zhang, H. Wei, Z. Guo

4:40 **PMSE 424.** Rheology of a high-performance biodegradable epoxy for use in composite resin infusion. J. Moeller, E. Reynaud, D.F. Schmidt

5:00 **PMSE 425.** Production of bacterial nanocellulose-based tubes for biomedical application. F. Hong, J. Tang, L. Bao, L. Chen

Section E

Westin Boston Waterfront
Faneuil

Celebrating 50 Years of Polymer Science and Engineering

T. Emrick, G. N. Tew, *Organizers*

E. B. Coughlin, *Organizer, Presiding*

T. J. McCarthy, *Presiding*

1:00 **PMSE 426.** Swelling-induced curling of elastic fibers wet by elastocapillary rise. D. Holmes

1:30 **PMSE 427.** Conjugated polymers: How did the UMSS experience lead us to where we are today? J.R. Reynolds

2:00 **PMSE 428.** Surface wrinkling metrology for soft materials. C.M. Stafford

2:30 Intermission.

3:00 **PMSE 429.** Electronic and optical devices via additive driven self-assembly and nanoimprint lithography: Toward solution-based R2R nanomanufacturing. J.J. Watkins

3:30 **PMSE 430.** Absence of density anomalies as a structural principle for semicrystalline polymers: The Importance of chain ends and chain tilt. K. Schmidt-Rohr, K. Fritzsche, K. Mao, A. Bosse

4:00 **PMSE 431.** Seeing the light at UMSS and beyond. Y.C. Simon

4:30 **PMSE 432.** Evolution of polymer science — a personal perspective. K.I. Winey

Polymer Concepts in Inorganic Chemistry Courses

Sponsored by CHED, Cosponsored by INOR, PMSE and POLY

Technical program information known at press time.

The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015

WEDNESDAY EVENING

Section A

Westin Boston Waterfront
Grand Blrm A/B

Joint PMSE/POLY Awards Reception and Plenary Lecture

Cosponsored by POLY†

C. L. Soles, *Organizer, Presiding*

5:30 **PMSE 433.** Polymers for optical technologies utilizing linear susceptibility. S.Z. Cheng, F.W. Harris

THURSDAY MORNING

Section A

Westin Boston Waterfront
Lewis

General Papers/New Concepts in Polymeric Materials

Polymer Thin Films, Interfaces, and Fibers

C. L. Soles, *Organizer, Presiding*

8:00 **PMSE 434.** Multilayer nanocoating incorporating aluminum hydroxide nanoparticles extinguishes flame on polyurethane foam. M.M. Haile, S. Fomete, I. Lopez, M. Leistner, J.C. Grunlan

8:20 **PMSE 435.** UV-nanoimprint lithography as a tool to develop flexible microfluidics for electrochemical detection. J. Chen, Y. Zhou, D. Wang, V.M. Rotello, K.R. Carter, J.J. Watkins, S.R. Nugen

8:40 **PMSE 436.** Functionalized nanoporous polymers containing sterically crowded comonomers. J. Huang, S.R. Turner

9:00 **PMSE 437.** Interfacial crosslinking reaction of catecholamine at air/water interface forming a free-standing, Janus-faced microfilms. S. Hong, Y. Wang, H. Lee

9:20 **PMSE 438.** Antimicrobial/Antifouling polycarbonate coatings: Role of block copolymer architecture, compositions and coating structure. D. Voo, M. Khan, J. Hedrick, Y. Yang

9:40 **PMSE 439.** Novel resistive volatile organic compound (VOC) sensor based on a composite structure of vertically aligned carbon nanotubes and oCVD/iCVD polymer films. X. Wang, A. Ugur, N. Chen, H. Goktas, N. Lachman, B.L. Wardle, K. Gleason

10:00 Intermission.

10:20 **PMSE 440.** Crystallization behavior of poly(butane adipate) confined in electrospun fibers. Y. Song, H. Ye, G. Lu, Q. Zhou

10:40 **PMSE 441.** Multiple responsive polyelectrolyte films prepared by layer by layer assembly. X. Hu, S.W. Thomas

11:00 **PMSE 442.** Thick growing multilayer nanobrick wall thin films: Super gas barrier with very few layers. T. Guin, J.C. Grunlan

11:20 **PMSE 443.** Boron nitride coated polymer films by interface trapping with improved barrier and dielectric properties. Z. Cui, Z. Cao, R. Ma, A.V. Dobrynin, D.H. Adamson

11:40 **PMSE 444.** Self-replenishing infused polymers as fouling-release surfaces. C. Howell, T.L. Vu, J. Lin, J. Alvarenga, J.C. Weaver, J. Aizenberg

Section B

Westin Boston Waterfront
Adams

Adhesion Science and Adhesive Materials

Bio-Inspired Adhesion

Financially supported by 3M Company, ExxonMobil Chemical Company

A. Crosby, *Organizer*

A. R. Fornof, R. Tripathy, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 **PMSE 445.** Defining the role of chemistry in the wet bioadhesion of mussels. H. Waite

9:25 **PMSE 446.** Role of water in adhesion and friction. A.N. Dhinojwala

10:00 Intermission.

10:15 **PMSE 447.** Developing new adhesive designs and capabilities from the biomimicry of pollen. J.C. Meredith, H. Lin, D. Shin

10:50 **PMSE 448.** Trying to be as smart as a shellfish: Understanding and copying natural adhesive. E. Alberts, C. Del Grosso, N. Hamada, C. Jenkins, M.L. Johnston, H. Meredith, M. North, J. Roman, J.J. Wilker

11:10 **PMSE 449.** Exploring bio-inspired adhesives via pendent catechols on maleimide-acrylate copolymers toward improved adhesion. M.A. Bartucci, J.A. Orlicki

11:30 **PMSE 450.** Bioinspired metal-coordination: Using more of nature's tricks to assemble multifunctional adhesive polymer materials. N. Holten-Andersen

11:50 Concluding Remarks.

Section C

Westin Boston Waterfront
Douglas

General Papers/New Concepts in Polymeric Materials

Semiconducting and Electronic Polymers

C. L. Soles, *Organizer, Presiding*

8:00 **PMSE 451.** Poly(vinyl carbonate sulfone)s with tunable thermal depolymerization for transient electronic packaging. O.P. Lee, H. Lopez Hernandez, N.R. Sottos, S. White, J.S. Moore

8:20 **PMSE 452.** Experimental and theoretical structure/property studies: Donor-acceptor polymers synthesized via acyclic diene metathesis. G. Singh, R.M. Peetz

8:40 **PMSE 453.** Synthesis and characterization of POSS-ProDOT₈ cross-linked PEDOT films. B. Wei, J. Liu, L. Ouyang, N.S. Bhagwat, D.C. Martin

9:00 **PMSE 454.** Hydrogen assisted growth of conducting polymer microstructures for supercapacitors. K.P. Diaz Orellana, M.E. Roberts

9:20 **PMSE 455.** New highly-emissive soluble dynamic Eu(III) coordination polymers for Ln(III) and transition metal sensing applications. A. Duerrbeck, A.T. Hor, N.J. Long

9:40 **PMSE 456.** Polypropylene dielectric nanocomposites with matrix compatible fillers containing anthracene. M. Mohammadkhani, T. Krentz, M.H. Bell, L. Schadler, B.C. Benicewicz, H. Hillborg, S. Zhao

10:00 Intermission.

10:20 **PMSE 457.** Hybrid TEOS-TIP-penta block copolymer composite membranes: Morphology, physical properties, and liquid transport. F. Huang, C.J. Cornelius

10:40 **PMSE 458.** High performance polymer supercapacitors utilizing electroactive polymers and CNT: From the concept of science to the prototypes of engineering. Y. Kim, J. Jung, S. Besic, M. Birschbach, V. Ebron, P.J. Kinlen, R. Mercado, H. Nguyen

11:00 **PMSE 459.** Design of assemblies based on polymer-coated quantum dots and organic dye. A. Machado, I. Moura, A.S. Abreu

11:20 **PMSE 460.** Random terpolymer, regular terpolymer, and ternary blend for polymer solar cells: A comparative study. Q. Zhang, M.A. Kelly, A. Hunt, W. You, H. Ade

11:40 **PMSE 461.** Odd-even effect of linear alkyl side-chains on BTTT monomers. E. Burnett, B.P. Cherniawski, S.P. Gido, A.L. Briseno

Section D

Westin Boston Waterfront
Alcott

General Papers/New Concepts in Polymeric Materials

Nanostructured and Porous Polymers

C. L. Soles, *Organizer, Presiding*

8:00 **PMSE 462.** Multicolor micropatterning of inverse opals by anisotropic thermal deformation. J. Lee, S. Kim

8:20 **PMSE 463.** Catalytic coatings of cytochrome P450-polymer diblock copolymers. A. Obermeyer, N. Colant, B.D. Olsen

8:40 **PMSE 464.** Self-assembly of nanostructured materials through irreversible covalent bond formation and their application. G. Yun, K. Kim

9:00 **PMSE 465.** Bridged silsesquioxane aerogels: A novel precursor, simple drying method and tunable properties. Z. Ning, Z. Wang, J. Xu

9:20 **PMSE 466.** Crystalline-driven self-assembly of biocompatible block copolymers. G. Cambridge, A. Pitto-Barry, R. O'Reilly

9:40 Intermission.

10:00 **PMSE 467.** Direct mapping of local director field of nematic liquid crystals at the nanoscale. Y. Xia, F. Serra, S. Yang

10:20 **PMSE 468.** Effects of processing parameters on jet diameter profiles during the electrospinning of poly(N-isopropylacrylamide) solutions. Y. Wang, C. Wang

10:40 **PMSE 469.** Removal of organic solvents from aqueous waste mixtures by novel covalent organic frameworks. M. Ullasan, S. Filikci, M. Citir, M.S. Yavuz

11:00 **PMSE 470.** Growth of 2D covalent organic framework thin films in flow. R.P. Bisbey, W. Dichtel

11:20 **PMSE 471.** Nanoscale friction of uniaxially stretched polymer films. X. Xu, R. Jin, D.F. Schmidt, E. Reynaud, M. Ruths

11:40 **PMSE 472.** Porous covalent organic frameworks made from polycyclic aromatic hydrocarbons. R. Smaidone, C.M. Thompson, G.T. McCandless, S.B. Alahakoon

Section E

Westin Boston Waterfront
Faneuil

General Papers/New Concepts in Polymeric Materials

Nanoparticles and Filled Polymers

C. L. Soles, *Organizer, Presiding*

8:00 PMSE 473. Preparation, cyclization, and pyrolysis of poly(methyl vinyl ketone) as a carbon fiber precursor polymer. J.W. Krumpfer, M. Klapper, A. Müller, M. Buchmeiser, K. Muellen

8:20 PMSE 474. Modular synthesis of functional polymer nanoparticles from poly(pentafluorophenyl methacrylate). Y. Lee, J. Lim, P. Theato, J. Pyun, K. Char

8:40 PMSE 475. Effects of polymer-grafted silica nanoparticles on the volume shrinkage and mechanical properties of cured vinyl ester resins. Y. Huang, W. Chung, M. Chung, J. Huang, Y. Lin

9:00 PMSE 476. Stimuli responsive polymer composites based on triggered release of inorganic fillers. B.M. Mosby, S. Shah, S. White, N.R. Sottos, P.V. Braun

9:20 PMSE 477. Withdrawn.

9:40 PMSE 478. Measuring temperature change on photothermal Au nanorod and nanocage upon laser irradiation. H. Cavusoglu, H. Sakalak, B. Buyukbekar, G. Demirel, M. Citir, M. Yavuz

10:00 Intermission.

10:20 PMSE 479. Functional magnetic nanoprobes: Novel nanotheranostics for the treatment of prostate carcinomas. D. Thompson, B. Heckert, S. Sulthana, S. Santra

10:40 PMSE 480. Exfoliated boron nitride polymer composites by a solvent trapping technique. C. Chapman, Z. Cui, A.V. Dobrynin, D.H. Adamson

11:00 PMSE 481. Cellulose nanocrystal-polyamide 6 nanocomposites with improved creep resistance prepared via in-situ polymerization. S. Kashani Rahimi, J. Otaigbe

11:20 PMSE 482. Redox polymer/carbon fiber hybrids for electrochemically responsive heterogeneous catalysis. X. Mao, W. Tian, J. Wu, G.C. Rutledge, T. Hatton

11:40 PMSE 483. Mechanical, morphological, and rheological properties of PBS/silica nanocomposites manufactured using a high-speed twin-screw compounder. X. Chen, M.J. Sobkowitz

THURSDAY AFTERNOON

Section A

Westin Boston Waterfront
Lewis

General Papers/New Concepts in Polymeric Materials

Fundamentals of Polymers

C. L. Soles, *Organizer, Presiding*

1:00 PMSE 484. High performance copoly(ester-imide)s. S. Jones, S. Meehan, S. Sankey, W. MacDonald, H. Colquhoun

1:20 PMSE 485. Rational design of covalent organic frameworks with triangular topology. S. Dalapati, D. Jiang

1:40 PMSE 486. Fast and accurate study of dynamical mechanical properties of polymers at the nanoscale. I. Sokolov, M. Dokukin

2:00 PMSE 487. Facile synthesis of nucleic acid-polymer amphiphiles and their self-assembly. F. Jia, X. Lu, X. Tan, K. Zhang

2:20 PMSE 488. Preparation and characterization of fully furan-based renewable thermosetting epoxy-amine systems. F. Hu, S. Yadav, J. La Scala, J.M. Sadler, G. Palmese

2:40 PMSE 489. Nanocapsules filled with reactive liquid amines for self-healing thermoset polymers. Y. Liu, B.M. Budhllal

3:00 Intermission.

3:20 PMSE 490. Modulating the thermal degradation of poly(vinyl *tert*-butyl carbonate sulfone) by small molecule additive. C. Possanza, O.P. Lee, H. Lopez Hernandez, N.R. Sottos, S. White, J.S. Moore

3:40 PMSE 491. Maintaining hand and improving fire resistance of cotton fabric through ultrasonication rinsing of multilayer nanocoating. T. Guin, A. Milhorn, J.C. Grunlan

4:00 PMSE 492. Techniques to improve adhesion between Kevlar fiber and rubber matrix using supercritical carbon dioxide. N. Kanbargi, A.J. Lesser

4:20 PMSE 493. Realizing reworkability in high performance thermosets for wind energy. W. Liu, E. Reynaud, D.F. Schmidt

4:40 PMSE 494. Thermal analyses of blends of poly(ethyl methacrylate) and cellulose acetate butyrate and their corresponding ternary hybrids in presence of a bentonite. S. Djadoun, K. Ouad, S. Kadi, T. Aouak, M. Ouladsmame

Section B

Westin Boston Waterfront
Adams

Adhesion Science and Adhesive Materials

Anti-Adhesion

Financially supported by 3M Company, ExxonMobil Chemical Company
A. Crosby, *Organizer*

A. R. Fornof, R. Tripathy, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 PMSE 495. Everything SLIPS: Anti-adhesive properties of liquid-infused surfaces. J. Aizenberg, P. Kim, T. Wong

2:25 PMSE 496. Stimulus-responsive superoleophobic polymer brushes showing excellent oil drop motion and low adhesion properties underwater. G. Dunderdale, M. England, C. Urata, A. Hozumi

2:45 Intermission.

3:00 PMSE 497. Mechanism-based approach to reduce biological adhesion. C. Del Grosso, T. McCarthy, C. Clark, J. Cloud, J.J. Wilker

3:20 PMSE 498. Effects of different kinds of curing agents on the surface properties of epoxy resin. Y. Jiang, C. Yu, A. Wei

3:40 Concluding Remarks.

Section C

Westin Boston Waterfront
Douglas

General Papers/New Concepts in Polymeric Materials

Fundamentals of Polymers

C. L. Soles, *Organizer, Presiding*

1:00 PMSE 499. Shedding light on new benefits. B. Tylkowski, M. Giambertini, S. Fernandez Prieto, J. Smets, T. Underiner

1:20 PMSE 500. Characterization of MgO-HA-PLLA nanocomposites as antibacterial scaffolds for orthopedic tissue engineering applications. D.J. Hickey, T. Webster

1:40 PMSE 501. Nonsmall-cell-lung-cancer treatment using Hsp90 inhibitor carrying magnetic nanotheranostics. J. Kallu, B. Heckert, S. Sulthana, S. Santra

2:00 PMSE 502. Light-responsive nucleic acid-drug nanostructures. X. Tan, B. Li, X. Lu, F. Jia, C. Santori, P. Menon, B. Zhang, H. Li, J. Zhao, K. Zhang

2:20 PMSE 503. DNA polymer amphiphiles as mRNA regulation agents: Properties and applications. S. Barnhill

2:40 PMSE 504. Turning bacteria's defense mechanism against them: Toward beta-lactamase-triggered release of antibiotics. Z.M. Hudson, A. McGrath, C.J. Hawker, D. Klinger

PROF

Division of Professional Relations

R. D. Libby, *Program Chair*

SOCIAL EVENTS:

Henry Hill Reception, 5:00 PM: Tuesday

PROF-LGBT Reception, 6:00 PM: Tuesday

BUSINESS MEETINGS:

Business Meeting, 2:00 PM: Tuesday

SUNDAY MORNING

National Science Foundation's Centers for Chemical Innovation

Sponsored by PRES, Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB

Opportunities for US/Cuba Collaboration in Chemistry, Chemical Engineering and Chemistry Education

Sponsored by IAC, Cosponsored by COMSCL and PROF

SUNDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 210C

Professional Legacy of Henry Hill

Cosponsored by CEPA, CMA, ETHC, HIST†, ORGN, PMSE, POLY†, PRES and SCHB†

E. A. Nalley, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 PROF 1. Division of Professional Relations Henry Hill Award: A Tribute to the Memory of Henry Hill. E.A. Nalley

2:00 PROF 2. Henry Hill, one of the founding fathers of professionalism. A.E. Pavlath

2:25 PROF 3. Continuing the legacy of Henry Hill: Through service to the profession and to industry. W. Carroll, Jr.

2:50 Intermission.

3:00 PROF 4. Facets of professionalism: Writing and editing. M. Orna

3:25 PROF 5. Howard Peters 2007, Henry Hill Awardee: Chemist2Lawyer2. H.M. Peters, S.B. Peters

3:50 PROF 6. The ACS Minority Scholars Program: How far we've come since the 1970's and the road ahead. J.D. Burke

4:15 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CIN†, COLL, ENFL, PROF and SOCED

National Science Foundation's Centers for Chemical Innovation

Sponsored by PRES, Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB

True Stories from Entrepreneurs: BRIC Edition

Sponsored by SCHB, Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 51

Getting Your First Industrial Job

Cosponsored by YCC†

N. A. LaFranzo, *Organizer*

A. C. Myers, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 PROF 7. Find the trampoline, avoid the black holes. K.C. Glasgow

8:55 PROF 8. Finding the career that fits: My life away from the bench. N.A. LaFranzo

9:15 PROF 9. Landing your first industrial position: The ACS Career Navigator as a competitive advantage. S.R. Meyers, B.D. Tweedy, M. Layazali

9:35 PROF 10. Alternate careers for chemists in sales and management. J.P. Stoner

9:55 Intermission.

10:05 PROF 11. Start-ups and research parks: Springboards to your chemical career. A.C. Myers

10:25 PROF 12. Uniqueness of working in a small business... or starting one. B.J. Streusand

10:45 PROF 13. Industry opportunities for the new graduate and a recruiter's perspective. K.M. Allen

11:05 Panel Discussion.

11:25 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CHED, CIN†, COLL, ENFL, PROF and SOCED

ACS Scholars: Rising Stars in Academe

Sponsored by PRES, Cosponsored by AGRO, CARB, CMA, COLL, ENFL, ENVF, PROF, SCHB and YCC

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits

Sponsored by CHED, Cosponsored by BMGT, CEI, ENVF, I&EC, MEDI, PROF, SCHB and YCC

The Chemistry Enterprise in 2015

Sponsored by BMGT, Cosponsored by PRES and PROF

Managing Transitions

Sponsored by WCC, Cosponsored by PROF

Memories of Henry Hill: His Legacy in Science and in Professional Service

Sponsored by HIST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES†, PROF and SCHB

True Stories from Entrepreneurs: BRIC Edition

Sponsored by SCHB, Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais

Sponsored by YCC, Cosponsored by CHED, IAC, PRES and PROF

MONDAY AFTERNOON**Section A**

Boston Convention & Exhibition Center
Room 51

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 Company Presentations.

3:00 Investment Discussion.

3:30 Open Forum.

4:00 Concluding Remarks.

ACS Scholars: Rising Stars in Industry

Sponsored by PRES, Cosponsored by AGRO, CARB, CMA†, COLL, ENFL, ENVR, PROF, SCHB and YCC

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector

Sponsored by SCHB, Cosponsored by CMA, COLL, HIST, I&EC, POLY, PRES and PROF

Leadership Skills as a Strategic Advantage: the Chemist's Competitive Edge

Sponsored by BMGT, Cosponsored by CEPA, PRES‡, PROF and YCC

Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais

Sponsored by YCC, Cosponsored by CHED, IAC, PRES and PROF

TUESDAY MORNING**Section A**

Boston Convention & Exhibition Center
Room 51

Checklist for Turning Thirty

Cosponsored by YCC‡

Financially supported by ACS Board of Trustees, Group Insurance Plans for ACS Members

J. A. Parr, *Organizer*

D. Chamot, *Presiding*

8:30 Introductory Remarks.

8:40 PROF 15. Career tune-up.
L.M. Balbes, L.B. Roberson

9:15 PROF 16. Work-life balance. B.W. Parks

9:35 PROF 17. Maximizing your volunteer experience. D.B. Hausner

9:55 Intermission.

10:10 PROF 18. Smart money moves in your 20's and 30's. S. Toscano

11:15 PROF 19. Finding the right insurance plan for your stage in life. K. Williams

11:30 Panel Discussion.

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Sponsored by POLY, Cosponsored by HIST, PMSE‡, PRES and PROF‡

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES‡, PROF and SCHB

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

Transforming University-Industry Partnerships for an Innovative Future**Envisioning, Enabling and Executing**

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

TUESDAY AFTERNOON**Section A**

Boston Convention & Exhibition Center
Room 51

Women in Innovation: Business and Commerce

Cosponsored by BMGT, SCHB, WCC and YCC

J. L. Bryant, *Organizer*

J. C. Giordan, *Organizer, Presiding*

1:30 PROF 20. Innovating women, business and commerce: Opening overview. J.C. Giordan

1:45 PROF 21. Innovating women, business and commerce: Moderated panel presentations and questions and answers.
D. Mason, J.C. Giordan, J.L. Bryant

2:45 Discussion.

3:45 Concluding Remarks.

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES‡, PROF and SCHB

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Sponsored by POLY, Cosponsored by HIST, PMSE‡, PRES and PROF‡

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Sponsored by SCHB, Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

Transforming University-Industry Partnerships for an Innovative Future**Energizing and Education**

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

RUBB**Rubber Division**

D. Ruch, *Program Chair*

MONDAY EVENING**From Raw to Varoom: The Science Behind Getting a Car on the Road**

Sponsored by CHED, Cosponsored by PMSE, POLY‡, RUBB and SCC‡

SCHB**Division of Small Chemical Businesses**

J. Sabol, *Program Chair*

OTHER SYMPOSIA OF INTEREST:**The Chemistry Enterprise in 2015 (see BMGT, Monday)**

Innovations in Analytical Chemistry and Their Application to National Security and Forensics (CBRNE) (see ANYL, Tuesday, Wednesday)

The Debate: How Do We Respond to Climate Change (see ENVR, Tuesday)

Innovative Platforms for Drug Discovery, Diagnostics & Target Validation (see BIOL, Tuesday)

Chemical Information Skills: The Essential Toolkit for Chemical Research (see CINP, Wednesday)

SOCIAL EVENTS:

Breakfast, 7:00 AM: Sunday

Luncheon, 11:45 PM: Sunday, Monday, Tuesday

Cannabis Chemistry Committee Social Hour, 3:00 PM: Tuesday

Henry Hill Reception, 5:00 PM: Tuesday

BUSINESS MEETINGS:

SCHB Division Executive Committee Meeting, 8:00 AM: Sunday

National Science Foundation's Centers for Chemical Innovation

Sponsored by PRES, Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB

SUNDAY AFTERNOON**Section A**

Westin Boston Waterfront
Webster

True Stories from Entrepreneurs: BRIC Edition

Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

Financially supported by Osha Liang, LLP
M. Chorghade, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 SCHB 6. The GelTex story. W. Mandeville

1:35 SCHB 7. Understanding, optimizing, and harnessing amphotericin B. M. Burke

2:05 SCHB 8. Engineering catalysts not just for chemical transformations but for building businesses BRIC by BRICK. G.D. Yadav

2:35 Intermission.

2:55 SCHB 9. Public private partnership: Recipe for discoveries. S.V. Malhotra

3:25 SCHB 10. Generating effective diagnostic technology for the developing world. G.M. Whitesides

3:55 SCHB 11. Withdrawn.

4:25 SCHB 12. Expanding chemistry frontiers: Efficient air-stable catalysts for aqueous chemistry water and chemosynthesis using "synthetic livers". A. Mehta, M. Chorghade

4:55 Concluding Remarks.

National Science Foundation's Centers for Chemical Innovation

Sponsored by PRES, Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB

Professional Legacy of Henry Hill

Sponsored by PROF, Cosponsored by CEPA, CMA, ETHC, HIST‡, ORGN, PMSE, POLY‡, PRES and SCHB‡

MONDAY MORNING**Section A**

Westin Boston Waterfront
Webster

True Stories from Entrepreneurs: BRIC Edition

Cosponsored by CARB, COLL, I&EC, IAC, PRES and PROF

Financially supported by Osha Liang, LLP
M. Chorghade, *Organizer, Presiding*

8:00 Networking.

8:30 Introductory Remarks.

8:35 SCHB 13. Chemical sensors: An ideal application for organic electronics. T.M. Swager

9:05 SCHB 14. Chemical management for safe, secure, and environmentally sound chemical facilities. N.B. Jackson

9:35 SCHB 15. Chemosynthetic livers: Predict, prepare, and prove the structure, activity, and toxicity of drug metabolites. M. Chorghade, R. Chorghade

10:05 Intermission.

10:25 SCHB 16. Perspectives on the science, technology, and innovation ecosystem as drivers of economic growth in BRIC countries. J. Margolis, S. Howerton, D. MacDonald

10:55 SCHB 17. Olefin metathesis chemistry as a catalyst for building businesses BRIC by BRIC. R.H. Grubbs

11:25 SCHB 18. Reverse pharmacology and systems approaches for chemical biology, drug discovery, and development: Inspiration from the wisdom of Mother Nature. M. Chorghade, R. Chorghade

11:55 Concluding Remarks.

ACS Scholars: Rising Stars in Academe

Sponsored by PRES, Cosponsored by AGRO, CARB, CMA†, COLL, ENFL, ENVR, PROF, SCHB and YCC

Memories of Henry Hill: His Legacy in Science and in Professional Service

Sponsored by HIST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES†, PROF and SCHB

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits

Sponsored by CHED, Cosponsored by BMGT, CEI, ENVR, I&EC, MEDI, PROF, SCHB and YCC

MONDAY AFTERNOON

Section A

Westin Boston Waterfront
Webster

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector

Cosponsored by CMA, COLL, HIST, I&EC, POLY, PRES and PROF

P. C. Kearney, *Organizer*

J. E. Sabol, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 SCHB 19. Antifouling marine and medical technology. M. Grunlan

1:50 SCHB 20. Olefin metathesis for commercial development of polymers on a commercial scale. R.H. Grubbs

2:20 SCHB 21. Polymer chemistry innovations from an academic start-up to where it is going. B. Gordon

2:50 Intermission.

3:10 SCHB 22. Organic growth of a polymer analysis business. J. Rancourt

3:40 SCHB 23. From university to reality. G.M. Whitesides

4:10 SCHB 24. Discovery and development of Renagel and WelChol. W. Mandeville

4:40 Concluding Remarks.

ACS Scholars: Rising Stars in Industry

Sponsored by PRES, Cosponsored by AGRO, CARB, CMA, COLL, ENFL, ENVR, PROF, SCHB and YCC

Chemical Angel Network: Chemists Investing in Chemical Companies

Sponsored by PROF, Cosponsored by SCHB

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Hall C

Sci-Mix

J. E. Sabol, *Organizer*

8:00 - 10:00

1-4. See previous listings.

Chemical Innovation and Design (CID) Talks: The Future of Innovation Now

Sponsored by MPPG, Cosponsored by AGFD, AGRO, BIOT, MEDI, PMSE and SCHB

TUESDAY MORNING

Section A

Westin Boston Waterfront
Webster

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

J. J. O'Neil, *Organizer*

P. C. Kearney, *Organizer, Presiding*

8:00 Networking.

8:30 Introductory Remarks.

8:35 SCHB 25. Delivery to biotech: Alkermes' and Transform's stories. J.F. Remenar

9:05 SCHB 26. Withdrawn.

9:35 SCHB 27. Calculario: The spin out process for an advanced organic materials computational discovery startup. A. Aspuru-Guzik, R. Gomez-Bombarelli, J. Aguilera-Iparaguire, T. Hirzel

10:05 Intermission.

10:25 SCHB 28. Catabasis: A biotech start up based on an innovative chemistry platform. M. Jirousek

10:55 SCHB 29. Career transitions in a rapidly evolving industry: Large company, small company, consulting, and virtual company. M.J. Tebbe

11:25 SCHB 30. Making molecular prosthetics with a small molecule synthesizer. M.D. Burke

11:55 Concluding Remarks.

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES†, PROF and SCHB

Transforming University-Industry Partnerships for an Innovative Future: Envisioning, Enabling and Executing

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

GMOs and the Entanglement of Intellectual Property Rights

Sponsored by AGRO, Cosponsored by CHAL, ENVR and SCHB

TUESDAY AFTERNOON

Section A

Westin Boston Waterfront
Webster

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry

Cosponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

P. C. Kearney, *Organizer*

J. J. O'Neil, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 SCHB 31. Intelligipigment™ hydrogen detection technology. N. Mohajeri

1:50 SCHB 32. Post start-up science: Weathering the seas of change. C.L. Campion

2:20 SCHB 33. Safer, high-performance electrolytes for next-generation lithium-ion batteries. R.J. Hamers, M.L. Usrey, A. Pena-Hueso, S. Guillot, R.C. West, M. Pollina

2:50 Intermission.

3:10 SCHB 34. YANACO: Yet another nano company, a lean start-up concept for chemicals and materials. R.N. Grass

3:40 SCHB 35. Building a microscale future at HD Sciences through high capacity magnetic nanoparticles for compound synthesis. P.C. Kearney

4:10 Concluding Remarks.

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace

Sponsored by IAC, Cosponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES†, PROF and SCHB

Transforming University-Industry Partnerships for an Innovative Future: Energizing and Education

Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MEDI, PROF and SCHB

Women in Innovation: Business and Commerce

Sponsored by PROF, Cosponsored by BMGT, SCHB, WCC and YCC

Immunochemistry Summit XII: Immunoassays and Other Bioanalytical Techniques

Sponsored by AGRO, Cosponsored by ANYL, ENVR and SCHB

WEDNESDAY MORNING

Section A

Westin Boston Waterfront
Webster

Big Chemistry from Small Businesses

Cosponsored by COLL, I&EC, PRES and PROF

J. H. Lauterbach, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 SCHB 36. XploSafe's technologies for a safer world. A.W. Applett, N.F. Materer

9:05 SCHB 37. Efforts to commercialize light and pH activated ruthenium anticancer compounds. E.T. Papish, D.L. Gerlach, S.E. Brown, J.J. Paul, E.J. Merino

9:35 SCHB 38. Sterically protected and electronically activated azamacrocyclic catalysts for lignin depolymerization: A new approach to biomass valorization. M. Chorghade

10:05 SCHB 39. Chemistry and toxicology of e-cigarettes and e-liquids. J.H. Lauterbach

10:35 Concluding Remarks.

CCS

Committee on Chemical Safety

E. Howson, *Program Chair*

SUNDAY AFTERNOON

Lab Safety 25 Years After Promulgation of the OSHA Laboratory Standard

Sponsored by CHAS, Cosponsored by CCS

MONDAY MORNING

Lab Safety 25 Years After Promulgation of the OSHA Laboratory Standard

Sponsored by CHAS, Cosponsored by CCS

MONDAY AFTERNOON

Chemical Health & Safety Awards

Sponsored by CHAS, Cosponsored by CCS

TUESDAY MORNING

Current Topics in Chemical Safety Information

Use Cases for Chemical Safety Information

Sponsored by CHAS, Cosponsored by AGFD, CCS, CHED and CINF†

TUESDAY AFTERNOON

Current Topics in Chemical Safety Information

Sponsored by CHAS, Cosponsored by CCS, CHED and CINF†

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CORP

Committee on
Corporation
Associates

D. Mason, Program Chair

TUESDAY MORNING

Academic Innovations for Tomorrow's
Industries: GSSPC SymposiumSponsored by CHED, Cosponsored by
ANYL‡, BIOL‡, BIOT‡, BMGT‡, CHED‡,
CORP‡, DAC‡, ENFL‡, PHYS‡ and POLY‡

TUESDAY AFTERNOON

Academic Innovations for Tomorrow's
Industries: GSSPC SymposiumSponsored by CHED, Cosponsored by
ANYL‡, BIOT‡, BMGT‡, CHED‡, CORP‡,
DAC‡, ENFL‡, PHYS‡ and POLY‡

DAC

Committee on
Divisional Activities

M. J. Morello, Program Chair

TUESDAY MORNING

Academic Innovations for Tomorrow's
Industries: GSSPC SymposiumSponsored by CHED, Cosponsored by
ANYL‡, BIOL‡, BIOT‡, BMGT‡, CHED‡,
CORP‡, DAC‡, ENFL‡, PHYS‡ and POLY‡

TUESDAY AFTERNOON

Academic Innovations for Tomorrow's
Industries: GSSPC SymposiumSponsored by CHED, Cosponsored by
ANYL‡, BIOT‡, BMGT‡, CHED‡, CORP‡,
DAC‡, ENFL‡, PHYS‡ and POLY‡

CEPA

Committee on
Economic and
Professional Affairs

D. Kneeland, Program Chair

SUNDAY AFTERNOON

Professional Legacy of Henry Hill

Sponsored by PROF, Cosponsored by
CEPA, CMA, ETHC, HIST‡, ORGN,
PMSE, POLY‡, PRES and SCHB‡

MONDAY AFTERNOON

Leadership Skills as a Strategic
Advantage: the Chemist's
Competitive EdgeSponsored by BMGT, Cosponsored
by CEPA, PRES‡, PROF and YCC

CEI

Committee on
Environmental
Improvement

C. Middlecamp, Program Chair

SUNDAY MORNING

Designing Safer Chemicals

Sponsored by ENVR, Cosponsored by CEI‡

New Challenges in Water Quality,
Treatment, Reuse and Sustainability:
Chemistry and Application of
Advanced Oxidation Processes for
Removal of Contaminants of Concern
and Transformation Products

Processes

Sponsored by ENVR, Cosponsored by CEI

Toxicology and Environmental Impact
in the Chemistry Curriculum: Science
and Strategies for Educators -
State of the Art Symposium

Sponsored by CHED, Cosponsored by CEI

SUNDAY AFTERNOON

Designing Safer Chemicals

Sponsored by ENVR, Cosponsored by CEI‡

Education for Sustainable
Development and Innovative
Technologies Across Culture

Sponsored by CHED, Cosponsored by CEI

New Challenges in Water Quality,
Treatment, Reuse and Sustainability:
Chemistry and Application of
Advanced Oxidation Processes for
Removal of Contaminants of Concern
and Transformation Products

Reactors

Sponsored by ENVR, Cosponsored by CEI

Toxicology and Environmental
Impact in the Chemistry Curriculum:
Science and Strategies for Educators
- State of the Art Symposium

Sponsored by CHED, Cosponsored by CEI

MONDAY MORNING

Citizens First: Using Real-World
Contexts for Engaging Students
in Learning Chemistry

Sponsored by CHED, Cosponsored by CEI

Careers for Young Professionals
in Green Chemistry: Breaking
Bad Chemistry HabitsSponsored by CHED, Cosponsored by BMGT,
CEI, ENVR, I&EC, MEDI, PROF, SCHB and YCCNew Challenges in Water Quality,
Treatment, Reuse and Sustainability:
Chemistry and Application of
Advanced Oxidation Processes for
Removal of Contaminants of Concern
and Transformation Products

Disinfection/Natural Organic Matter

Sponsored by ENVR, Cosponsored by CEI

Toxicology and Environmental
Impact in the Chemistry Curriculum:
Science and Strategies for Educators
- State of the Art Symposium

Sponsored by CHED, Cosponsored by CEI

MONDAY AFTERNOON

Citizens First: Using Real-World
Contexts for Engaging Students
in Learning Chemistry

Sponsored by CHED, Cosponsored by CEI

Incorporating Green Chemistry
Innovations and Applications into
the Classroom and OutreachSponsored by CHED, Cosponsored
by CEI‡, I&EC and SOCEDNew Challenges in Water Quality,
Treatment, Reuse and Sustainability:
Chemistry and Application of
Advanced Oxidation Processes for
Removal of Contaminants of Concern
and Transformation Products

Electrochemical/Inorganics

Sponsored by ENVR, Cosponsored by CEI

TUESDAY MORNING

Biological Inspiration for
Environmental Sustainability:
Bioinspired Approaches for Energy
Conversion, Storage and MaterialsElectron and Energy Transfer: From
Molecular to Device Engineering for
Minimizing Environmental ImpactsSponsored by ENVR, Cosponsored
by CEI, ENFL, ORGN and PHYSNew Challenges in Water Quality,
Treatment, Reuse and Sustainability:
Chemistry and Application of
Advanced Oxidation Processes for
Removal of Contaminants of Concern
and Transformation ProductsPharmaceuticals and Contaminants
of Emerging Concern

Sponsored by ENVR, Cosponsored by CEI

TUESDAY AFTERNOON

Biological Inspiration for
Environmental Sustainability:
Bioinspired Approaches for Energy
Conversion, Storage and MaterialsBioinspired Designs: From
Molecules to Functional MaterialsSponsored by ENVR, Cosponsored
by CEI, ENFL, ORGN and PHYSThe Debate: How Do We
Respond to Climate Change

Sponsored by ENVR, Cosponsored by CEI‡

New Challenges in Water Quality,
Treatment, Reuse and Sustainability:
Chemistry and Application of
Advanced Oxidation Processes for
Removal of Contaminants of Concern
and Transformation Products

Materials

Sponsored by ENVR, Cosponsored by CEI

WEDNESDAY MORNING

Biological Inspiration for
Environmental Sustainability:
Bioinspired Approaches for Energy
Conversion, Storage and MaterialsEnergy Storage, Solar Fuels, and
Biofuels: Satisfying the Energy Needs
While Decreasing the Carbon FootprintSponsored by ENVR, Cosponsored
by CEI, ENFL, ORGN and PHYS

WEDNESDAY AFTERNOON

Biological Inspiration for
Environmental Sustainability:
Bioinspired Approaches for Energy
Conversion, Storage and MaterialsArtificial Photosynthesis: Challenges
and Strategies to Meet Energy Needs
in an Environmentally Benign MannerSponsored by ENVR, Cosponsored
by CEI, ENFL, ORGN and PHYS

WEDNESDAY EVENING

Biological Inspiration for
Environmental Sustainability:
Bioinspired Approaches for Energy
Conversion, Storage and MaterialsSponsored by ENVR, Cosponsored
by CEI, ENFL, ORGN and PHYSNew Challenges in Water Quality,
Treatment, Reuse and Sustainability:
Chemistry and Application of
Advanced Oxidation Processes for
Removal of Contaminants of Concern
and Transformation Products

Sponsored by ENVR, Cosponsored by CEI

THURSDAY MORNING

Biological Inspiration for
Environmental Sustainability:
Bioinspired Approaches for Energy
Conversion, Storage and MaterialsBioinspired Designs: From
Molecules to Functional MaterialsSponsored by ENVR, Cosponsored
by CEI, ENFL, ORGN and PHYS

ETHC

Committee on Ethics

K. Vitense, Program Chair

SUNDAY AFTERNOON

Professional Legacy of Henry Hill

Sponsored by PROF, Cosponsored by
CEPA, CMA, ETHC, HIST‡, ORGN,
PMSE, POLY‡, PRES and SCHB‡

CMA

Committee on
Minority Affairs

J. Sarquis, Program Chair

SUNDAY AFTERNOON

Professional Legacy of Henry Hill

Sponsored by PROF, Cosponsored by
CEPA, CMA, ETHC, HIST‡, ORGN,
PMSE, POLY‡, PRES and SCHB‡

MONDAY MORNING

ACS Scholars: Rising Stars in Academe

Sponsored by PRES, Cosponsored by
AGRO, CARB, CMA‡, COLL, ENFL,
ENVR, PROF, SCHB and YCC

MONDAY AFTERNOON

ACS Scholars: Rising Stars in Industry

Sponsored by PRES, Cosponsored by
AGRO, CARB, CMA‡, COLL, ENFL,
ENVR, PROF, SCHB and YCCThe Legacy of Henry Hill: Commercial
Enterprises in the Polymer SectorSponsored by SCHB, Cosponsored by CMA,
COLL, HIST, I&EC, POLY, PRES and PROF

NTS

Committee on
Nomenclature,
Terminology
and Symbols

A. Censullo, Program Chair

WEDNESDAY MORNING

Chemistry and the International
System of Weights and MeasuresConsultative Committee on Metrology
in Chemistry and Biology: Who We Are,
What We Do, and Why You Should Care

Sponsored by CCQM, Cosponsored by NTS

WEDNESDAY AFTERNOON

Chemistry and the International
System of Weights and MeasuresRedefinition of the International
System of Units

Sponsored by CCQM, Cosponsored by NTS

COMSCI

Committee on
Science

K. C. Glasgow, Program Chair

SUNDAY MORNING

Opportunities for US/Cuba
Collaboration in Chemistry, Chemical
Engineering and Chemistry EducationSponsored by IAC, Cosponsored
by COMSCI, PRES and PROF

TUESDAY MORNING

Scientific Integrity: Can We Rely on
the Published Scientific Literature?

Integrity and Peer Review

Sponsored by CINP, Cosponsored by COMSCI

TUESDAY AFTERNOON

Scientific Integrity: Can We Rely on
the Published Scientific Literature?Publisher Safeguards to
Scientific Integrity

Sponsored by CINP, Cosponsored by COMSCI

IAC

International Activities
CommitteeH. N. Cheng and A. Rimando, Program
Chairs

OTHER SYMPOSIA OF INTEREST:

True Stories from Entrepreneurs:
BRIC Edition (see SCHB, Sunday, Monday)Younger Chemists Exchanging More
than Currency: First—Euros and
Dollars; Next—Rupees, Rands,
and Reais (see YCC, Monday)

BUSINESS MEETINGS:

Global Regional Networking: Asia
Pacific, 4:00 PM: SundayIAC International Welcoming
Reception, 5:30 PM: SundayGlobal Regional Networking: Americas
and Africa, 2:00 PM: MondayGlobal Regional Networking: Europe
and Middle East, 6:00 PM: Tuesday

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 109BOpportunities for US/Cuba
Collaboration in Chemistry, Chemical
Engineering and Chemistry Education

Cosponsored by COMSCI, PRES and PROF

R. S. Danchik, B. Miller, Organizers

L. Brown, Organizer, Presiding

8:00 Introductory Remarks.

8:15 IAC 1. ACS and Cuba: Past,
present, and future. B. Miller8:45 IAC 2. Chemistry between close
neighbors: A good practice. L. Montero9:15 IAC 3. Retracing footsteps
and developing new con-
tacts. T. Manning, C. LaPrade9:45 IAC 4. Internationalization of Cuban
doctoral programs in chemistry: An
opportunity for ACS-SCQ coopera-
tion. L. Brown, D. Garcia Rivera

10:15 Intermission.

10:30 IAC 5. Opportunities for US/
Cuba collaborations in biopharma-
ceutical development and manu-
facturing. R.G. Carbonell, S. Hill11:00 IAC 6. Bridging new generations
through chemistry: Challenges and oppor-
tunities toward the interchange between
undergraduate and young chemists from
ACS and SCQ. L. Brown, Y. Méndez11:30 IAC 7. Building relation-
ships between the University of
Alabama and the University of
Havana. P.A. Frantom, L. Brown12:00 IAC 8. Cuba-USA collabo-
ration can go nano. R. Cao

12:30 Concluding Remarks.

SUNDAY AFTERNOON

True Stories from Entrepreneurs:
BRIC EditionSponsored by SCHB, Cosponsored by
CARB, COLL, I&EC, IAC, PRES and PROF

MONDAY MORNING

True Stories from Entrepreneurs:
BRIC EditionSponsored by SCHB, Cosponsored by
CARB, COLL, I&EC, IAC, PRES and PROFYounger Chemists Exchanging
More than Currency: First—
Euros and Dollars; Next—
Rupees, Rands, and ReaisSponsored by YCC, Cosponsored by
CHED, IAC, PRES and PROF

MONDAY AFTERNOON

Younger Chemists Exchanging
More than Currency: First—
Euros and Dollars; Next—
Rupees, Rands, and ReaisSponsored by YCC, Cosponsored by
CHED, IAC, PRES and PROF

TUESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 210CInternational Entrepreneurship:
How To Start a Business and
Thrive in the Global MarketplaceCosponsored by AGFD, AGRO, BMGT,
CARB, CELL, INOR, MEDI, ORGN,
POLY, PRES‡, PROF and SCHBH. N. Cheng, A. M. Rimando, Organizers,
Presiding

8:30 Introductory Remarks.

8:40 IAC 9. Lessons in translating
university research to the mar-
ketplace. J.M. Desimone9:10 IAC 10. How to start a business
and thrive in the global marketplace: A
story from US/Taiwan/China. J. Shen9:35 IAC 11. From chemistry student
to chemical entrepreneur and
public company CEO. F. Jaksch

10:00 Intermission.

10:20 IAC 12. What it takes to be a chem-
istry entrepreneur. J. Garcia Martinez10:45 IAC 13. Creation of a glob-
ally sustainable generic pharma-
ceutical model. S.K. Nambiar11:10 IAC 14. It's a competitive
world out there: Factors for STEM
venture success. J.C. Giordan

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 208International Entrepreneurship:
How To Start a Business and
Thrive in the Global MarketplaceCosponsored by AGFD, AGRO, BMGT,
CARB, CELL, INOR, MEDI, ORGN,
POLY, PRES‡, PROF and SCHBH. N. Cheng, A. M. Rimando, Organizers,
Presiding1:30 IAC 15. From discovery to com-
mercialization. G.M. Whitesides2:00 IAC 16. Distributed alliances:
Strategic partnerships to access
markets and capital. N.J. Conti2:25 IAC 17. Knowledge-intensive business
services in Brazil: Entrepreneurship in
a stimulating scenario. T. Guaratini2:50 IAC 18. Tips for innovative
entrepreneurship. A. Ryan

3:15 Intermission.

3:35 IAC 19. International entrepreneur-
ship: Lessons from the road. S. Dugar4:00 IAC 20. Development of a global
small chemical business with
international marketing and out-
reach. S.V. Vercellotti, J.R. Vercellotti4:25 IAC 21. International proto-
type development. D.T. Daly

4:50 Concluding Remarks.

SCC

Senior Chemists
Committee

G. Heinze, Program Chair

MONDAY EVENING

From Raw to Varoom: The Science
Behind Getting a Car on the RoadSponsored by CHED, Cosponsored by
PMSE, POLY, RUBB and SCC‡

SOCED

Society Committee on Education

G. Muller, Program Chair

OTHER SYMPOSIA OF INTEREST:

Undergraduate Research Posters
(see CHED, Monday)

SOCIAL EVENTS:

Careers in Chemical Information and
Cheminformatics Panel Discussion
& Brunch, 2:00 PM: SundayNetworking with Graduate School
Recruiters, 2:00 PM: SundayEminent Scientist Luncheon,
12:00 PM: MondayStudent Speed Networking with Chemistry
Professionals, 4:00 PM: Monday

SUNDAY MORNING

High School Program

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

SUNDAY AFTERNOON

21st Century Chemistry Education:
Formal and InformalSponsored by PRES, Cosponsored by
AGRO, CARB, CHAS, CHED, CINF,
COLL, ENFL, PROF and SOCED

Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

MONDAY MORNING

21st Century Chemistry Education:
Formal and InformalSponsored by PRES, Cosponsored by
AGRO, CARB, CHAS, CHED, CINF,
COLL, ENFL, PROF and SOCED

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 52A

What's in Your Chemical Toolbox?

Cosponsored by ENFL and ENVR

G. Muller, Organizer, Presiding

12:00 **SOCEC 1.** Eminent Scientist
Lecture: What's in your chemical
toolbox? J.C. WarnerTechnical program information
known at press time.The official technical program
for the 250th ACS National
Meeting is available at:
www.acs.org/boston2015Incorporating Green Chemistry
Innovations and Applications into
the Classroom and OutreachSponsored by CHED, Cosponsored
by CEI, I&EC and SOCED

Undergraduate Research Posters

Sponsored by CHED, Cosponsored
by AGFD and SOCED

MONDAY EVENING

Successful Student Chapters

Sponsored by CHED, Cosponsored by SOCED

WCC

Women Chemists
CommitteeK. Wozniak and A. Debaille, Program
Chairs

SOCIAL EVENTS:

WCC Breakfast, 7:30 AM: Monday

WCC/Eli Lilly Travel Award Poster
Session, 11:00 AM: TuesdayWCC Luncheon, 12:00 PM: Tuesday
Just Cocktails, 4:00 PM: Tuesday

BUSINESS MEETINGS:

WCC Division Executive Session,
7:30 PM: Saturday

MONDAY MORNING

Section A

Sheraton Boston Hotel
Hampton A/B

Managing Transitions

Cosponsored by PROF

M. J. Shultz, Organizer, Presiding

N. Bridges, Presiding

9:15 Introductory Remarks.

9:20 **WCC 1.** After school: Diverse paths
in the chemical enterprise. K.L. Lee9:30 **WCC 2.** Diverse paths in the
chemical enterprise: A career
in publishing. H.L. Tierney9:40 **WCC 3.** Still love science, but don't
want to DO science? H. Ertelcher9:50 **WCC 4.** Withdrawn.

10:00 Discussion.

10:45 Intermission.

11:00 **WCC 5.** Mid-career reflections:
New direction? New company?
Re-commitment? M. Ollson11:15 **WCC 6.** Successful strategies for next
steps: What should I do now? S.N. Collins11:30 **WCC 7.** It's about the journey:
Adventures in the new chemistry job
market and advice for successfully
managing career changes. K.M. George

11:45 Discussion.

12:25 Concluding Remarks.

TUESDAY AFTERNOON

Women in Innovation:
Business and CommerceSponsored by PROF, Cosponsored by
BMGT, SCHB, WCC and YCC

YCC

Younger Chemists
Committee

A. Gavrilenko and T. Matos, Program Chairs

MONDAY MORNING

Section A

Seaport Hotel and World Trade Center
Seaport Blrm BYounger Chemists Exchanging
More than Currency: First—
Euros and Dollars; Next—
Rupees, Rands, and Reais

Cosponsored by CHED, IAC, PRES and PROF

J. Breffke, A. V. Gavrilenko, L. L. Johnson,
Organizers

F. R. Lucci, Presiding

8:45 Introductory Remarks.

8:55 **YCC 1.** Chemistry in Germany,
educational and research opportuni-
ties: How to get connected and how
to continue. E. Kapatsina, B. Weber9:25 **YCC 2.** European Young Chemists'
Network bridging the gap between aca-
demia and industry. F. Backaert, A. Walshe9:45 **YCC 3.** Ripple effect of global student
exchanges: How the exchange program
founded and developed by NESACS and
the GDCh has evolved and influenced
our peers along the way. L.L. Johnson

10:05 Intermission.

10:15 **YCC 4.** Community engage-
ment: Benefits for science, society,
and myself. M. Kavanagh10:35 **YCC 5.** Partners for progress
and prosperity: Promoting interna-
tional collaborations. M.P. Wu10:55 **YCC 6.** Spirit of scientific net-
working: Examples, given by a
lifestyle full of rewards. C. Janaky

11:15 Discussion.

11:25 Concluding Remarks.

ACS Scholars: Rising Stars in Academe

Sponsored by PRES, Cosponsored by
AGRO, CARB, CMA+, COLL, ENFL,
ENVR, PROF, SCHB and YCCCareers for Young Professionals
in Green Chemistry: Breaking
Bad Chemistry HabitsSponsored by CHED, Cosponsored by BMGT,
CEI, ENVR, I&EC, MEDI, PROF, SCHB and YCC

Getting Your First Industrial Job

Sponsored by PROF, Cosponsored by YCC‡

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by YCC

MONDAY AFTERNOON

Section A

Seaport Hotel and World Trade Center
Seaport Blrm BYounger Chemists Exchanging
More than Currency: First—
Euros and Dollars; Next—
Rupees, Rands, and Reais

Cosponsored by CHED, IAC, PRES and PROF

A. V. Gavrilenko, L. L. Johnson, Organizers

J. Breffke, Organizer, Presiding

1:30 Introductory Remarks.

1:40 **YCC 7.** Chemistry communities in
an international context: The expan-
sion of cultural representation among
ACS student chapters. N. Di Fabio2:00 **YCC 8.** Expanding beyond the Boston
area for young chemists. F.R. Lucci2:20 **YCC 9.** Young Chemists' section
of the German Chemical Society:
"JungChemiker Forum". M.M. Linden,
A.U. Augustin, F. Pfeiffer, C. Schrapel, T. John

2:40 Intermission.

2:50 **YCC 10.** Where chemistry meets wan-
derlust: A continuing journey. C. Dunne3:10 **YCC 11.** Chemistry without
borders: International activities
at ACS. H. Cheng, B. Miller3:30 **YCC 12.** Formation of the International
Young Chemists Network (IYCN).
L.B. Roberson, C. Janaky, J. Breffke

3:50 Discussion.

4:00 Concluding Remarks.

ACS Scholars: Rising Stars in Industry

Sponsored by PRES, Cosponsored by
AGRO, CARB, CMA+, COLL, ENFL,
ENVR, PROF, SCHB and YCC

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by YCC

Leadership Skills as a Strategic
Advantage: the Chemist's
Competitive EdgeSponsored by BMGT, Cosponsored
by CEPA, PRES+, PROF and YCC

TUESDAY MORNING

Checklist for Turning Thirty

Sponsored by PROF, Cosponsored by YCC‡

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by YCC

Starting-Up & Spinning-Out:
Commercializing Innovative ChemistrySponsored by SCHB, Cosponsored by
AGRO, COLL, I&EC, PRES, PROF and YCC

TUESDAY AFTERNOON

Starting-Up & Spinning-Out:
Commercializing Innovative ChemistrySponsored by SCHB, Cosponsored by
AGRO, COLL, I&EC, PRES, PROF and YCCWomen in Innovation:
Business and CommerceSponsored by PROF, Cosponsored by
BMGT, SCHB, WCC and YCC

WEDNESDAY EVENING

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by YCC

Consultative Committee on Metrology in Chemistry and Biology

R. Wielgosz and W. May, *Program Chairs*

WEDNESDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 109B

Chemistry and the International System of Weights and Measures

Consultative Committee on Metrology in Chemistry and Biology: Who We Are, What We Do, and Why You Should Care

Cosponsored by NTS

W. E. May, R. Wielgosz, *Organizers*

R. M. Parris, *Presiding*

9:00 **CCQM 1.** Introduction to the international system of weights and measures. W.E. May

9:20 **CCQM 2.** The CCQM, what it does, what it has achieved and why it is important to you. R. Kaarls

9:50 **CCQM 3.** CCQM activities and impact in healthcare. W.E. May

10:20 Intermission.

10:50 **CCQM 4.** CCQM activities and impact in environment and climate. R. Wielgosz

11:20 **CCQM 5.** CCQM activities and impact in food safety and nutrition. S.A. Wise

11:50 Discussion.

WEDNESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 109B

Chemistry and the International System of Weights and Measures

Redefinition of the International System of Units

Cosponsored by NTS

W. E. May, R. Wielgosz, *Organizers*

P. F. Rusch, *Presiding*

1:30 **CCQM 6.** Linking the international system of units to fundamental constants. J. Ullrich

2:00 **CCQM 7.** Units and accurate measurements in chemistry. R. Wielgosz

2:30 Intermission.

3:00 **CCQM 8.** Progress in the redefinition of the mole. B. Güttler

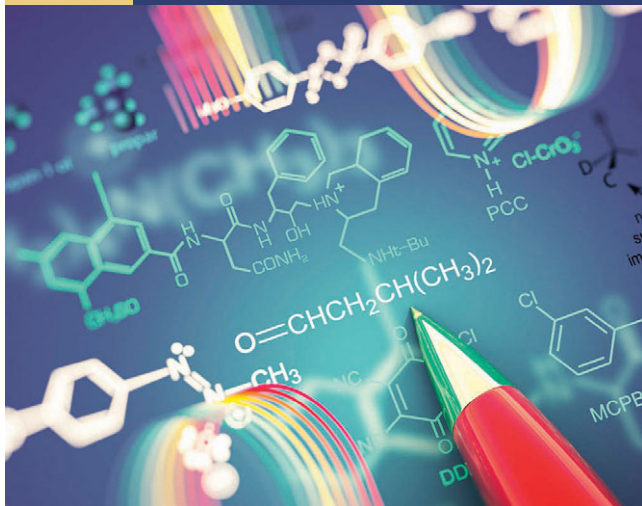
3:30 **CCQM 9.** Redefinition of the kilogram. R. Davis

4:00 Discussion.

4:30 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.

FEDERAL FUNDERS SYMPOSIUM & SPEED COACHING



TUESDAY, AUGUST 18 • 1:00 PM–5:00 PM
BOSTON CONVENTION & EXHIBITION CENTER, ROOM 102AB



1:00 PM–3:00 PM

FEDERAL FUNDERS SYMPOSIUM

Learn about agency priorities, initiatives, programs, and how to participate!

Meet the Federal Funders from the National Science Foundation (NSF CHE, DMR, CBET, MCB and OISE), Department of Energy (DOE BES), National Institutes of Health (NIH NIGMS), Air Force Office of Scientific Research (AFOSR), and the Environmental Protection Agency (EPA)



3:00 PM–5:00 PM

SPEED COACHING

Join speed coaching — one-on-one interactions with federal funders to discuss research, education, and outreach activities.

All are welcome — registration not required!
For additional information, email: cheminfo@nsf.gov

NEW

Sci-Mix Posters:

Monday, August 17 • 8–10 pm
Hall C—Convention Center
Posters ORGN 340–342



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EXHIBIT HOURS

Sunday, August 16 • 6:00 pm – 8:30 pm

Monday, August 17 • 9:00 am – 5:00 pm

Tuesday, August 18 • 9:00 am – 5:00 pm

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.

EXPOSITION HIGHLIGHTS

SEE WHAT'S NEW INSIDE THE

EXPOSITION. Visit the ACS National Exposition at the BCEC, Halls A & B1, from Sunday, August 16, through Tuesday, August 18. 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/boston2015 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 BCEC. These workshops will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications that may improve your productivity.

Presentations, Prizes & Special Events. Visit the Daily Prize Raffle area (#255) 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 Welcome Celebration. Need a digital headshot for social media networks? Stop by the ACS ProShot Social Media Lounge inside the Town Center for a FREE headshot, Sunday through Tuesday during the Exposition.

Meet the President-Elect candidates inside the exposition on Monday, from 1:00 to 4:00 PM.

Visit the Networking Lounge from Sunday through Tuesday to connect with your colleagues. On Tuesday, stop by the

Town Center for the Division of Energy & Fuels (ENFL) poster session from 2:00 to 4:00 PM and the ACS Division of Agricultural Food and Chemistry (AGFD) poster session from 3:00 to 5:00 PM.

To celebrate the ACS 250th National Meeting pick up a commemorative lapel pin Sunday through Tuesday during exposition.

Internet & Technology. Use free Internet access, and leave messages for one another at the Meeting Mail terminals located throughout the exposition and BCEC. Also, enjoy free Wi-Fi service throughout the BCEC.

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 BCEC, North Lobby.



ACS Exposition

EXHIBITORS

The following list exhibitors, as of July 15, 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/boston2015 to download the updated exhibitor list and access product information.

A ChemTek, Inc., 100 Barber Ave., Worcester, MA, United States 014606, 508-856-7100, fax: 508-845-9201, Internet: www.achemtek.com A ChemTek locates in Worcester MA provides chemicals, analytical, purification products and services to world-wide pharmaceutical researchers in an Easy, Economic, Efficient & Express way. The major products include Amino Acids, Bioactive Reference Compounds, Nature Products, Building Blocks; HPLC/prep-HPLC/flash columns, chromatography systems, TLC, silica gel, syringe filters, vials etc. **941**

AAAS/Science & Technology Policy Fellowship, 1200 New York Ave., NW, Washington, DC 20005, 202-326-6700, fax: 202-289-4950, Internet: <http://aaas.org/stpf> The AAAS Science & Technology Policy Fellowships provide scientists and engineers with a unique opportunity to apply their knowledge and skills to national and international issues, while learning first-hand about establishing and implementing policy. Fellows serve yearlong assignments in all three branches of the federal government in Washington, D.C. **1241**

AAPS (Amer Assoc. of Pharm Sci.), 2107 Wilson Blvd., Suite 700, Arlington, VA 22201, 703-243-2800, Internet: www.aaps.org **648**

Accela ChemBio Co. Ltd., 9883 Pacific Heights Blvd., Suite H, San Diego, CA, United States 92121, 858-699-3322, fax: 858-769-6322 or 858-876-1948, e-mail: info@accelachem.com, Internet: www.accelachem.com Founded in 2007, Accela ChemBio is a Quality R&D Chemical Supplier for use in scientific research, industrial development and analysis. Our established business sites are located in San Diego, US and Shanghai, China, respectively. Accela specializes in providing advanced pharmaceutical intermediates, building blocks, synthetic reagents and other specialty chemicals to R&D laboratories in the pharmaceutical, material, chemical and petrochemical industries, as well as academic institutions. In addition to its extensive catalog products, Accela also offers process research, custom manufacturing, and consulting services. With rigorous quality control, unique product lines, and dependability, Accela attracted 1400 global customers. **1105**

Ace Glass, Inc., 1430 N. West Blvd., POBox 688, Vineland, NJ 08360, 800-223-4524, fax: 800-543-6752, e-mail: sales@aceglass.com, Internet: www.aceglass.com Ace Glass is a leader and innovator of scientific glassware, lab equipment and glass apparatus- manufacturing glass systems up to 200L in size, complete with all controls and accessory equipment. In addition to our standard product offerings, Ace Glass also fabricates custom laboratory glassware to customer necessary specifications. **1400**

ACS Career Navigator, 1155 16th Street, NW, Washington, DC 20036, 202-872-6031, e-mail: k_redmond@acs.org, Internet: www.acs.org/content/acs/en/careers/profdev.html The ACS Career Navigator™ is home to career services,

leadership development, professional education courses and market intelligence resources. Tools provided help you find a job, discover a new career path, and compare your salary. Courses available help refresh skills or branch into new areas of science and develop leadership abilities. **625**

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 Chemistry and the Law (CHAL), Shelterpoint Business Center, 591 Redwood Highway, Mill Valley, CA 94941, 415-389-8900, fax: 415-381-4301, e-mail: carl@lippenbergerlaw.com, Internet: www.acs-chal.org/ The lawyer is in. As part of his "Enterprise 2015" project, Bill Carroll, past ACS president, challenged the Division of Chemistry and the Law to help ACS members with their legal needs. CHAL responded with a lawyer referral service and a speaker's bureau. For the referral service, CHAL members will answer legal questions from ACS members, refer them to an attorney who can help them, or if appropriate, represent them. For the speaker's bureau, CHAL will provide attorneys to speak to ACS members about topics of mutual interest. To request a referral or a speaker, e-mail Carl Lippenberger at carl@lippenbergerlaw.com. **348**

ACS Division of Small Chemical Businesses (SCHB), 4344 Moorpark Ave., Ste # 1, San Jose, CA, United States 95129, 408-834-8597, fax: 408-351-7900, e-mail: expo-booth@acs-schb.org, Internet: www.acs-schb.org The ACS Division of Small Chemical Businesses (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. Cannabis chemistry group is here. **1033**

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Microtrac Inc.	948
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PSS USA, Inc.	750
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2-Amino-4-bromobenzaldehyde, 59278-65-8

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Berry & Associates

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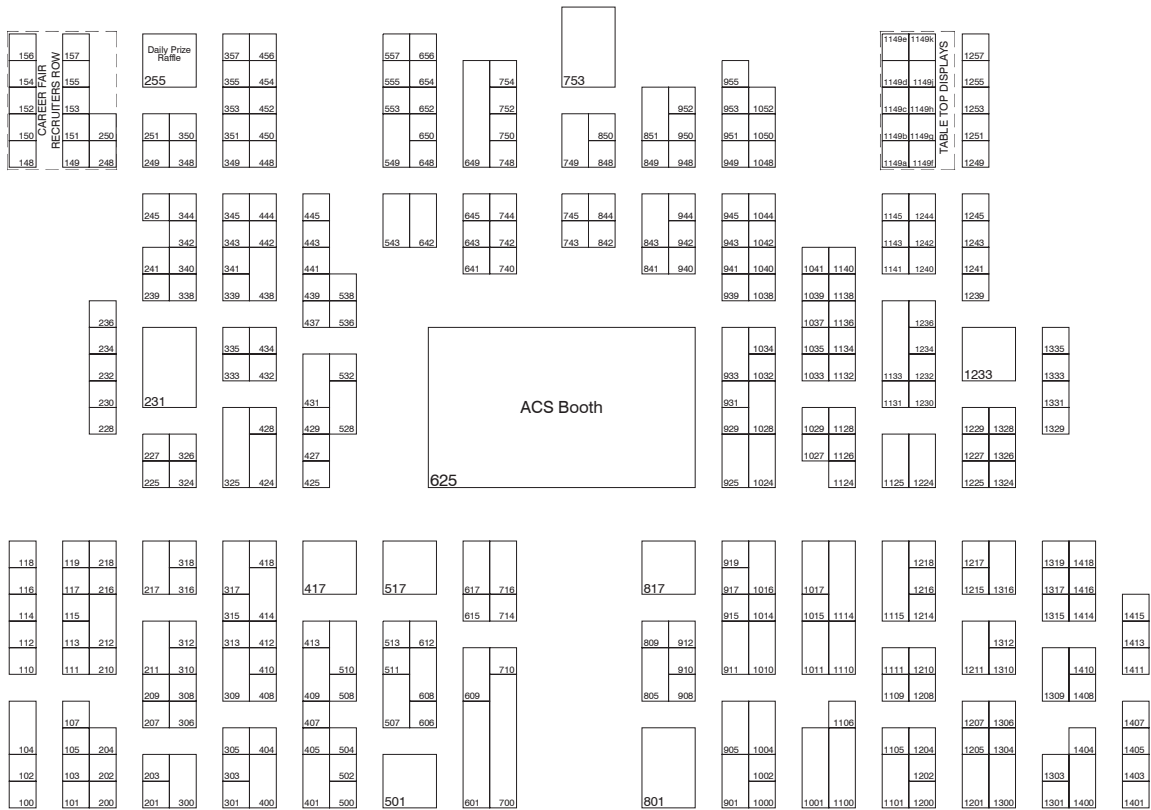
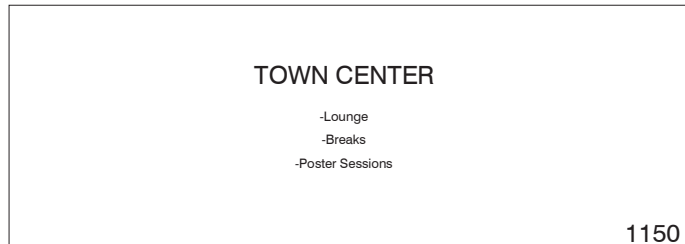
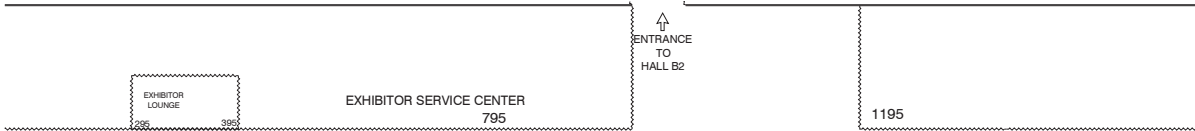
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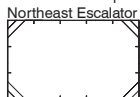
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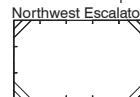


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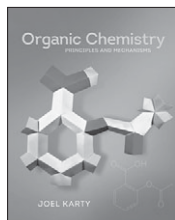


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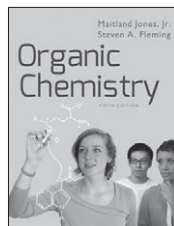


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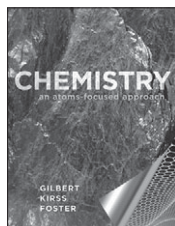
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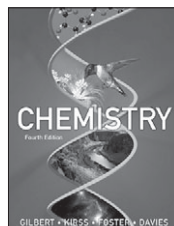
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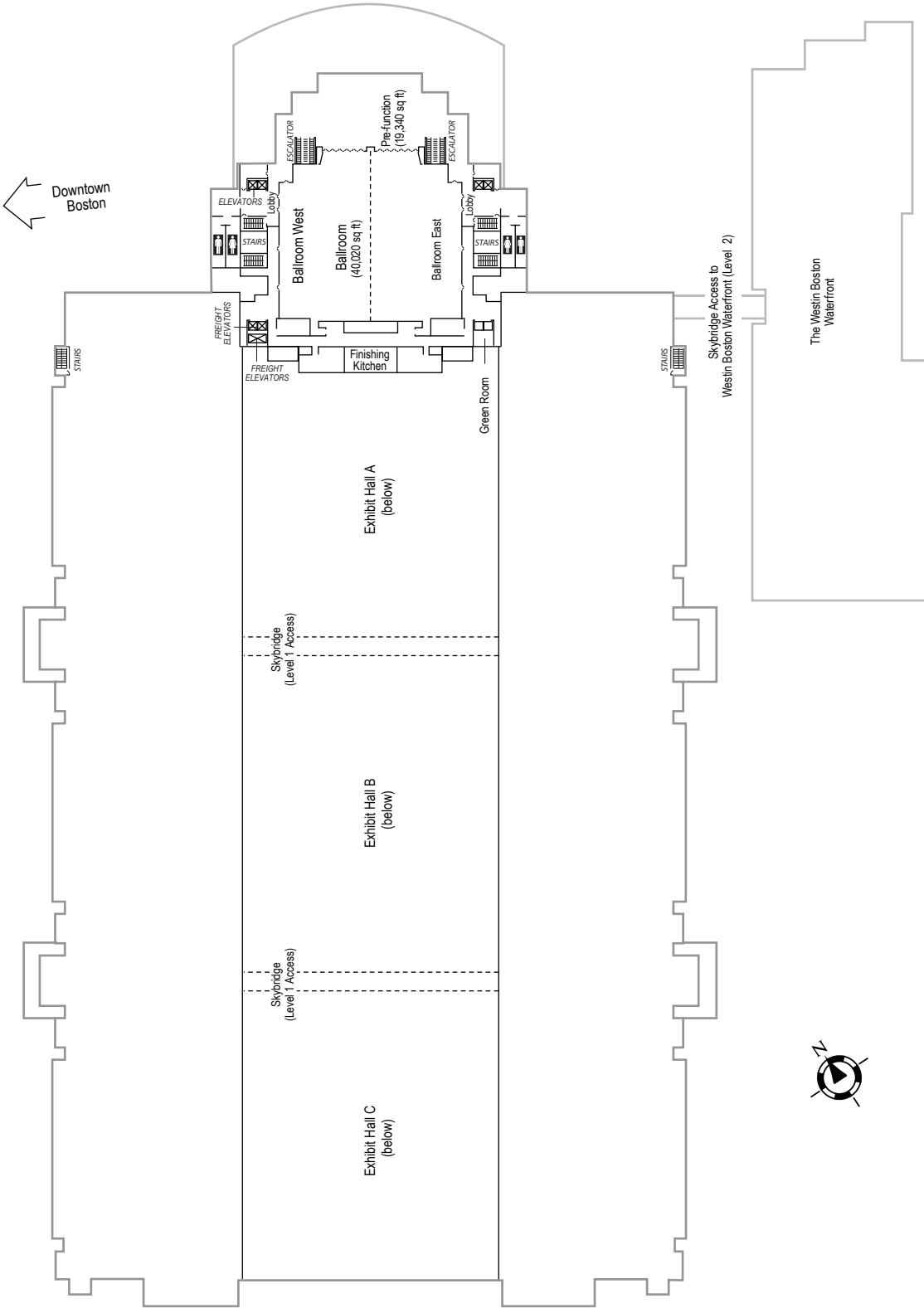
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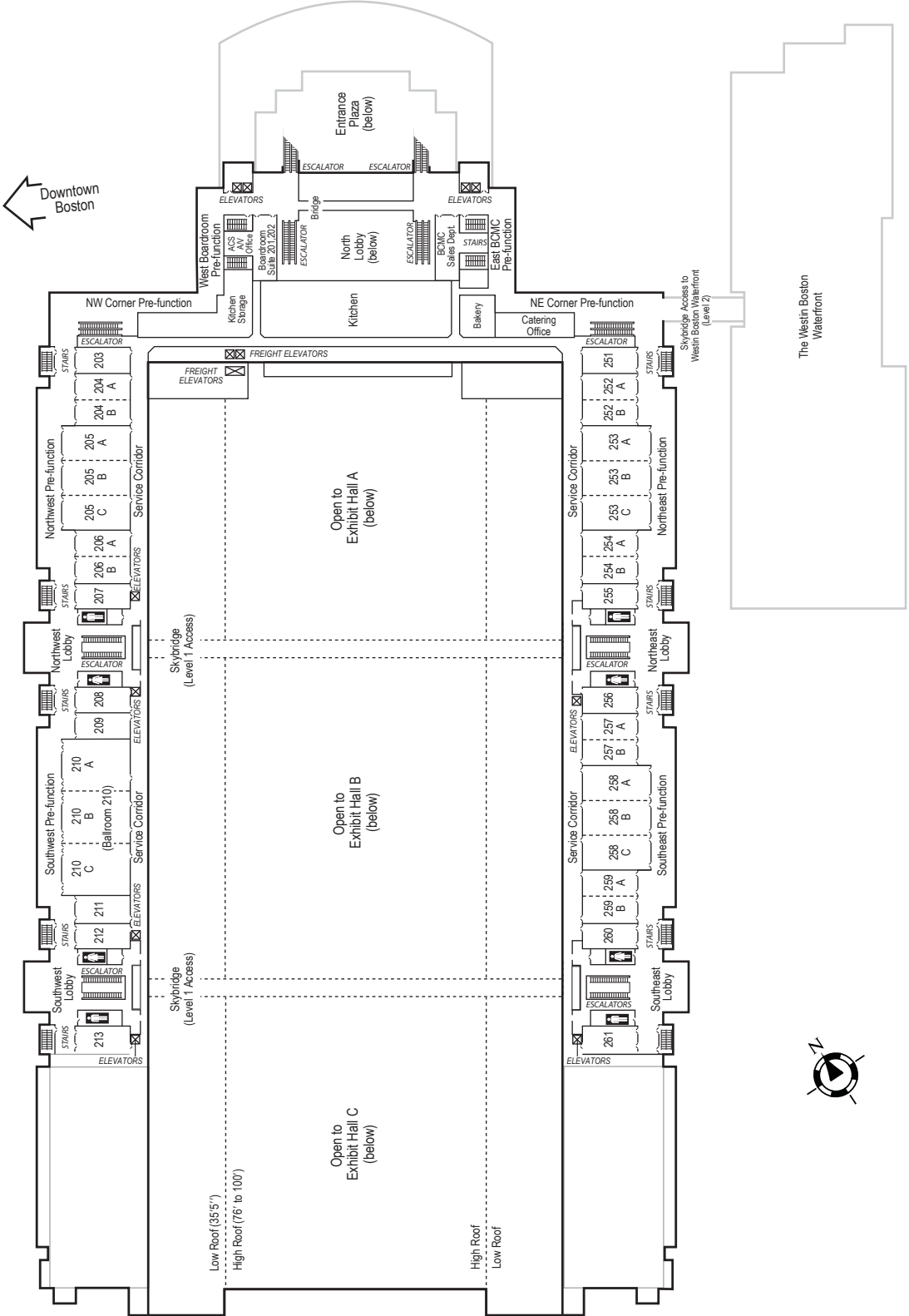
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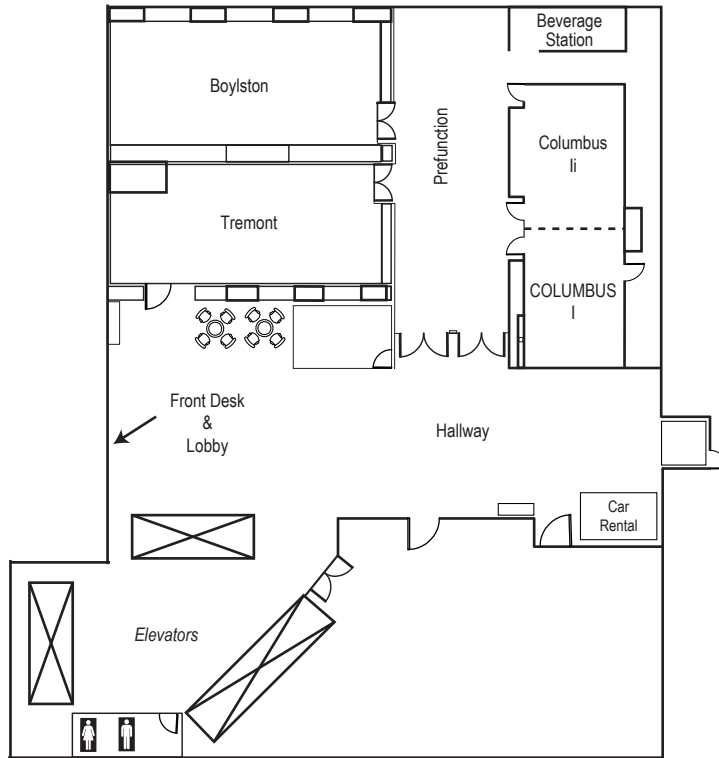
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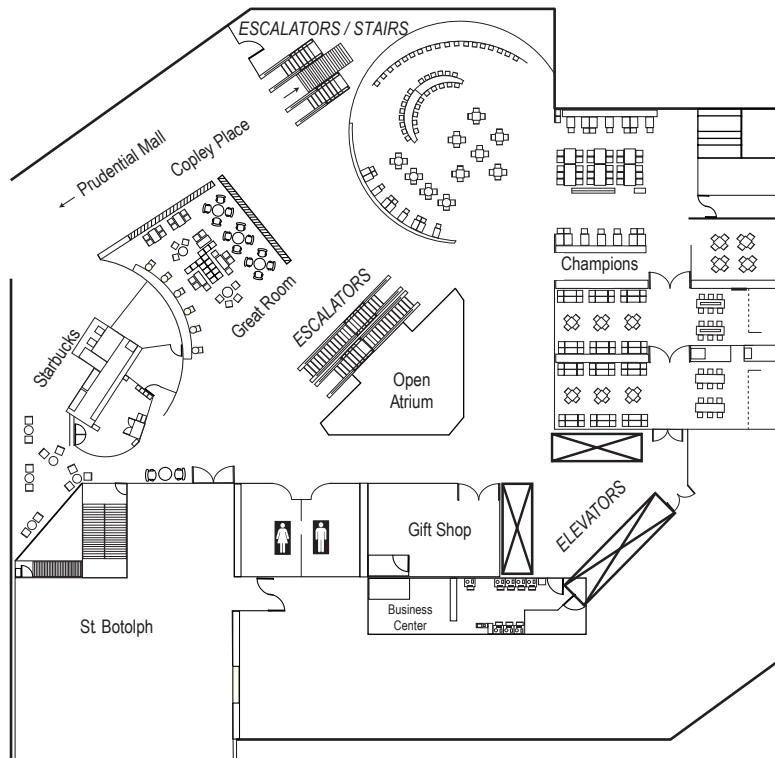


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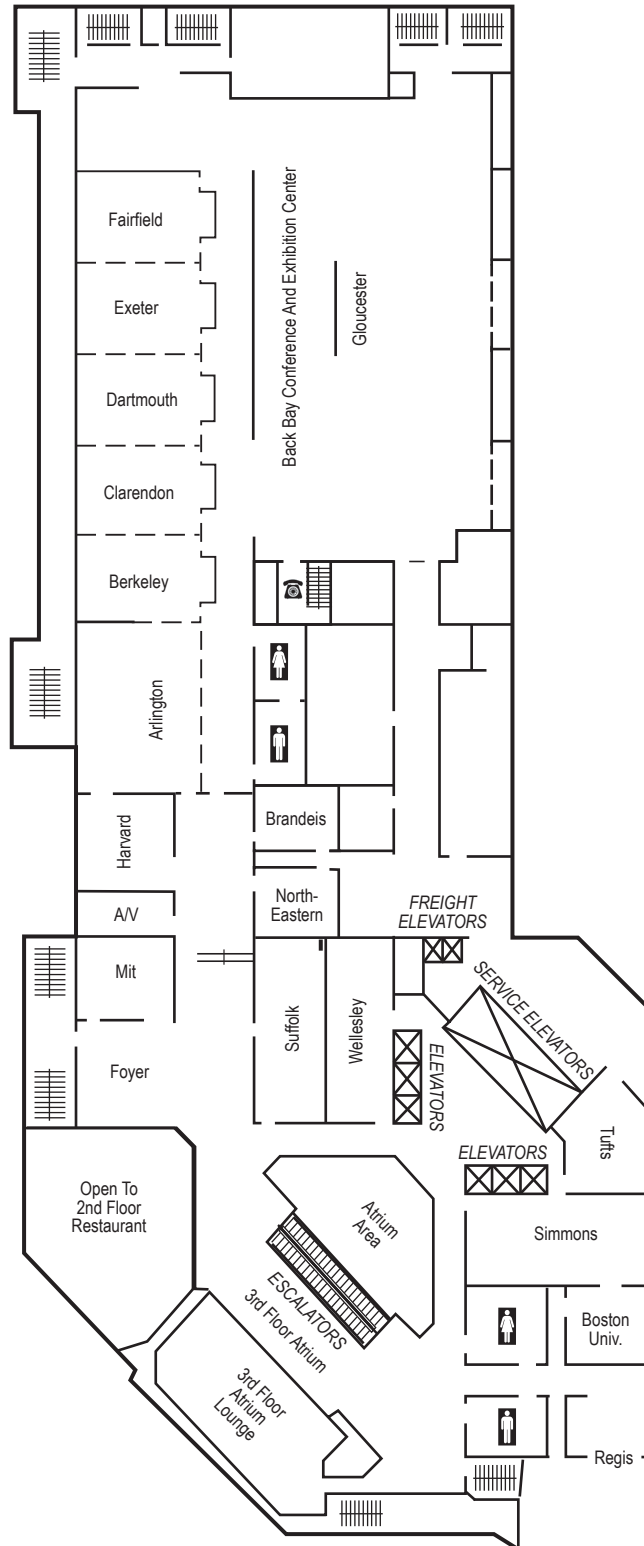


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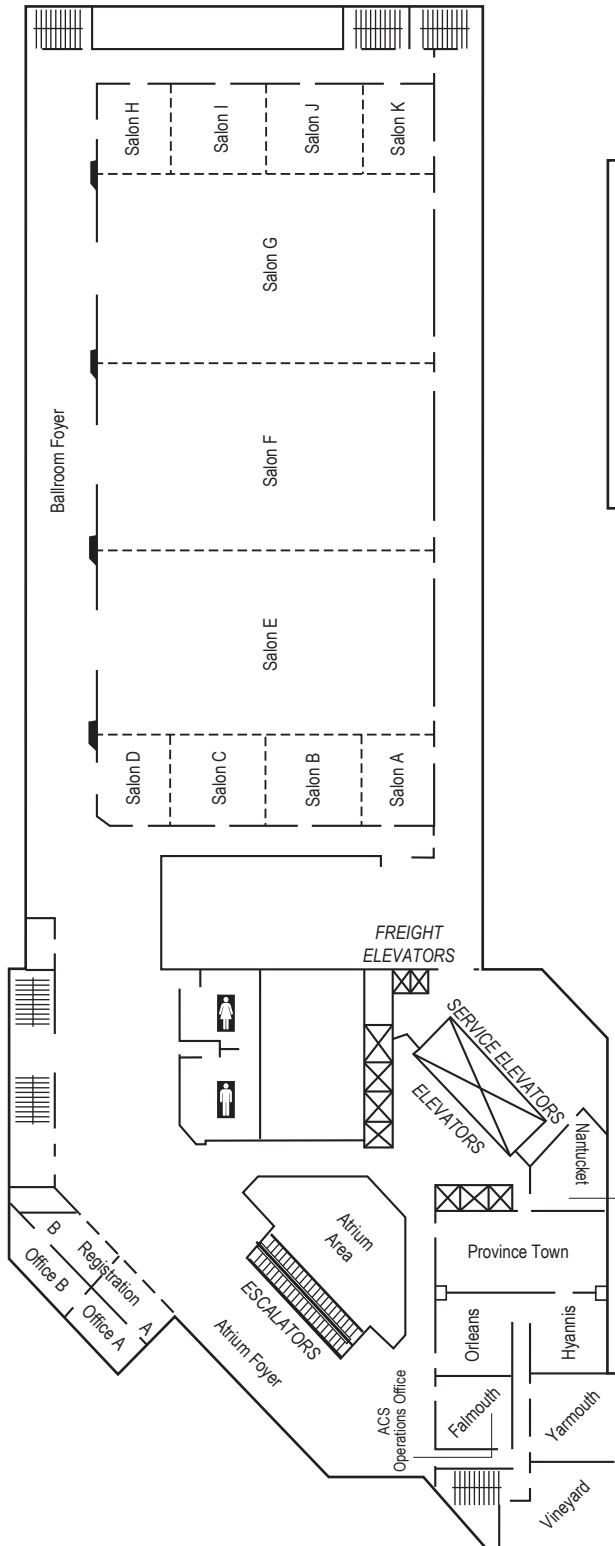
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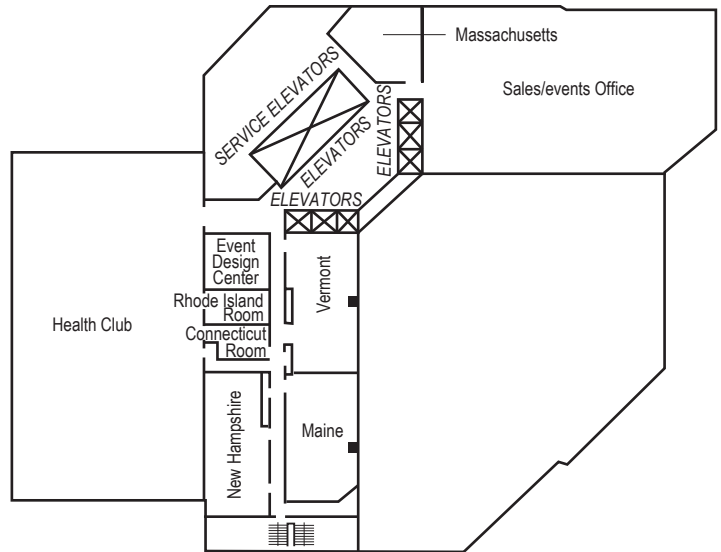


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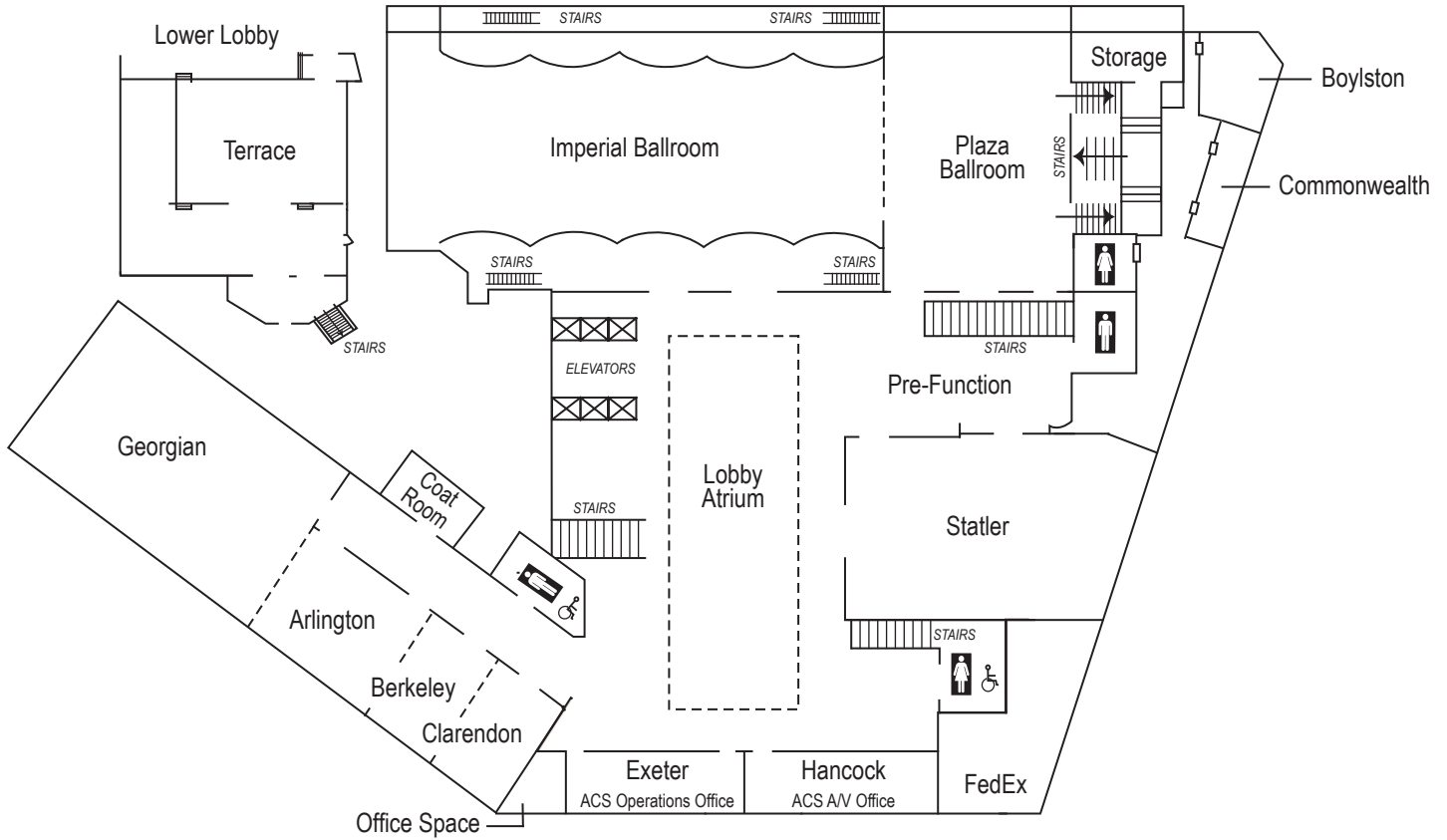


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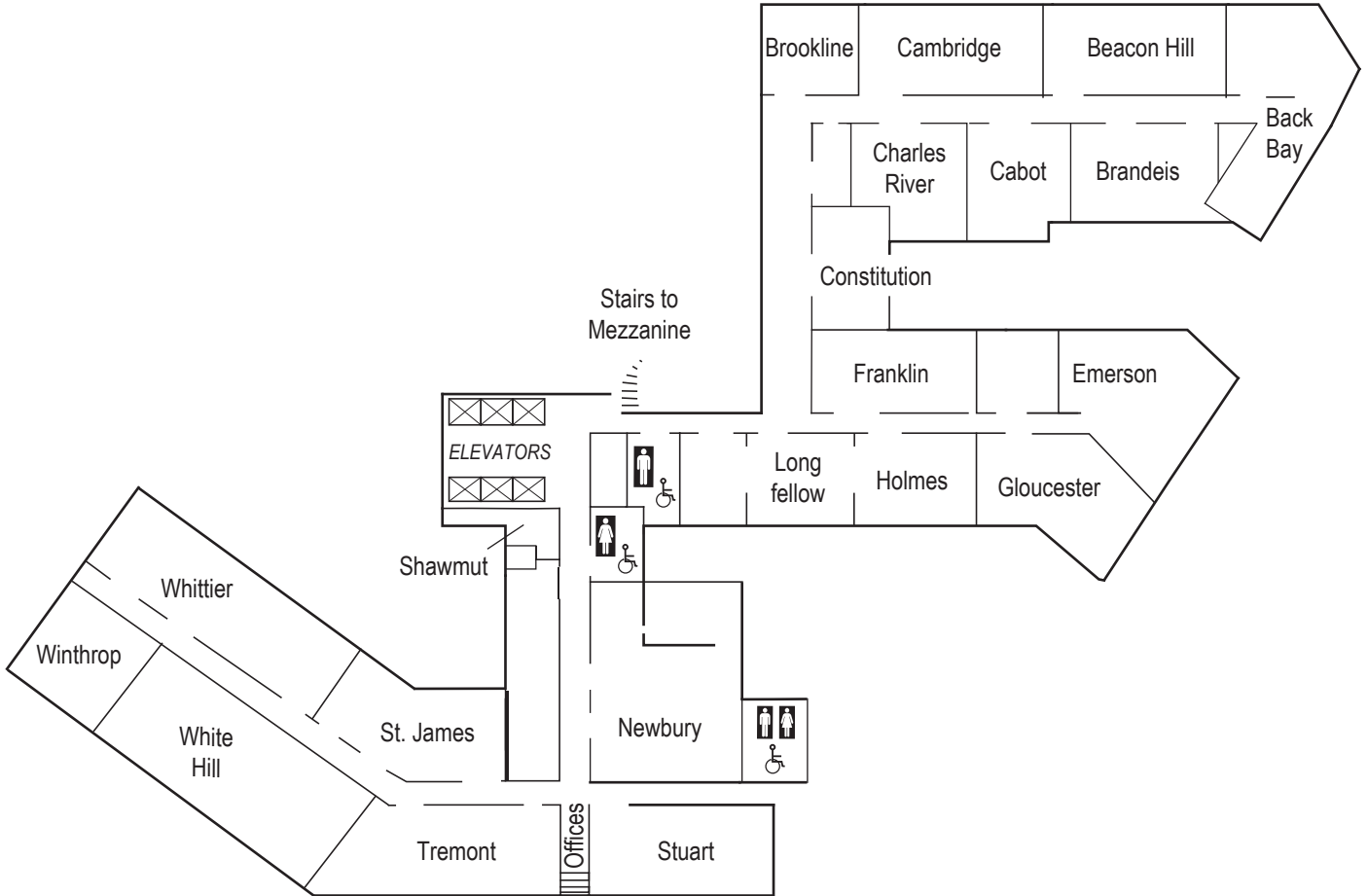
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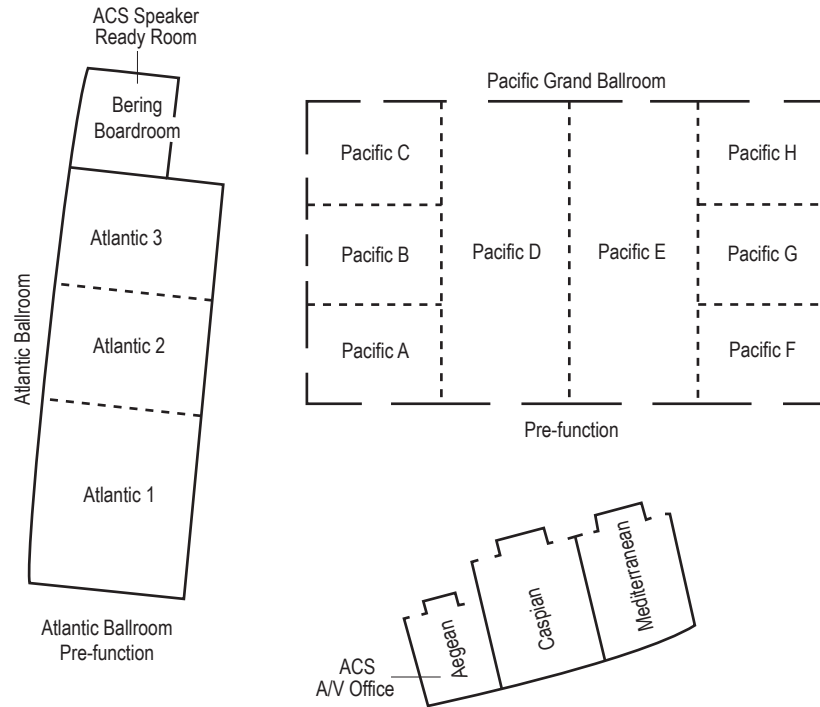
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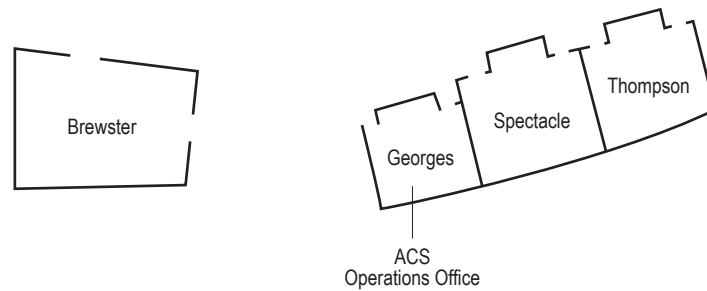


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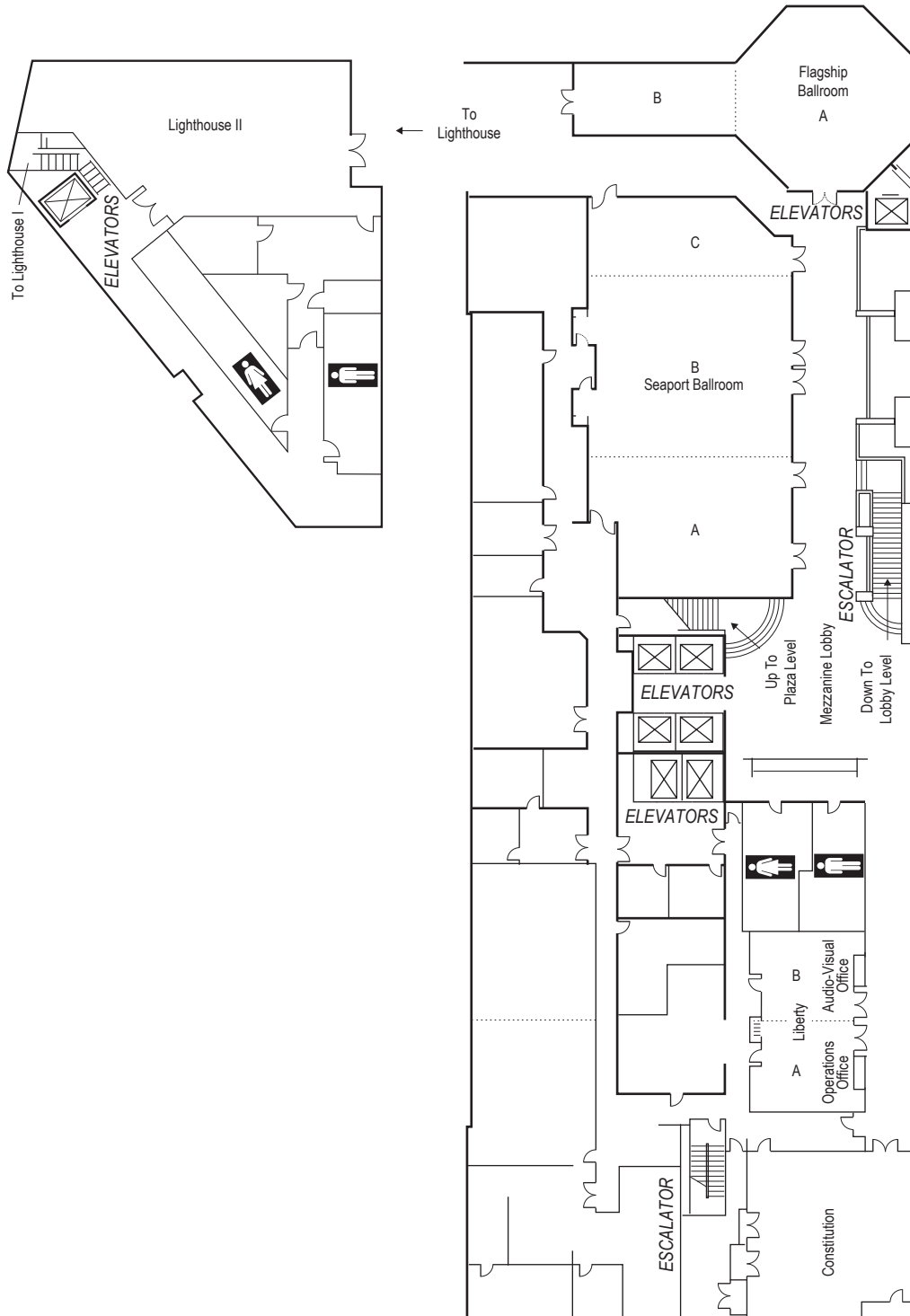


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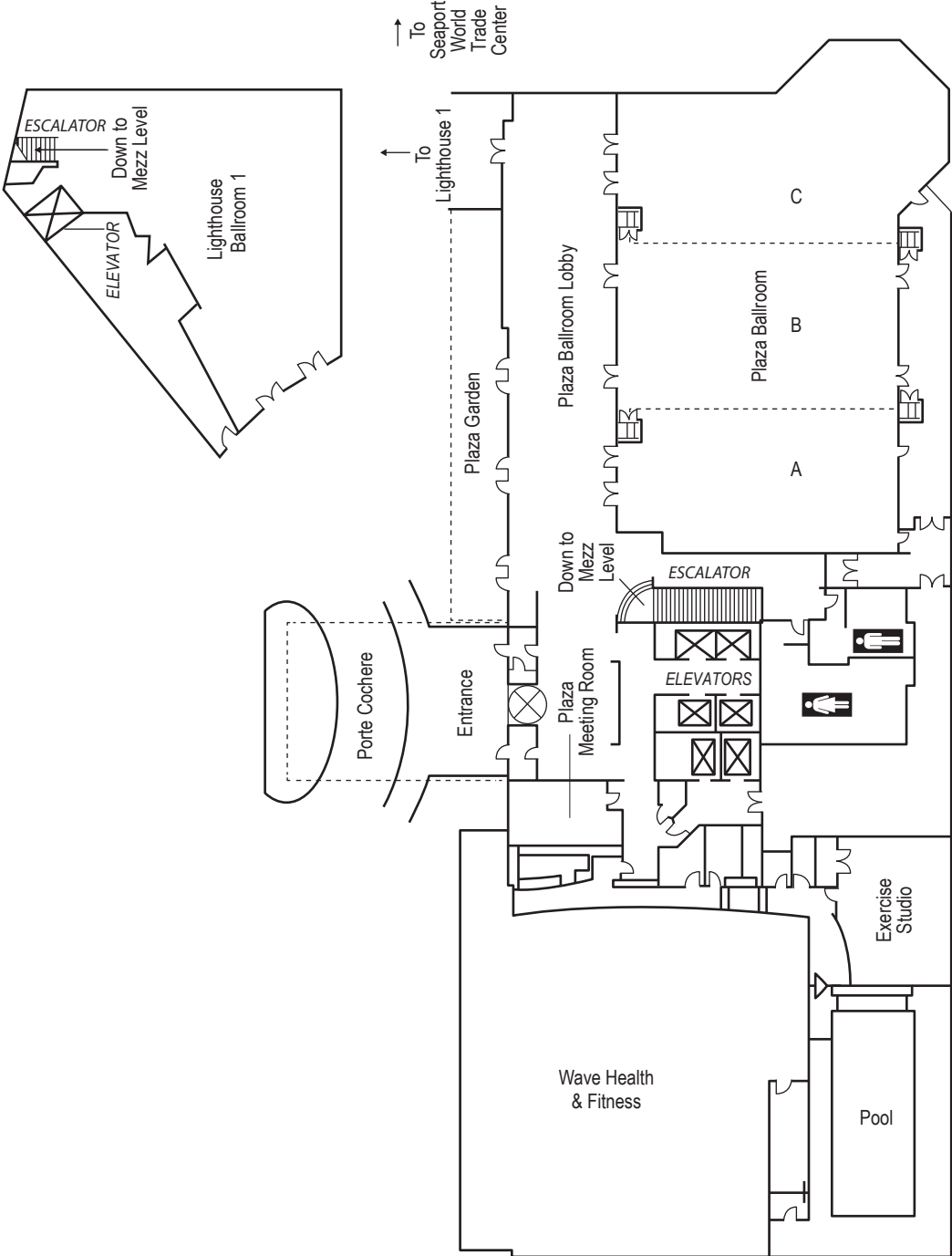
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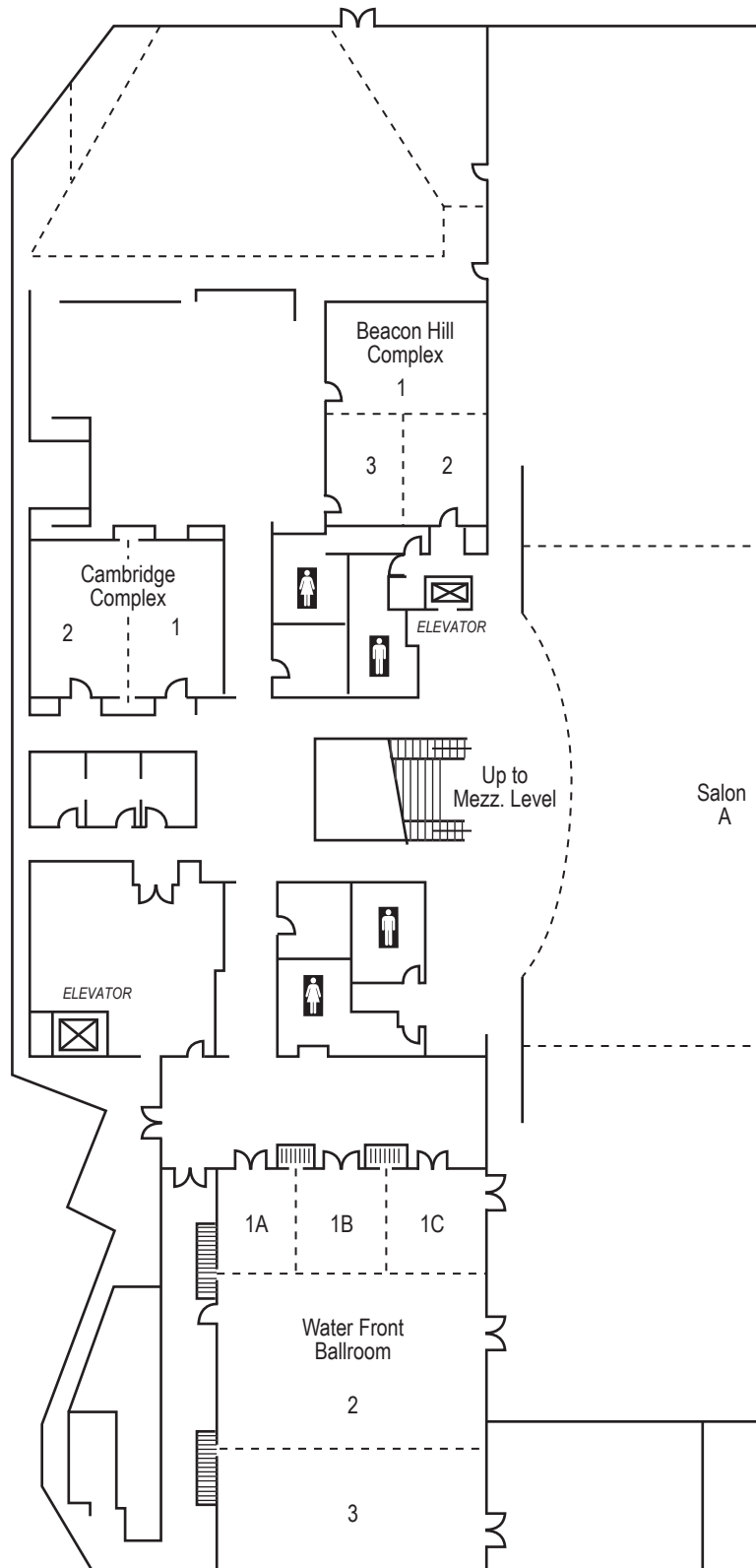
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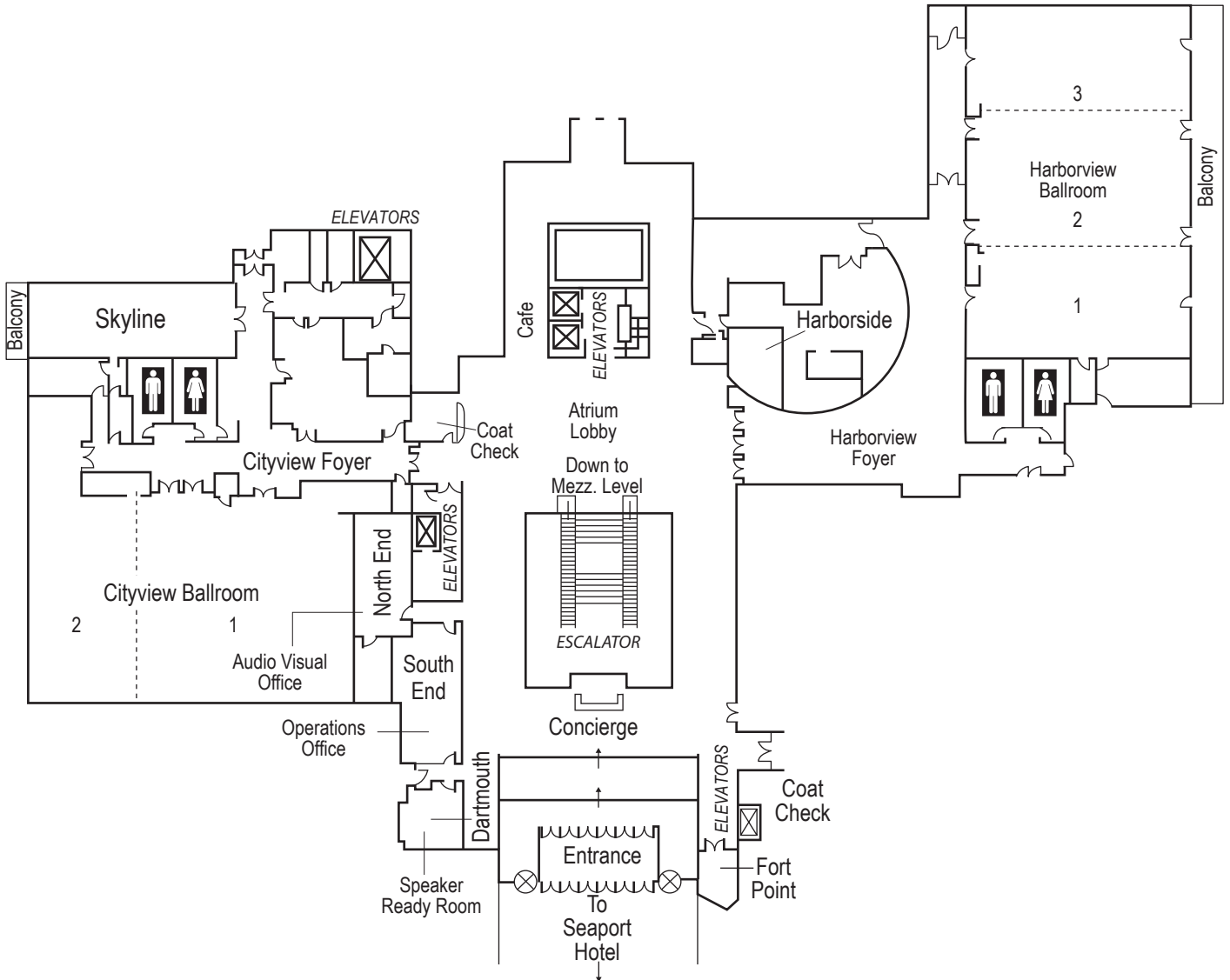
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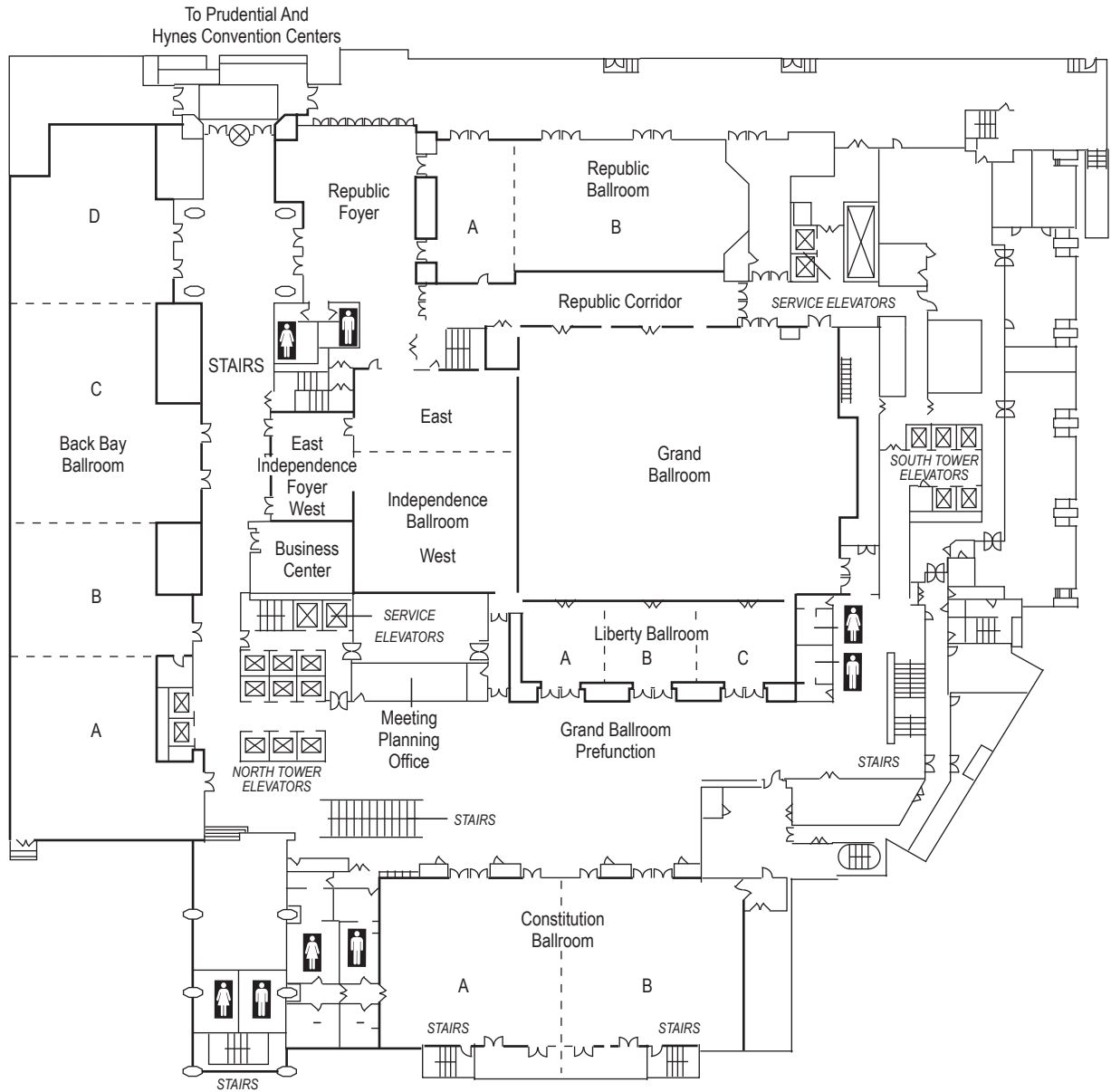
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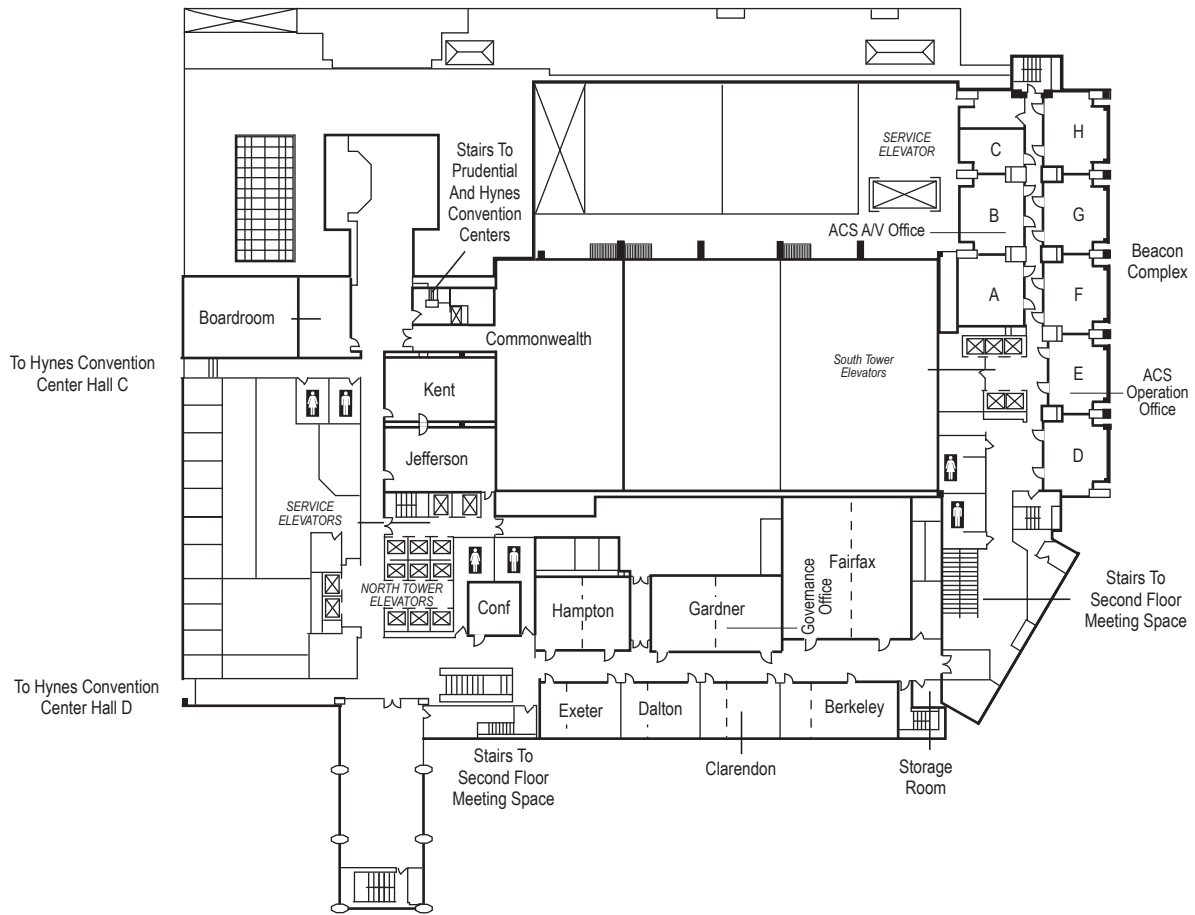
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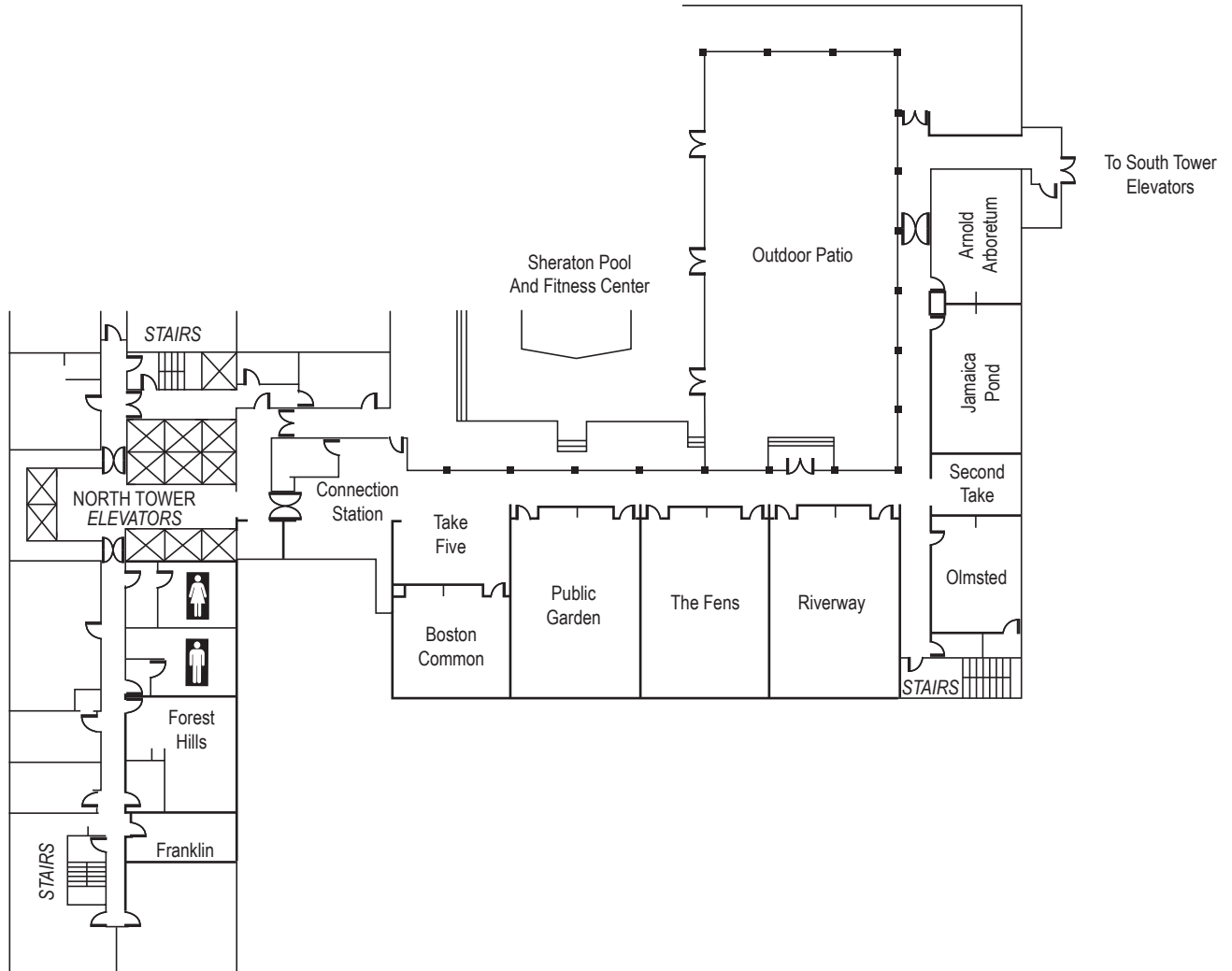
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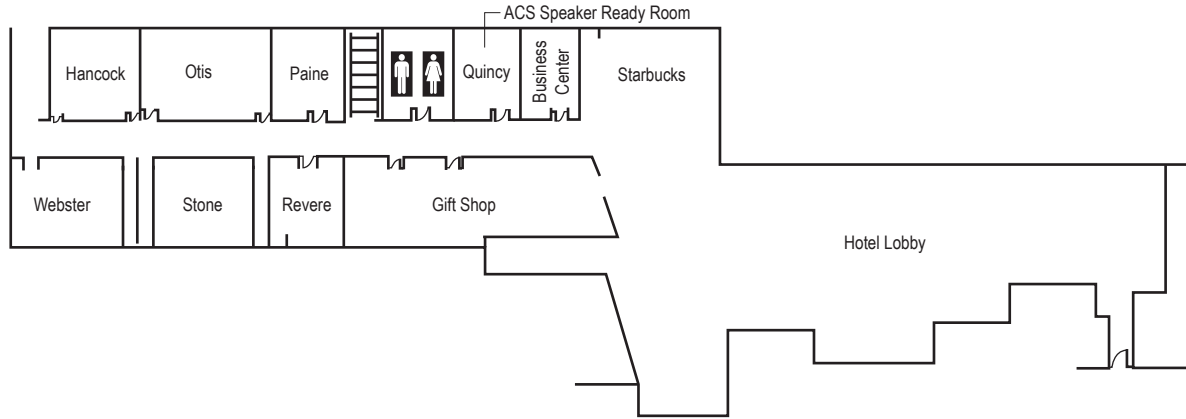
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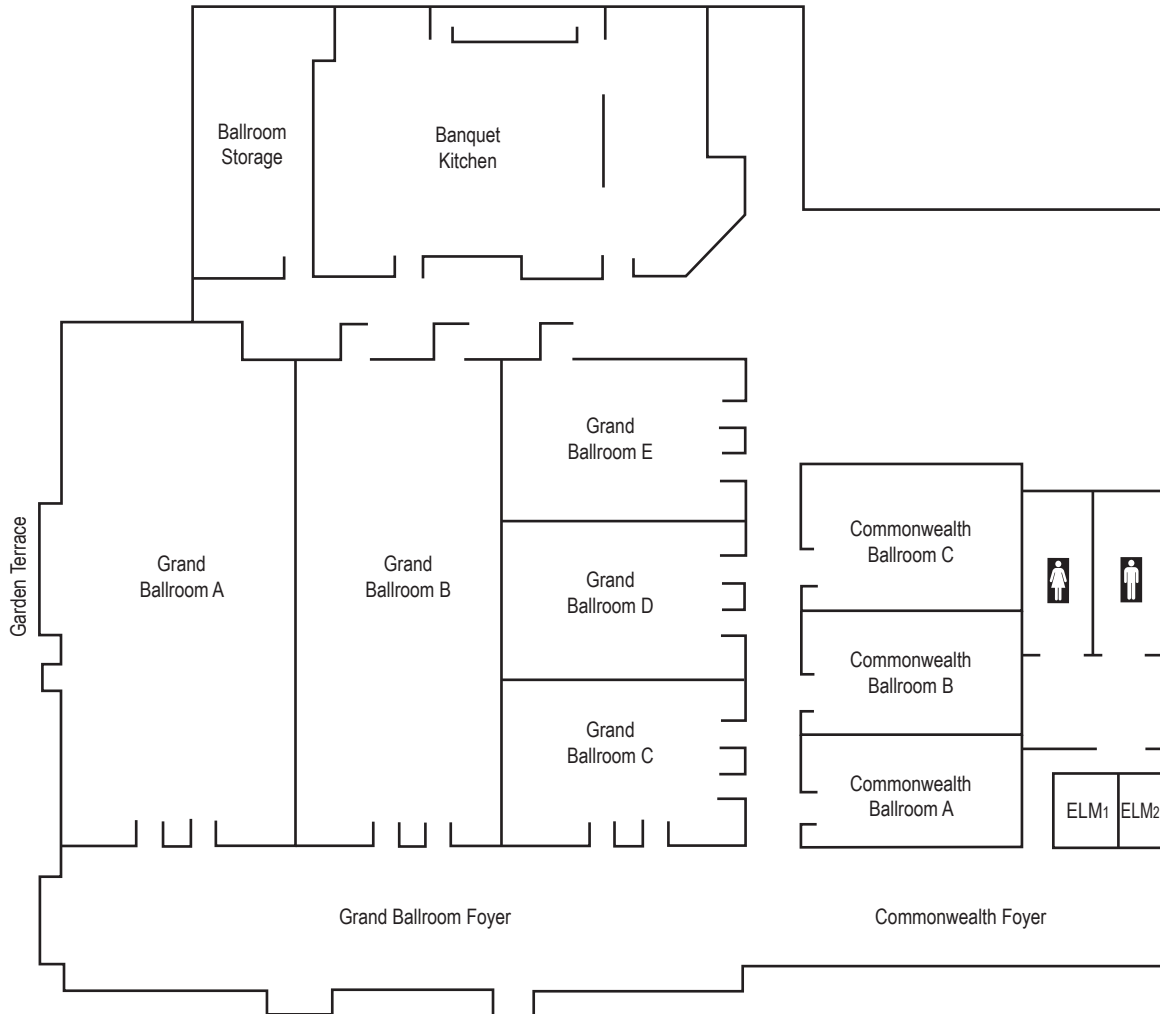


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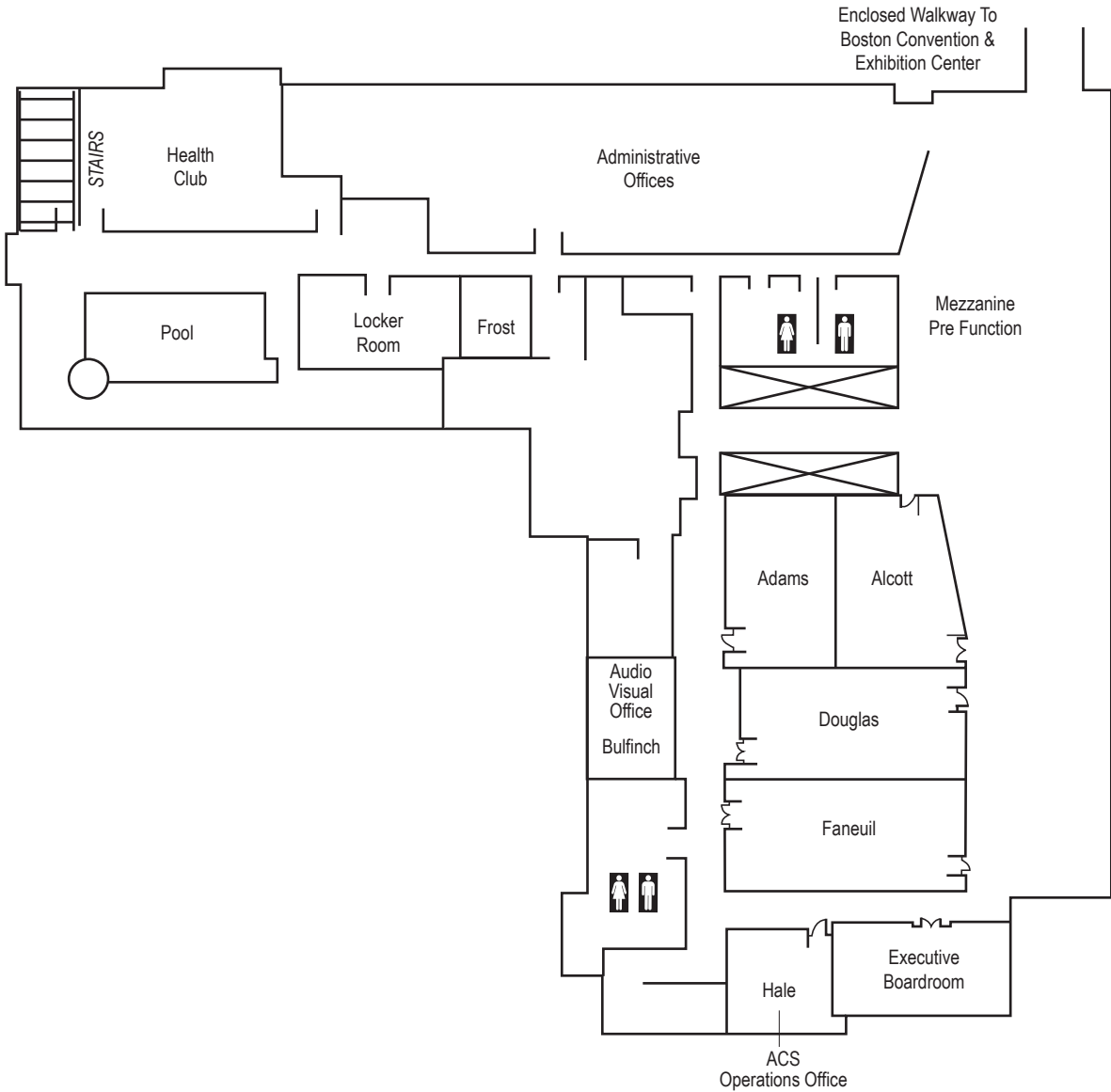


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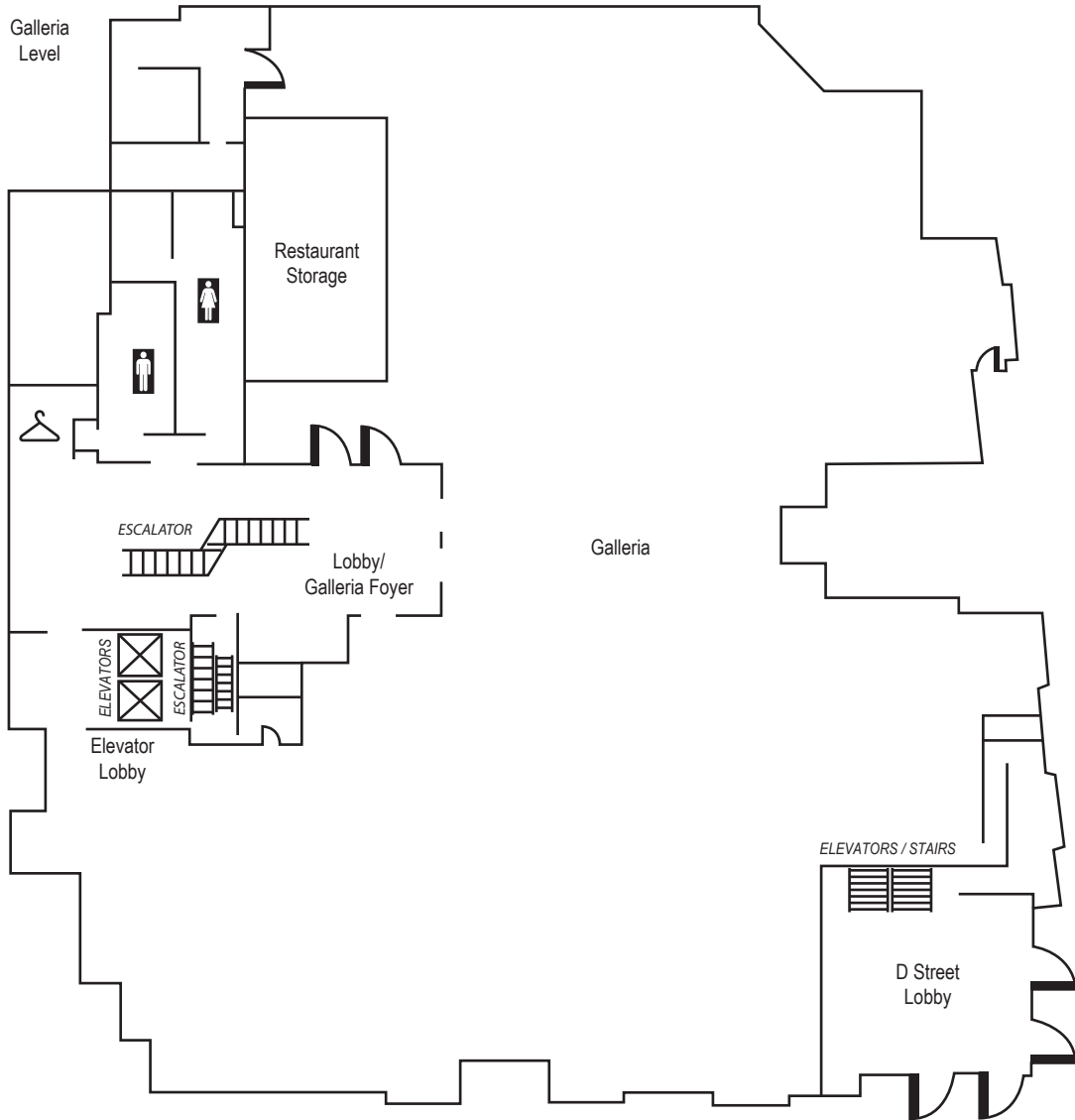
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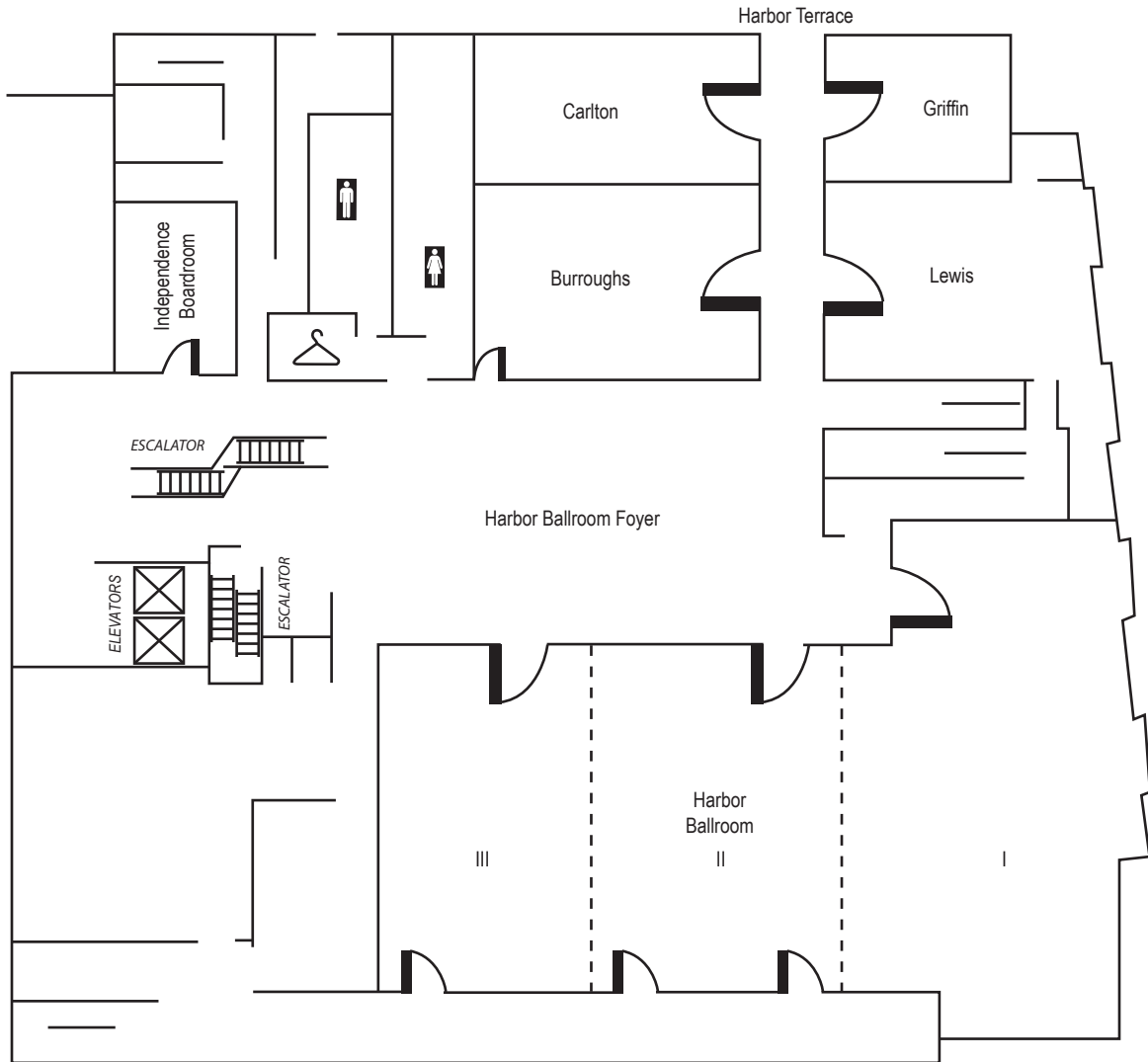
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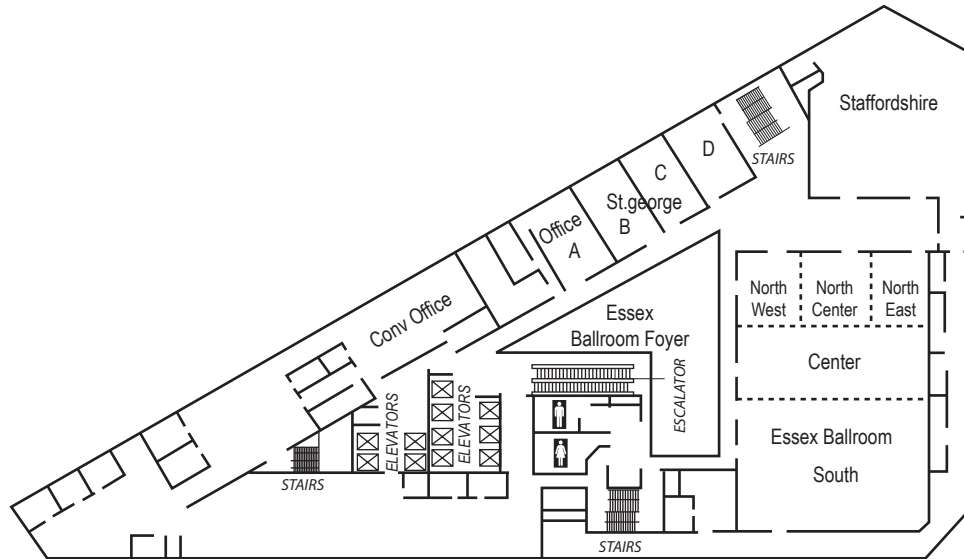
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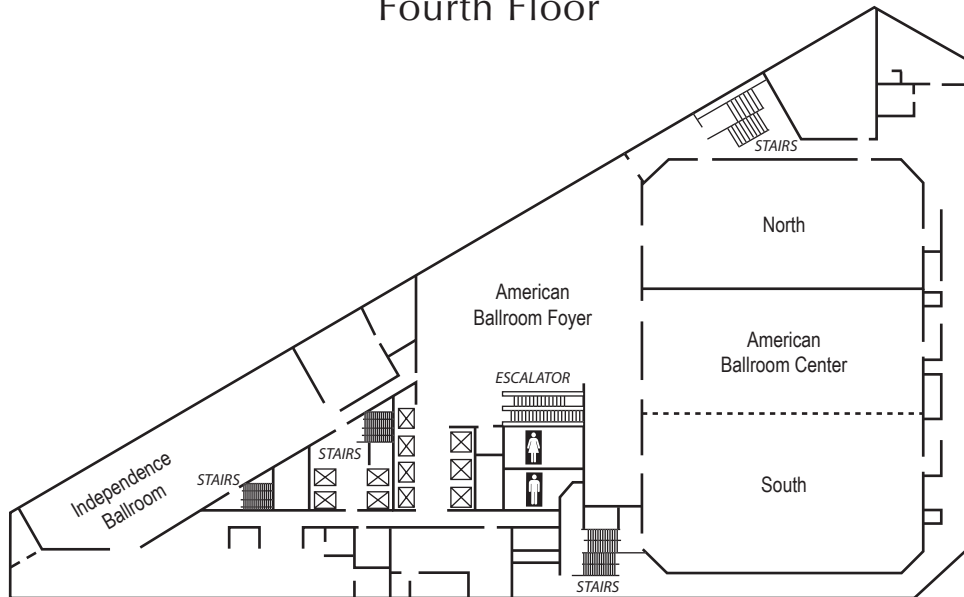


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7:00 AM – 10:00 AM 15 minute intervals
10:00 AM – 4:00 PM 30 minute intervals
4:00 PM – 11:00 PM 15 minute intervals

TUESDAY, AUGUST 18

7:00 AM – 10:00 AM 15 minute intervals
10:00 AM – 4:00 PM 30 minute intervals
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● Route 5 ● Walk to Convention Center
✕ Boarding Location

  For all shuttle enquiries and wheelchair assistance, please call 1-866-439-8564.

 Shuttle Services managed and operated by Transportation Management Services.

 Carbon Neutral Shuttles.

Scan here to download a copy of the shuttle schedule:



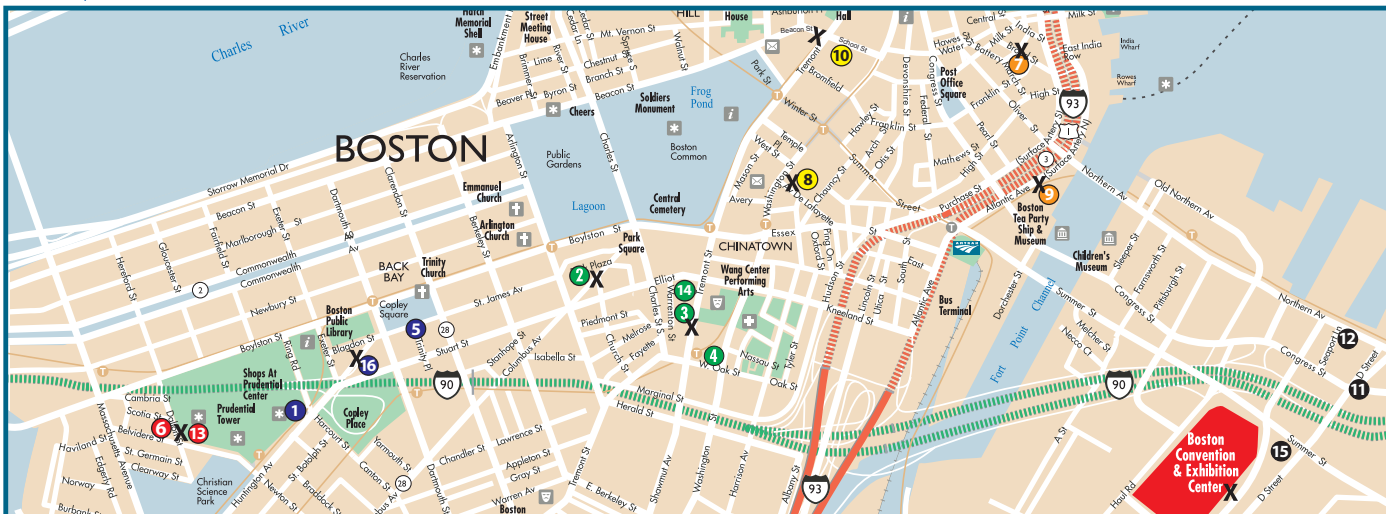


ACS
Chemistry for Life®

250th ACS National Meeting & Exposition

August 16 - 20, 2015 | Boston, MA | www.acs.org/boston2015 | [#acsBoston](https://twitter.com/acsBoston)

SHUTTLE SERVICE SCHEDULE



LEGEND ● ROUTE 1 ● ROUTE 2 ● ROUTE 3 ● ROUTE 4 ● ROUTE 5 ● WALKING X BOARDING LOCATION

HOURS OF OPERATION

Sunday, August 16

7:00 AM - 10:00 AM 15 minute intervals
 10:00 AM - 4:00 PM 30 minute intervals
 4:00 PM - 7:00 PM 15 minute intervals
 7:00 PM - 11:00 PM 15 minute intervals

Monday, August 17

7:00 AM - 10:00 AM 15 minute intervals
 10:00 AM - 4:00 PM 30 minute intervals
 4:00 PM - 11:00 PM 15 minute intervals

Tuesday, August 18

7:00 AM - 10:00 AM 15 minute intervals
 10:00 AM - 4:00 PM 30 minute intervals
 4:00 PM - 11:00 PM 15 minute intervals

Wednesday, August 19

7:00 AM - 11:00 PM 30 minute intervals

Thursday, August 20

7:00 AM - 6:00 PM 60 minute intervals



Scan here to download a copy of the shuttle schedule.



For all shuttle inquiries and wheelchair assistance, please call: **1-866-439-8564**



Shuttles are operated by Transportation Management Services. Carbon Neutral Shuttles ♻️

HOTEL ROUTE INFORMATION

Map#	Hotels	Route
1	Boston Marriott Copley Place <i>Boarding: Walk to Westin Copley Place</i>	1
2	Boston Park Plaza Hotel and Towers <i>Boarding: Valet Entrance on Columbus Avenue</i>	2
3	Courtyard Boston Downtown <i>Boarding: Curbside on Tremont Street</i>	2
4	Doubletree by Hilton Hotel Boston- Downtown <i>Boarding: Walk to Courtyard Boston Downtown</i>	2
5	Fairmont Copley Plaza <i>Boarding: Walk to Westin Copley Place</i>	1
6	Hilton Boston Back Bay <i>Boarding: Cross Dalton Street to Sheraton</i>	3
7	Hilton Boston Downtown / Faneuil Hall <i>Boarding: Curbside on Broad Street</i>	4
8	Hyatt Regency Boston <i>Boarding: Curbside on Avenue DeLafayette</i>	5
9	InterContinental Boston <i>Boarding: Curbside on Atlantic Avenue</i>	4
10	Omni Park House Hotel <i>Boarding: Corner of Beacon St. - at the Citizen Bank</i>	5
11	Renaissance Boston Waterfront <i>Walk to Boston Convention & Exhibition Center</i>	W
12	Seaport Hotel <i>Walk to Boston Convention & Exhibition Center</i>	W
13	Sheraton Boston Hotel <i>Boarding: Curbside on Dalton Street</i>	3
14	W Boston <i>Boarding: Walk to Courtyard Boston Downtown</i>	2
15	Westin Boston Waterfront <i>Walk to Boston Convention & Exhibition Center</i>	W
16	Westin Copley Place <i>Boarding: Curbside on Huntington Avenue</i>	1



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Exposition, Town Center

Boston Convention & Exhibition Center, Town Center, Halls A & B1

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through

Innovation & Passion

TUESDAY AUGUST 18TH



Westin Copley Place Hotel

BOSTON MASSACHUSETTS

Poster Session

Essex Ballroom • 8pm

ChemLuminary Awards Ceremony

America Ballroom • 9pm

Celebration

America Ballroom • 10pm

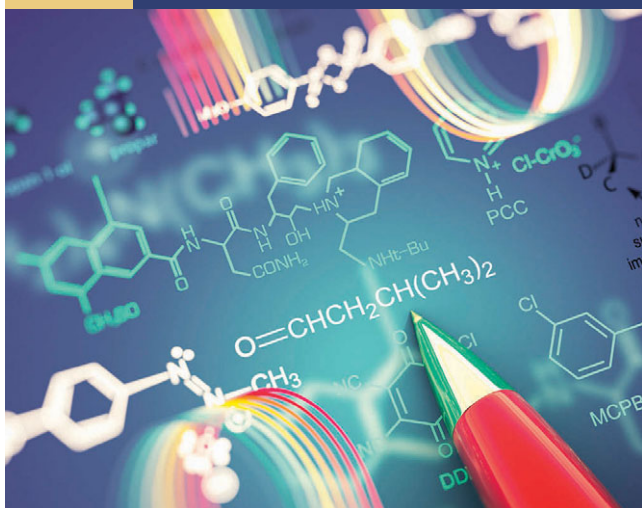


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FEDERAL FUNDERS SYMPOSIUM & SPEED COACHING



TUESDAY, AUGUST 18 • 1:00 PM–5:00 PM
BOSTON CONVENTION & EXHIBITION CENTER, ROOM 102AB



1:00 PM–3:00 PM

FEDERAL FUNDERS SYMPOSIUM

Learn about agency priorities, initiatives, programs, and how to participate!

Meet the Federal Funders from the National Science Foundation (NSF CHE, DMR, CBET, MCB and OISE), Department of Energy (DOE BES), National Institutes of Health (NIH NIGMS), Air Force Office of Scientific Research (AFOSR), and the Environmental Protection Agency (EPA)



3:00 PM–5:00 PM

SPEED COACHING

Join speed coaching — one-on-one interactions with federal funders to discuss research, education, and outreach activities.

All are welcome — registration not required!
For additional information, email: cheminfo@nsf.gov

NEW

Sci-Mix Posters:
Monday, August 17 • 8–10 pm
Hall C—Convention Center
Posters ORGN 340–342





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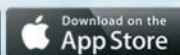
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Onsite Support – Hours of Operation

Sunday, August 16 from 8AM – 5PM
Monday, August 17 from 8AM – 5PM
Tuesday, August 18 from 8AM – 3PM
Learn more at www.acs.org/meetingapp

Boston Convention & Exhibition Center, North Lobby

Check with your division for your deadline.
Presenters – Abstract submission varies by division.

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