For meeting updates
click here.

250th American Chemical Society National Meeting & Exposition

BOSTON
August 16-20, 2015
BOSTON, MA
www.acs.org/boston2015
#acsBoston

INNOVATION from Discovery to Application

Put this book in your pocket!
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.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACS Volunteer/National Meeting</td>
<td>2</td>
</tr>
<tr>
<td>Attendee Conduct Policy</td>
<td></td>
</tr>
<tr>
<td>ACS President’s Welcome</td>
<td>4</td>
</tr>
<tr>
<td>Thematic Organizer’s Welcome</td>
<td>5</td>
</tr>
<tr>
<td>Governor’s Welcome</td>
<td>6</td>
</tr>
<tr>
<td>Mayor’s Letter</td>
<td>7</td>
</tr>
<tr>
<td>General Meeting Information</td>
<td></td>
</tr>
<tr>
<td>• Registration</td>
<td>12</td>
</tr>
<tr>
<td>• Accommodations</td>
<td>13</td>
</tr>
<tr>
<td>• Travel &amp; Transportation</td>
<td>16</td>
</tr>
<tr>
<td>• Member Services</td>
<td>17</td>
</tr>
<tr>
<td>• On-Site Arrangements</td>
<td>17</td>
</tr>
<tr>
<td>Governance &amp; Business Meetings</td>
<td></td>
</tr>
<tr>
<td>• Board of Directors &amp; Council Meetings</td>
<td>22</td>
</tr>
<tr>
<td>• Division Officers &amp; Councilor Caucus Meetings</td>
<td>22</td>
</tr>
<tr>
<td>• Governance Committee Meetings &amp; Agendas</td>
<td>22</td>
</tr>
<tr>
<td>• Division Meetings &amp; Social Events</td>
<td>26</td>
</tr>
<tr>
<td>Social &amp; Educational Events</td>
<td></td>
</tr>
<tr>
<td>• Presidential Events</td>
<td>32</td>
</tr>
<tr>
<td>• Social &amp; Ticketed Events</td>
<td>32</td>
</tr>
<tr>
<td>• Student &amp; Teacher Activities</td>
<td>35</td>
</tr>
<tr>
<td>• Workshops</td>
<td>36</td>
</tr>
<tr>
<td>• ACS Career Navigator</td>
<td>37</td>
</tr>
<tr>
<td>• ACS Career Fair</td>
<td>38</td>
</tr>
<tr>
<td>• ACS Professional Educational Short Courses</td>
<td>39</td>
</tr>
<tr>
<td>• 2015 Leadership Development System Course Offerings</td>
<td>39</td>
</tr>
<tr>
<td>• Exposition</td>
<td>41</td>
</tr>
<tr>
<td>• Exhibitor Workshops</td>
<td>41</td>
</tr>
<tr>
<td>Technical Program Summary</td>
<td></td>
</tr>
<tr>
<td>• Speaker Instructions</td>
<td>47</td>
</tr>
<tr>
<td>• Abstracts &amp; Preprints</td>
<td>47</td>
</tr>
<tr>
<td>• Technical Program Summary</td>
<td>49</td>
</tr>
<tr>
<td>Full Technical Program</td>
<td></td>
</tr>
<tr>
<td>• How to Read the Technical Program</td>
<td>68</td>
</tr>
<tr>
<td>• Index of Organizing Groups</td>
<td>69</td>
</tr>
<tr>
<td>• Technical Program (Listing of Papers)</td>
<td>70</td>
</tr>
<tr>
<td>Exposition</td>
<td></td>
</tr>
<tr>
<td>• Exposition Highlights</td>
<td>247</td>
</tr>
<tr>
<td>• Exhibitor Directory (Listing of Exhibitors)</td>
<td>248</td>
</tr>
<tr>
<td>• Exposition Floor Plan</td>
<td>267</td>
</tr>
<tr>
<td>Attendee Resources</td>
<td></td>
</tr>
<tr>
<td>• Floor Plans (Convention Center &amp; Meeting Hotels)</td>
<td>270</td>
</tr>
<tr>
<td>• Acknowledgements &amp; Thank You to Our Volunteers</td>
<td>293</td>
</tr>
<tr>
<td>• Official ACS Properties &amp; Shuttle Schedule (Addresses, Phone Numbers &amp; Map)</td>
<td>294</td>
</tr>
</tbody>
</table>

## 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

1155 16th Street, NW, Washington, DC 20036
Tel: 800-227-5558 (US only) or 202-872-4600
Fax: 202-872-4615 E-mail: help@acs.org Website: www.acs.org

The American Chemical Society is a self-governed individual membership organization of more than 158,000 members at all degree levels and in all fields of chemistry. The Society provides a broad range of opportunities for peer interaction and career development, regardless of professional or scientific interests. The programs and activities conducted by ACS today are the products of a tradition of excellence in meeting member needs that dates from the Society’s founding in 1876.

This On-site Meeting Program is published by the American Chemical Society as a service to its attendees. Information contained herein is subject to change without notice. While every effort is made to ensure accuracy, ACS makes no warranties, expressed or implied, related to the information. For the official technical program for the 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.

Adopted by the Board of Directors 12/6/13
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 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 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
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,

CHARLES D. BAKER
GOVERNOR

KARYN E. POLITO
LIEUTENANT GOVERNOR
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

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)

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, ENV, 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)
Download Your Free Boston Mobile App Today!

ACS Boston
2015 Mobile App

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

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.

American Chemical Society
PRESIDENTIAL SYMPOSIA AND EVENTS
Recommended by the 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.

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 standard registration rates, see below.

MEETING INFO ON THE WEB

Registration, housing, technical programming, special events, participating exhibitors, and other meeting details are available at www.acs.org/boston2015.

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.

<table>
<thead>
<tr>
<th>REGISTRATION CATEGORY</th>
<th>EARLY BY JAN. 30</th>
<th>STANDARD AFTER FEB. 13</th>
</tr>
</thead>
<tbody>
<tr>
<td>MEMBERS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ACS member or society affiliate</td>
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<td>$470</td>
</tr>
<tr>
<td>Postdoctoral member</td>
<td>390</td>
<td>470</td>
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<tr>
<td>Emeritus or retired member</td>
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<tr>
<td>50-year member</td>
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<td>Unemployed member (Dues waiver required)</td>
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<td>Premedical teacher</td>
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</tr>
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</tr>
<tr>
<td>Undergraduate</td>
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<td>100</td>
</tr>
<tr>
<td>One-day registrant</td>
<td>195</td>
<td>235</td>
</tr>
<tr>
<td>NONMEMBERS</td>
<td>$685</td>
<td>$825</td>
</tr>
<tr>
<td>Chemical scientist</td>
<td>390</td>
<td>470</td>
</tr>
<tr>
<td>Postdoctoral scientist</td>
<td>685</td>
<td>825</td>
</tr>
<tr>
<td>Visitor: Nonchemical scientist or chemical technician</td>
<td>390</td>
<td>470</td>
</tr>
<tr>
<td>Premedical teacher</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Graduate student</td>
<td>195</td>
<td>195</td>
</tr>
<tr>
<td>Undergraduate</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>One-day registrant</td>
<td>195</td>
<td>235</td>
</tr>
<tr>
<td>Guest of registrant*</td>
<td>40</td>
<td>40</td>
</tr>
<tr>
<td>EXPOSITION-ONLY VISITORS</td>
<td>$50</td>
<td>$50</td>
</tr>
<tr>
<td>Adult, exhibition only</td>
<td>$25</td>
<td>$25</td>
</tr>
<tr>
<td>Student, exhibition only</td>
<td>25</td>
<td>25</td>
</tr>
</tbody>
</table>

*Registration is restricted to a spouse or family member of registered attendees 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.
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 BCCEC. 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!)

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.
Make the greener meetings Pledge

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.
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, Halis A & B1.

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

**GENERAL INFORMATION**

**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: CD02CB26E8
- **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
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.

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**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.

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**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 coverages 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.

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**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 (TTD) 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.

**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
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 something 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. 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.

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 opportunities. 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
- Finance Office: Halls A & B1
- Exposition: Westin Boston Waterfront, Frost Boardroom
- Host Local Section Center: North Lobby
- Member Services: North Lobby
- Finance Office: Westin Boston Waterfront, Frost Boardroom
- 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

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.
Free Exhibitor-Sponsored Workshops

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 – 5PM

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

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

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

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 SOCITIES &
THE AMERICAN CHEMICAL SOCIETY INVITE YOU TO

PACIFICHEM 2015

Chemical Networking: Building Bridges Across The Pacific

Honolulu, Hawaii • December 15 - 20, 2015
Housing & Registration Now Open

Become an exhibitor and reserve booth space now.
Contact expo@acs.org

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

Learn more at www.pacificchem.org
GOVERNANCE & BUSINESS MEETINGS

Many members participate in meetings concerning the business of the Society, technical divisions, and governance committees in conjunction with the meeting. On the following pages, you will find a listing of the open meetings scheduled for 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.
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.

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.

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.

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
4. 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
CHEMISTRY & PUBLIC AFFAIRS
Susan B. Butts, chair; sbbuttersdc@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 Meeting
Monday, August 17, 1:30 to 2:15 PM
Sheraton Boston, Back Bay D
1. Welcome
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; gheard@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 Marriot 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; PO. 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 Vitenos, 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
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. Chair 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. ILPAC Reports
5. Update to Kilogram, Amount of Substance and Mole issues
6. Task Force on new SI definitions
7. New Business

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. Updates from ACS Publications Division

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

Open Meeting
Sunday, August 16, 4:00 to 5:00 PM
Sheraton 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

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, dsgottfried@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 — CPA, 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 Glascock, chair; Nomacor 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
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

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

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
   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
   e. Planning and Priorities
      1. SCC Fall Strategic Planning Retreat
   5. Old Business
      a. Senior Chemists Breakfast
      b. 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

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

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
## DIVISION MEETINGS & SOCIAL EVENTS

### Division of Agricultural & Food Chemistry — AGFD

<table>
<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Room</th>
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</thead>
<tbody>
<tr>
<td>Special Committee Meeting - Awards</td>
<td>Sunday, August 16</td>
<td>12:00 PM - 1:00 PM</td>
<td>Room 102A, BCEC</td>
</tr>
<tr>
<td>Executive Committee Meeting</td>
<td>Sunday, August 16</td>
<td>5:00 PM - 8:00 PM</td>
<td>Room 158, BCEC</td>
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<tr>
<td>Future Programs Planning Meeting</td>
<td>Monday, August 17</td>
<td>12:00 PM - 1:00 PM</td>
<td>Room 211, BCEC</td>
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<tr>
<td>Business Meeting</td>
<td>Tuesday, August 18</td>
<td>12:00 PM - 1:00 PM</td>
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### Division of Agrochemicals — AGRO

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<tr>
<th>Event</th>
<th>Date</th>
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<tbody>
<tr>
<td>Social/ Posters (AM Sessions)</td>
<td>Sunday, August 16</td>
<td>10:00 AM - 10:45 AM</td>
<td>Terrace Room, Boston Park Plaza</td>
</tr>
<tr>
<td>Social/ Posters (PM Sessions)</td>
<td>Sunday, August 16</td>
<td>3:00 PM - 3:45 PM</td>
<td>Terrace Room, Boston Park Plaza</td>
</tr>
<tr>
<td>General Posters</td>
<td>Sunday, August 16</td>
<td>1:00 PM - 5:00 PM</td>
<td>Terrace Room, Boston Park Plaza</td>
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<tr>
<td>Business Meeting</td>
<td>Sunday, August 16</td>
<td>5:00 PM - 9:00 PM</td>
<td>Imperial Blrm, Boston Park Plaza</td>
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<tr>
<td>Social/ Posters (AM Sessions)</td>
<td>Monday, August 17</td>
<td>10:00 AM - 10:45 AM</td>
<td>Terrace Room, Boston Park Plaza</td>
</tr>
<tr>
<td>General Posters</td>
<td>Monday, August 17</td>
<td>8:00 AM - 10:00 AM</td>
<td>Terrace Room, Boston Park Plaza</td>
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<tr>
<td>Graduate Student Luncheon</td>
<td>Monday, August 17</td>
<td>12:00 PM - 1:20 PM</td>
<td>Boylston Room, Boston Park Plaza</td>
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<tr>
<td>General Posters</td>
<td>Monday, August 17</td>
<td>1:00 PM - 5:00 PM</td>
<td>Terrace Room, Boston Park Plaza</td>
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<tr>
<td>General Posters</td>
<td>Tuesday, August 18</td>
<td>8:00 AM - 10:00 AM</td>
<td>Terrace Room, Boston Park Plaza</td>
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<tr>
<td>Social/ Posters (AM Sessions)</td>
<td>Tuesday, August 18</td>
<td>8:00 AM - 10:00 AM</td>
<td>Terrace Room, Boston Park Plaza</td>
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<tr>
<td>USDAARS Sterling B. Hendricks Reception</td>
<td>Tuesday, August 18</td>
<td>1:00 PM - 1:30 PM</td>
<td>Boylston Room, Boston Park Plaza</td>
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<tr>
<td>General Posters</td>
<td>Wednesday, August 19</td>
<td>8:00 AM - 10:00 AM</td>
<td>Terrace Room, Boston Park Plaza</td>
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<tr>
<td>Blues-N-Brews</td>
<td>Wednesday, August 19</td>
<td>5:15 PM - 7:00 PM</td>
<td>Boylston Room, Boston Park Plaza</td>
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<tr>
<td>Social/ Posters (AM Sessions)</td>
<td>Wednesday, August 19</td>
<td>10:00 AM - 10:45 AM</td>
<td>Terrace Room, Boston Park Plaza</td>
</tr>
<tr>
<td>Social/ Posters (PM Sessions)</td>
<td>Wednesday, August 19</td>
<td>3:00 PM - 3:45 PM</td>
<td>Terrace Room, Boston Park Plaza</td>
</tr>
<tr>
<td>Awards Social</td>
<td>Wednesday, August 19</td>
<td>6:00 PM - 8:00 PM</td>
<td>Boylston Room, Boston Park Plaza</td>
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### Division of Analytic Chemistry — ANYL

<table>
<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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<tbody>
<tr>
<td>Long Range Planning Meeting (Closed Meeting)</td>
<td>Friday, August 14</td>
<td>6:00 PM - 10:00 PM</td>
<td>Atlantic Blrm 3, Renaissance Boston Waterfront</td>
</tr>
<tr>
<td>General Analytical Posters</td>
<td>Saturday, August 15</td>
<td>9:00 AM - 5:00 PM</td>
<td>Atlantic Blrm 3, Renaissance Boston Waterfront</td>
</tr>
<tr>
<td>Executive Committee Meeting</td>
<td>Sunday, August 16</td>
<td>6:00 PM - 8:00 PM</td>
<td>Room 52 A/B, BCEC</td>
</tr>
<tr>
<td>Analytical Division Dinner (Ticketed Event)</td>
<td>Tuesday, August 17</td>
<td>4:00 PM - 7:00 PM</td>
<td>Spectacle Room, Renaissance Boston Waterfront</td>
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### Division of Biological Chemistry — BIOL

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<th>Event</th>
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<tr>
<td>Poster Session</td>
<td>Sunday, August 16</td>
<td>5:30 PM - 7:30 PM</td>
<td>Cityview Blrm, Seaport Hotel &amp; World Trade Center</td>
</tr>
<tr>
<td>Poster Session</td>
<td>Tuesday, August 18</td>
<td>6:00 PM - 8:00 PM</td>
<td>Galleria, Westin Boston Waterfront</td>
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Note: Due to space limitations, hotel abbreviations are used in these tables.
### Division of Business Development & Management — BMGT

<table>
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<th>Event</th>
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<tbody>
<tr>
<td>Annual Open Meeting</td>
<td>Tuesday, August 18</td>
<td>10:00 AM - 11:00 AM</td>
<td>Pacific Birm C, Renaissance Boston Waterfront</td>
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### Division of Catalysis and Surface Science — CATL

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<tr>
<td>Business Meeting</td>
<td>Monday, August 17</td>
<td>5:00 PM - 7:00 PM</td>
<td>Pacific Birm A, Renaissance Boston Waterfront</td>
</tr>
<tr>
<td>Catalysis Poster Session</td>
<td>Monday, August 17</td>
<td>6:00 PM - 8:00 PM</td>
<td>Galleria, Westin Boston Waterfront</td>
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### Division of Chemistry and Law — CHAL

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<th>Event</th>
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<tr>
<td>Drug &amp; Power Luncheon</td>
<td>Monday, August 17</td>
<td>12:00 PM - 1:30 PM</td>
<td>Room 52B, BCEC</td>
</tr>
<tr>
<td>CHAL Reception</td>
<td>Monday, August 17</td>
<td>5:00 PM - 8:00 PM</td>
<td>Room 152, BCEC</td>
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### Division of Chemical Health & Safety — CHAS

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<tr>
<td>Laboratory Safety Workshop</td>
<td>Friday, August 14</td>
<td>8:00 AM - 5:00 PM</td>
<td>Room 157A, BCEC</td>
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<tr>
<td>Laboratory Waste Management</td>
<td>Friday, August 14</td>
<td>8:00 AM - 5:00 PM</td>
<td>Room 157B, BCEC</td>
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<tr>
<td>Reactive Chemical Management</td>
<td>Saturday, August 15</td>
<td>8:00 AM - 5:00 PM</td>
<td>Room 157B, BCEC</td>
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<tr>
<td>Hazard Analysis Workshop</td>
<td>Saturday, August 15</td>
<td>8:00 AM - 5:00 PM</td>
<td>Room 157A, BCEC</td>
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<tr>
<td>How to be a More Effective Chemical Hygiene Officer Workshop</td>
<td>Saturday, August 15</td>
<td>8:00 AM - 5:00 PM</td>
<td>Room 157C, BCEC</td>
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<tr>
<td>Executive Committee Meeting</td>
<td>Sunday, August 16</td>
<td>7:15 AM - 11:30 AM</td>
<td>Seaport Birm A, Seaport Hotel &amp; World Trade Center</td>
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### Division of Chemical Education — CHED

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

<table>
<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
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<tbody>
<tr>
<td>Education Committee Meeting (Closed Meeting)</td>
<td>Saturday, Aug 15</td>
<td>1:00 PM - 3:00 PM</td>
<td>Room 107C, BCEC</td>
</tr>
<tr>
<td>Program Committee Meeting (Closed Meeting)</td>
<td>Saturday, Aug 15</td>
<td>1:00 PM - 3:00 PM</td>
<td>Room 108, BCEC</td>
</tr>
<tr>
<td>Awards Committee Meeting (Closed Meeting)</td>
<td>Saturday, Aug 15</td>
<td>1:00 PM - 3:00 PM</td>
<td>Room 109A, BCEC</td>
</tr>
<tr>
<td>Executive Meeting (Closed Meeting)</td>
<td>Saturday, Aug 15</td>
<td>3:00 PM - 6:00 PM</td>
<td>Room 107B, BCEC</td>
</tr>
<tr>
<td>Chemical Structure Association Trust (CSAT) Meeting</td>
<td>Sunday, Aug 16</td>
<td>12:00 PM - 2:00 PM</td>
<td>Adams Room, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Welcoming Reception &amp; Poster Session</td>
<td>Sunday, Aug 16</td>
<td>6:30 PM - 8:30 PM</td>
<td>Lighthouse 1, Seaport Hotel &amp; World Trade Center</td>
</tr>
<tr>
<td>Division Luncheon (Ticketed Event)</td>
<td>Tuesday, Aug 18</td>
<td>12:00 PM - 1:30 PM</td>
<td>Room 52A, BCEC</td>
</tr>
<tr>
<td>Herman Skolnik Award Reception Honoring Dr. Jurgen Bajorath</td>
<td>Tuesday, Aug 18</td>
<td>6:30 PM - 8:30 PM</td>
<td>Room 254A, BCEC</td>
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### Division of Colloid & Surface Chemistry — COLL

<table>
<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>Program/Executive Committee Meeting</td>
<td>Saturday, Aug 15</td>
<td>5:00 PM - 7:00 PM</td>
<td>Room 151B, BCEC</td>
</tr>
<tr>
<td>Social Hour/Open Business/Poster Session</td>
<td>Sunday, Aug 16</td>
<td>5:30 PM - 8:00 PM</td>
<td>Galleria, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Luncheon (Ticketed Event)</td>
<td>Tuesday, Aug 18</td>
<td>12:00 PM - 1:30 PM</td>
<td>Stone Room, Westin Boston Waterfront</td>
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### Division of Computers in Chemistry — COMP

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<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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<tbody>
<tr>
<td>Executive &amp; Program Meeting</td>
<td>Saturday, Aug 15</td>
<td>3:00 PM - 6:00 PM</td>
<td>Commonwealth A Room, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Poster Session</td>
<td>Tuesday, Aug 18</td>
<td>6:00 PM - 8:00 PM</td>
<td>Galleria, Westin Boston Waterfront</td>
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### Division of Energy & Fuel — ENFL

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<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
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<tbody>
<tr>
<td>Program Meeting</td>
<td>Sunday, Aug 16</td>
<td>12:00 PM - 2:00 PM</td>
<td>Room 102B, BCEC</td>
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<tr>
<td>Business Meeting</td>
<td>Monday, Aug 17</td>
<td>5:00 PM - 8:00 PM</td>
<td>Room 158, BCEC</td>
</tr>
<tr>
<td>Division Dinner (Ticketed Event)</td>
<td>Tuesday, Aug 18</td>
<td>6:30 PM - 9:30 PM</td>
<td>Morton's Steak House</td>
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### Division of Environmental Chemistry — ENVR

<table>
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<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>Program Planning Committee Meeting</td>
<td>Sunday, Aug 16</td>
<td>2:00 PM - 3:00 PM</td>
<td>Brookline Room, Boston Park Plaza</td>
</tr>
<tr>
<td>Long Range Planning Committee Meeting</td>
<td>Sunday, Aug 16</td>
<td>3:00 PM - 5:00 PM</td>
<td>Brookline Room, Boston Park Plaza</td>
</tr>
<tr>
<td>Business Meeting</td>
<td>Sunday, Aug 16</td>
<td>7:00 PM - 7:30 PM</td>
<td>Boylston Room, Boston Park Plaza</td>
</tr>
<tr>
<td>Executive Committee Meeting</td>
<td>Sunday, Aug 16</td>
<td>7:30 PM - 10:00 PM</td>
<td>Boylston Room, Boston Park Plaza</td>
</tr>
<tr>
<td>Social &amp; Reception (Ticketed Event)</td>
<td>Tuesday, Aug 18</td>
<td>6:00 PM - 7:30 PM</td>
<td>Back Bay Harry's</td>
</tr>
<tr>
<td>Division Dinner (Ticketed Event)</td>
<td>Tuesday, Aug 18</td>
<td>8:00 PM - 10:00 PM</td>
<td>Back Bay Harry's</td>
</tr>
<tr>
<td>General Posters</td>
<td>Wednesday, Aug 19</td>
<td>6:00 PM - 8:00 PM</td>
<td>Hall C, BCEC</td>
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### Division of Geochemistry — GEOC

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<thead>
<tr>
<th>Event</th>
<th>Date</th>
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<th>Location</th>
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<tbody>
<tr>
<td>Executive Committee Meeting (Closed Meeting)</td>
<td>Sunday, Aug 16</td>
<td>6:00 PM - 8:00 PM</td>
<td>Beacon Hill 1, Seaport Hotel &amp; World Trade Center</td>
</tr>
<tr>
<td>Division Reception</td>
<td>Tuesday, Aug 18</td>
<td>5:30 PM - 7:30 PM</td>
<td>Flagship A, Seaport Hotel &amp; World Trade Center</td>
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## Division of Industrial & Engineering Chemistry — I&EC

<table>
<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>Executive Committee Meeting (Closed Meeting)</td>
<td>Sunday, August 16</td>
<td>2:30 PM - 6:00 PM</td>
<td>Pacific Blrm E, Renaissance Boston Waterfront</td>
</tr>
<tr>
<td>I&amp;EC Graduate Symposia Luncheon (Ticketed Event)</td>
<td>Tuesday, August 18</td>
<td>11:45 AM - 12:45 PM</td>
<td>Mediterranean, Renaissance Boston Waterfront</td>
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<tr>
<td>General Posters Session</td>
<td>Tuesday, August 18</td>
<td>6:00 PM - 8:00 PM</td>
<td>Hall C, BCEC</td>
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## Division of Medicinal Chemistry — MEDI

<table>
<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>Executive Meeting (Closed Meeting)</td>
<td>Sunday, August 16</td>
<td>8:30 AM - 1:00 PM</td>
<td>Room 151B, BCEC</td>
</tr>
<tr>
<td>LRPC Meeting (Closed Meeting)</td>
<td>Monday, August 17</td>
<td>5:30 PM - 9:30 PM</td>
<td>Room 253A, BCEC</td>
</tr>
<tr>
<td>Hall of Fame Ceremony</td>
<td>Tuesday, August 18</td>
<td>5:30 PM - 7:30 PM</td>
<td>Room 52A/B, BCEC</td>
</tr>
<tr>
<td>General Poster Session</td>
<td>Sunday, August 16</td>
<td>7:00 PM - 9:00 PM</td>
<td>Galleria, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Joint MEDI/ORGN Poster Session</td>
<td>Wednesday, August 19</td>
<td>7:00 PM - 9:00 PM</td>
<td>Ballroom, BCEC</td>
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## Division of Nuclear Chemistry & Technology — NUCL

<table>
<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>Executive Committee Meeting</td>
<td>Sunday, August 16</td>
<td>5:00 PM - 7:00 PM</td>
<td>Constitution, Seaport Hotel &amp; World Trade Center</td>
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<tr>
<td>Business Meeting</td>
<td>Tuesday, August 18</td>
<td>5:00 PM - 6:00 PM</td>
<td>Waterfront 2, Seaport Hotel &amp; World Trade Center</td>
</tr>
<tr>
<td>Social Hour</td>
<td>Tuesday, August 18</td>
<td>6:00 PM - 8:00 PM</td>
<td>Cityview 1, Seaport Hotel &amp; World Trade Center</td>
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## Division of Organic Chemistry — ORGN

<table>
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<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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<tbody>
<tr>
<td>Executive Committee Meeting (Closed Meeting)</td>
<td>Sunday, August 16</td>
<td>1:00 PM - 5:00 PM</td>
<td>Seaport Blrm A, Seaport Hotel &amp; World Trade Center</td>
</tr>
<tr>
<td>Poster Session</td>
<td>Sunday, August 16</td>
<td>8:00 PM - 10:00 PM</td>
<td>Hall C, BCEC</td>
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<tr>
<td>Poster Session</td>
<td>Tuesday, August 18</td>
<td>8:00 PM - 10:00 PM</td>
<td>Hall C, BCEC</td>
</tr>
<tr>
<td>Joint MEDI/ORGN Poster Session</td>
<td>Wednesday, August 19</td>
<td>7:00 PM - 9:00 PM</td>
<td>Ballroom, BCEC</td>
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## Division of Physical Science — PHYS

<table>
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<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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<tbody>
<tr>
<td>Workshop for Undergraduates</td>
<td>Sunday, August 16</td>
<td>8:00 AM - 12:30 PM</td>
<td>Room 254A, BCEC</td>
</tr>
<tr>
<td>Poster Session</td>
<td>Wednesday, August 19</td>
<td>6:00 PM - 8:00 PM</td>
<td>Hall C, BCEC</td>
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## Division of Polymeric Materials Science & Engineering — PMSE

<table>
<thead>
<tr>
<th>Event</th>
<th>Date</th>
<th>Time</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>Membership Desk</td>
<td>Sunday, August 16</td>
<td>8:00 AM - 5:00 PM</td>
<td>Mezz Foyer, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Monday, August 17</td>
<td>8:00 AM - 5:00 PM</td>
<td>Mezz Foyer, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Tuesday, August 18</td>
<td>8:00 AM - 5:00 PM</td>
<td>Mezz Foyer, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Business Meeting &amp; PMSE/POLY Coordinatiation Meeting</td>
<td>Tuesday, August 18</td>
<td>5:00 PM - 6:00 PM</td>
<td>Douglas Room, Westin Boston Waterfront</td>
</tr>
<tr>
<td>PMSE/POLY Poster Session</td>
<td>Tuesday, August 18</td>
<td>6:00 PM - 8:00 PM</td>
<td>Ballroom West, BCEC</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Wednesday, August 19</td>
<td>8:00 AM - 5:00 PM</td>
<td>Mezz Foyer, Westin Boston Waterfront</td>
</tr>
<tr>
<td>PMSE/POLY Award Lecture Reception</td>
<td>Wednesday, August 19</td>
<td>6:00 PM - 9:00 PM</td>
<td>Grand Blrm A/B, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Thursday, August 20</td>
<td>8:00 AM - 5:00 PM</td>
<td>Mezz Foyer, Westin Boston Waterfront</td>
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</table>
## Division of Polymer Chemistry — POLY

<table>
<thead>
<tr>
<th>Event</th>
<th>Date/Time</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>Board Meeting</td>
<td>Sunday, August 16 12:00 PM - 2:00 PM</td>
<td>Harbor Blrm 1, Westing Boston Waterfront</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Sunday, August 16 9:00 AM - 5:00 PM</td>
<td>Elm 1, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Monday, August 17 9:00 AM - 5:00 PM</td>
<td>Elm 1, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Tuesday, August 18 9:00 AM - 5:00 PM</td>
<td>Elm 1, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Programming Meeting</td>
<td>Tuesday, August 18 12:00 PM - 2:00 PM</td>
<td>Harbor Blrm 1, Westing Boston Waterfront</td>
</tr>
<tr>
<td>POLY/PMSE Poster Session</td>
<td>Tuesday, August 18 6:00 PM - 8:00 PM</td>
<td>Ballroom West, BCEC</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Wednesday, August 19 9:00 AM - 5:00 PM</td>
<td>Elm 1, Westin Boston Waterfront</td>
</tr>
<tr>
<td>POLY/PMSE Award Lecture Reception</td>
<td>Wednesday, August 19 6:00 PM - 9:00 PM</td>
<td>Grand Blrm A/B, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Membership Desk</td>
<td>Thursday, August 20 9:00 AM - 5:00 PM</td>
<td>Elm 1, Westin Boston Waterfront</td>
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## Division of Professional Relations — PROF

<table>
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<tr>
<th>Event</th>
<th>Date/Time</th>
<th>Location</th>
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</thead>
<tbody>
<tr>
<td>Professional Relations - Executive Committee &amp; Open Meeting</td>
<td>Tuesday, August 18 2:00 PM - 4:00 PM</td>
<td>Room 157C, BCEC</td>
</tr>
<tr>
<td>Henry Hill’s 100th Anniversary Reception &amp; Award Program</td>
<td>Tuesday, August 18 5:00 PM - 7:00 PM</td>
<td>Plaza Blrm AB, Seaport Hotel &amp; World Trade Center</td>
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</table>

## Division of Small Chemical Business — SCHB

<table>
<thead>
<tr>
<th>Event</th>
<th>Date/Time</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>Member Breakfast</td>
<td>Sunday, August 16 7:00 AM - 8:00 AM</td>
<td>Griffin Room, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Executive Committee Meeting</td>
<td>Sunday, August 16 8:00 AM - 11:30 AM</td>
<td>Griffin Room, Westin Boston Waterfront</td>
</tr>
<tr>
<td>SCHB Luncheon</td>
<td>Sunday, August 16 11:45 AM - 1:00 PM</td>
<td>Commonwealth A, Westin Boston Waterfront</td>
</tr>
<tr>
<td>SCHB Luncheon</td>
<td>Monday, August 17 11:45 AM - 1:15 PM</td>
<td>Griffin Room, Westin Boston Waterfront</td>
</tr>
<tr>
<td>SCHB Luncheon</td>
<td>Tuesday, August 18 11:45 AM - 1:15 PM</td>
<td>Griffin Room, Westin Boston Waterfront</td>
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## Division of Toxicology — TOXI

<table>
<thead>
<tr>
<th>Event</th>
<th>Date/Time</th>
<th>Location</th>
</tr>
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<tbody>
<tr>
<td>Keynote Address</td>
<td>Tuesday, August 18 5:00 PM - 6:00 PM</td>
<td>Harbor Blrm III, Westin Boston Waterfront</td>
</tr>
<tr>
<td>Keynote Reception</td>
<td>Tuesday, August 18 5:00 PM - 6:30 PM</td>
<td>Harbor Blrm III, Westin Boston Waterfront</td>
</tr>
<tr>
<td>General Poster Session Dinner</td>
<td>Tuesday, August 18 6:30 PM - 10:30 PM</td>
<td>Grand Blrm A/B, Westin Boston Waterfront</td>
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</table>
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.

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-Academia. On Tuesday, an all-day symposium with a special symposium of past scholars throughout both industry and academia. On Tuesday, an all-day symposium will cover “Transforming University-Academia. On Tuesday, an all-day symposium with a special symposium of past scholars throughout both industry and academia.

SOCIAL & EDUCATIONAL EVENTS

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<th>Event</th>
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<tbody>
<tr>
<td>Friday, August 14</td>
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<tr>
<td>CHAS Workshop: Laboratory Waste Management Workshop</td>
<td>8:00 AM to 5:00 PM</td>
<td>BCEC, Room 157B</td>
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<tr>
<td>CHAS Workshop: How to be a More Effective CHO</td>
<td>8:00 AM to 5:00 PM</td>
<td>BCEC, Room 157A</td>
<td></td>
</tr>
<tr>
<td>COACh Workshop: COACh the COACh Training</td>
<td>8:30 AM to 5:00 PM</td>
<td>Renaissance Boston Waterfront, Pacific Blrm F&amp;G</td>
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<tr>
<td>COACh Workshop: COAChing Powerful Postdocs: Career Launch &amp; Acceleration</td>
<td>8:30 AM to 5:00 PM</td>
<td>Renaissance Boston Waterfront, Pacific Blrm F&amp;G</td>
<td></td>
</tr>
<tr>
<td>COACh Workshop: Basics of Entrepreneurship and Commercialization of Research</td>
<td>8:30 AM to 5:00 PM</td>
<td>Renaissance Boston Waterfront, Mediterranean</td>
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<tr>
<td>COACh Reception</td>
<td>5:00 to 7:00 PM</td>
<td>Renaissance Boston Waterfront, Caspian</td>
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<td>Sunday, August 16</td>
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<tr>
<td>Undergraduate Hospitality Center</td>
<td>8:00 AM to 5:00 PM</td>
<td>BCEC, Room 205A</td>
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<tr>
<td>Tuesday, August 18</td>
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<tr>
<td>ACS Career Fair</td>
<td>9:00 AM to 4:30 PM</td>
<td>BCEC, Hall B2</td>
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<tr>
<td>ACS Career Fair Workshop Room</td>
<td>9:00 AM to 6:00 PM</td>
<td>BCEC, Room 103</td>
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<tr>
<td>ACS Career Fair Workshop: Career Pathways I</td>
<td>9:00 AM to 6:00 PM</td>
<td>BCEC, Room 104C</td>
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<tr>
<td>Graduate School Reality Check: Getting in! Part 1</td>
<td>11:00 AM to 12:15 PM</td>
<td>BCEC, Room 50</td>
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<tr>
<td>ACS Board Luncheon &amp; Meeting</td>
<td>11:45 AM to 1:00 PM</td>
<td>BCEC, Ballroom West</td>
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<tr>
<td>CHED High School-College Interface Luncheon/SE-05/$45</td>
<td>Noon to 1:00 PM</td>
<td>BCEC, Room 253C</td>
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<tr>
<td>Graduate School Reality Check: You’re in Now What! Part 2</td>
<td>12:15 to 1:30 PM</td>
<td>BCEC, Room 50</td>
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<tr>
<td>SCHB Poster Session</td>
<td>1:00 to 2:00 PM</td>
<td>Westin Boston Waterfront, Webster</td>
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<tr>
<td>Mystery of Matter PBS Preview</td>
<td>1:30 to 3:00 PM</td>
<td>BCEC, Room 52AB</td>
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<tr>
<td>Networking Social with Graduate School and Research Opportunity Representatives</td>
<td>2:00 to 5:00 PM</td>
<td>BCEC, East Registration</td>
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<tr>
<td>PRES Poster Session</td>
<td>3:00 to 6:00 PM</td>
<td>Westin Boston Waterfront, Galleria</td>
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<tr>
<td>International and Domestic Chapters Panel Discussions</td>
<td>4:00 to 5:30 PM</td>
<td>BCEC, Room 205A</td>
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<tr>
<td>Regional Networking Event: Asia Pacific</td>
<td>4:00 to 5:00 PM</td>
<td>Sheraton Boston Hotel, Liberty A</td>
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</table>
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 Halls 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
SciFind® 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 205A
CHAL Drug & Power Luncheon/SE-13/$40
Noon to 1:30 PM, BCEC, Room 258A
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, BCEC, Constitution A/B
University of Rochester Alumni Social Hour
3:00 to 4:00 PM, Westin Boston Waterfront, Revere
<table>
<thead>
<tr>
<th>Event</th>
<th>Time</th>
<th>Location</th>
<th>Sponsor/Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACS Career Fair Workshop:</td>
<td>8:00 AM to 6:00 PM</td>
<td>BCEC, Room 106</td>
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<tr>
<td>Career Pathways III</td>
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<tr>
<td>ACS Career Fair</td>
<td>9:00 AM to 5:00 PM</td>
<td>BCEC, Hall B2</td>
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<tr>
<td>ACS Exposition</td>
<td>9:00 AM to 5:00 PM</td>
<td>BCEC, Halls A/B1</td>
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<tr>
<td>ACS Career Fair Workshop:</td>
<td>9:00 AM to 6:00 PM</td>
<td>BCEC, Room 104C</td>
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<td>Career Pathways I</td>
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<tr>
<td>Elsevier — How to Successfully Publish Scientific Articles</td>
<td>9:30 AM to 12:00 PM</td>
<td>BCEC, Room 52AB</td>
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<tr>
<td>CDD Vision Workshop, Sponsor: Collaborative Drug Discovery</td>
<td>9:30 AM-12:00 PM</td>
<td>BCEC, Exhibit Halls A &amp; B1</td>
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<td>Exhibitor Workshop Room 1</td>
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<tr>
<td>What's New from Waters, Sponsor: Waters</td>
<td>9:30 AM to 12:00 PM</td>
<td>BCEC, Exhibit Halls A &amp; B1</td>
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<td>Exhibitor Workshop Room 2</td>
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<tr>
<td>FTIR, atomic spectroscopy, HPLC, GC, and Mass Spectrometry, Sponsor:</td>
<td>9:30 AM to 6:00 PM</td>
<td>BCEC, Room 101</td>
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<td>Agilent Technologies</td>
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<tr>
<td>SciFinder® Skill Builder: Substance Searching, Sponsor: CAS</td>
<td>10:00 AM to 11:00 AM</td>
<td>BCEC, Room 258B</td>
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<tr>
<td>WCC/Eli Lilly Poster Session</td>
<td>11:00 AM to 12:00 PM</td>
<td>Sheraton Boston Hotel, Republic A/B</td>
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<td>Alpha Chi Sigma Luncheon/$20 (RSVP to <a href="mailto:gpa@alphachisigmas.org">gpa@alphachisigmas.org</a>)</td>
<td>11:30 AM to 1:30 PM</td>
<td>Atlantic Beer Garden</td>
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<tr>
<td>I&amp;EC Graduate Symposia Luncheon/$40</td>
<td>11:45 AM to 12:45 PM</td>
<td>Renaissance Boston Waterfront, Mediterranean</td>
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<tr>
<td>The State-Of-The-Art in Infrared and Raman Analysis, Sponsor: Bruker</td>
<td>12:30 PM to 3:00 PM</td>
<td>BCEC, Room 258B</td>
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<td>Research in Germany Science Lunch, Sponsor: Research in Germany</td>
<td>12:30 PM to 3:00 PM</td>
<td>BCEC, Exhibit Halls A &amp; B1</td>
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<tr>
<td>Exhibitor Workshop Room 1</td>
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<tr>
<td>New Applications in High Resolution Accurate Mass (HR/AM) Mass Spectrometry, Sponsor: Thermo Scientific</td>
<td>12:30 PM to 3:00 PM</td>
<td>BCEC, Exhibit Halls A &amp; B1</td>
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<tr>
<td>AGFD Poster Session</td>
<td>3:00 to 5:00 PM</td>
<td>BCEC, Halls A/B1</td>
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<tr>
<td>WCC ’Just Cocktails’ Open Meeting</td>
<td>4:00 to 5:00 PM</td>
<td>Westin Boston Waterfront, Stone</td>
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<td>Division Councilors &amp; Officers Caucus</td>
<td>4:00 to 5:30 PM</td>
<td>BCEC, Room 107A</td>
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<tr>
<td>Committee on Science Networking Session &amp; Panel</td>
<td>4:00 to 6:30 PM</td>
<td>BCEC, Liberty A/B</td>
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<tr>
<td>I&amp;EC Poster Session</td>
<td>5:00 to 6:30 PM</td>
<td>BCEC, Hall C</td>
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<tr>
<td>Henry Hill’s 100th Anniversary Reception and Award Program</td>
<td>5:00 to 7:00 PM</td>
<td>Seaport Hotel and World Trade Center, Plaza Blrm A/B</td>
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<tr>
<td>University of New Hampshire Chemistry Reception</td>
<td>5:00 to 7:30 PM</td>
<td>Westin Boston Waterfront, Revere</td>
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<tr>
<td>AGRO Blues-N-Brew</td>
<td>5:30 to 6:30 PM</td>
<td>Boston Park Plaza, Boylston Room</td>
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</table>
### 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

### 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

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**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

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**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

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**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 BION), 2:00 to 4:00 PM

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 OFFICE. The Graduate & Postdoctoral Scholars Office with support from the Graduate Education Advisory Board and ACS Corporation Associates, 4:00 to 5:30 PM

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 list. Participation is open to all interested registrants.

Division of Chemical Health & Safety (CHAS)-sponsored workshop fees (unless otherwise indicated). CHAS members: full registration $375/early registration $300; non-CHAS members: 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 skills to assess 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: Samuel 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-
erating 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.

**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 mindset 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 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 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
DISPERSSIONS 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.

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 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.
Free Exhibitor-Sponsored Workshops

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 – 5PM

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

- 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!
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 GOG 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-
For more confident analyses.

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.


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.

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 & 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 applications 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:** Thales Nano 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:** PANalitical, 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 \( P \), \( pK_a \), 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.
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

www.acs.org/boston2015
#acsBoston
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
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*
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 & AUDIOVISUAL 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.


Polymer Chemistry. Kathy Mitchem, e-mail: kathyl@vt.edu
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
## Presidential Events

*Diane Grob Schmidt, Program Chair*

<table>
<thead>
<tr>
<th>Event</th>
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<tr>
<td>National Science Foundation’s Centers for Chemical Innovation** &lt;sup&gt;IDA&lt;/sup&gt;</td>
<td>Boston Convention &amp; Exhibition Center</td>
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<td>21st Century Chemistry Education: Formal &amp; Informal**</td>
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<td>ACS Scholars: Rising Stars in Academe**</td>
<td>Boston Convention &amp; Exhibition Center</td>
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<td>ACS Scholars: Rising Stars in Industry**</td>
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<td>Transforming University-Industry Partnerships for an Innovative Future**</td>
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<td>Professional Legacy of Henry Hill* (PROF)</td>
<td>Boston Convention &amp; Exhibition Center</td>
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<td>The Chemistry Enterprise in 2015* (BMGT)</td>
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<td>Memories of Henry Hill: His Legacy in Science &amp; in Professional Service* (HIST)</td>
<td>Boston Convention &amp; Exhibition Center</td>
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<td>Younger Chemists Exchanging More than Currency: First—Euros &amp; Dollars; Next—Rupees, Rands &amp; Reais* (YCC)</td>
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<td>Leadership Skills as a Strategic Advantage: The Chemist’s Competitive Edge* (BMGT)</td>
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<td>The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector * (SCHB)</td>
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<td>Henry A. Hill Centennial Symposium: Innovation in Polymer Science* (POLY)</td>
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<td>International Entrepreneurship: How To Start a Business &amp; Thrive in the Global Marketplace* (IAC)</td>
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## Multidisciplinary Program Planning Group (continued)

*R. Wagner, Program Chair*

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<td>Innovation in Health &amp; Medicine** &lt;sup&gt;IDA&lt;/sup&gt;</td>
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## National Science Foundation’s Centers for Chemical Innovation** <sup>IDA</sup>

- **Public Perception of the Chemistry Enterprise**<sup>IDA</sup>
- **The Fred Kavli Innovations in Chemistry Lecture**<sup>IDA</sup>
- **The Kavli Foundation Emerging Leader in Chemistry Lecture**<sup>IDA</sup>
- **The Future of Innovation Now**<sup>IDA</sup>
- **Fifty Years of Innovation: The Legacy of the Westheimer Report**<sup>IDA</sup>
- **Innovation in Materials for Emerging Uses**<sup>IDA</sup>
- **Innovation in Chemical Synthesis**<sup>IDA</sup>
### Division of Agricultural & Food Chemistry (continued)

**B. Park, Program Chair**

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<td>Browned Flavors: Analysis, Formation &amp; Physiology</td>
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<td>Recovery of Bioactive Compounds from Processing By-Products</td>
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<td>Chemistry &amp; Bioactivities of Natural Polymethoxyflavones</td>
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<td>The Future of Innovation Now* (MPPG)</td>
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<td>Journal of Agricultural &amp; Food Chemistry Best Paper Awards* (AGRO)</td>
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<td>Current Topics in Chemical Safety Information* (CHAS)</td>
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<td>Nanoparticles in Food, Agricultural &amp; Environmental Settings* (COLL)</td>
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### Division of Agrochemicals

**P. Rice, Program Chair**

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<td>Innovations in Agrochemical Discovery &amp; 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</td>
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<td>Combining Scientific Evidence for Health Policy &amp; Regulation**</td>
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<td>Pesticide Dose: Effects on the Environment &amp; Target &amp; Non-Target Organisms**</td>
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<td>Insecticide Action on Ion Channels: A Tribute to Professor Toshio Narahashi</td>
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<td>Urban Agriculture: Turf, Ornamentals, Household Products &amp; Water Re-Use**</td>
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<td>Global Research Needs: Identifying &amp; Prioritizing Efforts To Sustain Environmental Quality**</td>
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<td>Metabolites from Endophytic Microorganism To Combat Biotic Stress in Crop Plants**</td>
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<td>Environmental Fate, Transport &amp; Modeling of Agricultural Chemicals**</td>
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<td>Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications**</td>
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<td>Innovation in Metabolism, Bioavailability &amp; Formulations Research Leading to the Discovery of Agrochemicals: Symposium Honoring Dr. Keith D. Wing; AGRO International Award for Research in Agrochemicals**</td>
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<td>Biochemical Biopesticides: Discovery &amp; Regulation of New &amp; Potential Products**</td>
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<td>Endangered Species Risk Assessment for Pesticides: Advances in Methods &amp; Process**</td>
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### Division of Agrochemicals (continued)

**P. Rice, Program Chair**

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<td>USDA-ARS Sterling B. Hendricks Memorial Lectureship: James H. Tumlinson**</td>
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<td>Immunochemistry Summit XII: Immunoassays &amp; Other Bioanalytical Techniques**</td>
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<td>Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis &amp; Ecological Effects**</td>
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<td>Pollinators &amp; Agrochemicals**</td>
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<td>Pesticides &amp; Hydrophobic Compounds in Sediment**</td>
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<td>Environmental Fate, Management &amp; Mitigation of Nitrogen in Agricultural Systems**</td>
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<td>Degradation of Halogenated Compounds in the Environment**</td>
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<td>Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage &amp; Monitoring Data**</td>
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<td>Recent Advances in the Analysis of Environmental Contaminants in Foods &amp; Feeds**</td>
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<td>Formulation Technologies for Improved Crop Protection**</td>
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<td>Structure Elucidation in Metabolism Studies: Plant, Animal &amp; Soil**</td>
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<td>Spray Application Technology**</td>
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<td>Data to Decisions: Software Solutions for Modern Analytical Workflows**</td>
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<td>Biomonitoring for Pesticide Exposures**</td>
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<td>Hydrothermal Carbonization: Possibilities &amp; Limits for Feedstocks, Processes &amp; Applications* (ENVR)</td>
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<td>National Science Foundation’s Centers for Chemical Innovation* (PRES)</td>
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<td>21st Century Chemistry Education: Formal &amp; Informal* (PRES)</td>
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<td>Memories of Henry Hill: His Legacy in Science &amp; in Professional Service* (HIST)</td>
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### Division of Agrochemicals (continued)

**P. Rice, Program Chair**

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<td>ACS Scholars: Rising Stars in Academe* (PRES)</td>
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<td>Sensing of Environmentally Relevant Contaminants* (ENVR)</td>
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<td>ACS Scholars: Rising Stars in Industry* (PRES)</td>
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<td>The Future of Innovation Now* (MPPG)</td>
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<td>Reclamation, Remediation, Restoration: Novel Approaches to Environmental Challenges* (ENVR)</td>
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<td>Microorganism-Membrane Interactions: Towards Understanding Pathogen Removal &amp; Membrane Biofouling* (ENVR)</td>
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<td>Transforming University-Industry Partnerships for an Innovative Future* (PRES)</td>
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<td>Starting-Up &amp; Spinning-Out: Commercializing Innovative Chemistry* (SCHB)</td>
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<td>Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas &amp; Professor Mehmet A. Oturan* (ENVR)</td>
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<td>Computational Toxicology: From QSAR Models to Adverse Outcome Pathways* (CINF)</td>
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<td>Detection &amp; Fate of Health-Related Microorganisms in Water* (ENVR)</td>
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<td>Using Passive Sampling Techniques To Detect Organic Contaminants* (ENVR)</td>
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*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
### Division of Analytical Chemistry

**D. Duckworth, Program Chair**

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

**C. Crews, V. Bandarian, Program Chairs**

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<td>Gordon Hammes Award Lecture</td>
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<td>Repligen Award for the Chemistry of Biological Processes</td>
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<td>Chemical Biology Approaches to Probe Ubiquitin-like Signaling</td>
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<td>Innovative Platforms for Drug Discovery, Diagnostics &amp; Target Validation</td>
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<td>Eli Lilly Award in Biological Chemistry</td>
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<td>Graduate Student &amp; Postdoctoral Symposium</td>
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<td>Advances in Oligonucleotide Therapeutics* (CARB)</td>
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<td>Metabolites from Endophytic Microorganisms To Combat Biotic Stress in Crop Plants* (AGRO)</td>
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<td>Biochemical Biopesticides: Discovery &amp; Regulation of New &amp; Potential Products* (AGRO)</td>
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### Division of Business Development & Management

**K. Allen, J. Bryant, Program Chairs**

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<td>Leadership Skills as a Strategic Advantage: The Chemist’s Competitive Edge**</td>
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<td>Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)</td>
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<td>Academic Innovations for Tomorrow’s Industries: GSSPC Symposium* (CHED)</td>
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<td>Women in Innovation: Business &amp; Commerce* (PROF)</td>
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### Division of Carbohydrate Chemistry (continued)

**E. Rozners, Program Chair**

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<td>Fundamental &amp; Applied Aspects of Glyconanotechnology</td>
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<td>New Strategies &amp; Applications of Aminoglycosides**</td>
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<td>Glycolipid Immunostimulants**</td>
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<td>Carbohydrate Synthesis for Medicinal Chemistry &amp; Biology</td>
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<td>National Science Foundation’s Centers for Chemical Innovation* (PRES)</td>
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<td>True Stories from Entrepreneurs: BRIC Edition* (SCHB)</td>
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<td>21st Century Chemistry Education: Formal &amp; Informal* (PRES)</td>
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### Division of Catalysis Science & Technology

**K. Ramasamy, Program Chair**

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<td>Symposium Honoring Gary Haller</td>
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<td>Role of the Outer Coordination Sphere on the Activity of Enzymes &amp; Molecular Catalysts</td>
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<td>Metal Organic Frameworks for Catalysis Applications</td>
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<td>In Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles</td>
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<td>CO₂ Reduction &amp; Utilization</td>
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<td>Catalytic Upgrading of Biomass</td>
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<td>Energy Storage Applications of Ammonia: Synthesis, Storage, Cracking &amp; Utilization</td>
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<td>Biofuels for Powering the World: Discovery to Application* (ENFL)</td>
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<td>Innovative Chemistry &amp; Electrocatalysis for Low-Carbon Energy &amp; Fuels: Discovery to Application* (ENFL)</td>
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## Division of Catalysis Science & Technology (continued)

**K. Ramasamy, Program Chair**

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<td>Advances in Ceria-Based Catalysis: Structural, Electronic &amp; Chemical Properties Tailored for Chemical Conversion* (ENFL)</td>
<td>Renaissance Boston Waterfront</td>
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## Division of Chemical Education (continued)

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

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## Division of Chemical Health & Safety

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

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### Division of Chemical Information

**E. Davis, Program Chair**

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### Division of Chemical Toxicology

**A. C. Bryant-Friedrich, Program Chair**

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*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
## Division of Chemistry & the Law

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

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## Division of Colloid & Surface Chemistry

R. Nagarajan, Program Chair

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### Division of Computers in Chemistry

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

**Boston Convention & Exhibition Center**

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<td>Computational Study of Water</td>
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*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.

**Primary organizer of a cosponsored symposium.

IDA: Innovation from Discovery to Application

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### Division of Computers in Chemistry (continued)

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

**Boston Convention & Exhibition Center**

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<td>From Diradicals &amp; Polyradicals to Functionalized Materials: Theory Meets Experiment* (PHYS)</td>
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<td>Electronic Structure Methods for Large Systems* (PHYS)</td>
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<td>Undergraduate Research Posters* (CHED)</td>
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<td>Computational Toxicology: From QSAR Models to Adverse Outcome Pathways* (CINF)</td>
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### Division of Energy & Fuels

**A. Park, X. Wang, Program Chairs**

**Boston Convention & Exhibition Center**

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<td>Solar Energy &amp; Solar Cells</td>
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<td>Biofuels for Powering the World: Discovery to Application**</td>
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<td>Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization &amp; Storage**</td>
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<td>Innovative Chemistry &amp; Electrocatalysis for Low-Carbon Energy &amp; Fuels: Discovery to Application**</td>
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<td>Porous Materials for Energy &amp; Sustainability from Discovery to Application</td>
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<td>Energy &amp; Fuels Joint Award for Excellence in Publication: Honoring Phillip E. Savage</td>
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### Division of Energy & Fuels (continued)

**A. Park, X. Wang, Program Chairs**

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<td>International Symposium on Mesoporous Zeolites**</td>
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<td>Advances in Analytical Methods for Petroleum Upstream Applications</td>
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<td>Innovative Utilization Pathways for Natural Gas**</td>
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<td>Next Generation Nanomaterials: Advances &amp; Perspectives for Biomedicine, Energy &amp; Environmental Protection* (ENVR)</td>
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<td>National Science Foundation’s Centers for Chemical Innovation* (PRES)</td>
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<td>21st Century Chemistry Education: Formal &amp; Informal* (PRES)</td>
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<td>Memories of Henry Hill: His Legacy in Science &amp; in Professional Service* (HIST)</td>
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<td>ACS Scholars: Rising Stars in Academe* (PRES)</td>
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<td>What’s in Your Chemical Toolbox?* (SOCED)</td>
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<td>ACS Scholars: Rising Stars in Industry* (PRES)</td>
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<td>Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage &amp; Materials* (ENVR)</td>
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<td>Transforming University-Industry Partnerships for an Innovative Future* (PRES)</td>
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<td>Academic Innovations for Tomorrow’s Industries: GSSPC Symposium* (CHED)</td>
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<td>Advances in Chemistry for Carbon Capture, Utilization &amp; Sequestration* (ENVR)</td>
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IDA: Innovation from Discovery to Application

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### Division of Environmental Chemistry

**D. Dionysiou, Program Chair**

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<td>Assessing Transformation Products by Non-Target &amp; Suspected Target Screening: The New Frontier in Environmental Chemistry &amp; Engineering</td>
<td>Boston Park Plaza Hotel &amp; Towers</td>
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<td>New Challenges in Water Quality, Treatment, Reuse &amp; Sustainability: Chemistry &amp; Application of Advanced Oxidation Processes for Removal of Contaminants of Concern &amp; Transformation Products**</td>
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<td>Hydrothermal Carbonization: Possibilities &amp; Limits for Feedstocks, Processes &amp; Applications**</td>
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<td>Advances in Drinking Water Disinfection: By-products' Occurrence, Formation, Treatment, Health Effects, Epidemiology &amp; Regulation</td>
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<td>Nano-enabled Environmental Technologies</td>
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<td>Designing Safer Chemicals**</td>
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<td>Heterogeneous Catalysis for Environmental Applications**</td>
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<td>Green Chemistry &amp; the Environment**</td>
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<td>Sensing of Environmentally Relevant Contaminants**</td>
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<td>Advanced Materials &amp; Technologies for Desalination &amp; Wastewater Reuse</td>
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<td>ACS Award for Creative Advances in Environmental Science &amp; Technology: Honoring Dr. Paul B. Shepson</td>
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<td>Reclamation, Remediation, Restoration: Novel Approaches to Environmental Challenges**</td>
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<td>Microorganism-Membrane Interactions: Toward Understanding Pathogen Removal &amp; Membrane Biofouling**</td>
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<td>Next Generation Nanomaterials: Advances &amp; Perspectives for Biomedicine, Energy &amp; Environmental Protection**</td>
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<td>Environmental Applications &amp; Implications of Graphene-Based Nanomaterials</td>
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### Division of Environmental Chemistry (continued)

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<td>Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas &amp; Professor Mehmet A. Oturan**</td>
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<td>C. Ellen Gonter Awards Symposium</td>
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<td>The Debate: How Do We Respond to Climate Change?**</td>
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<td>Status &amp; Trends of Biological &amp; Persistent Organic Chemicals in the Great Lakes</td>
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<td>Anaerobic Sewage Treatment: Dissolved Methane &amp; Nitrogen Control</td>
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<td>Environmental Transformation of Nanoparticles: Processes, Mechanisms &amp; Ecological Impacts</td>
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<td>Resource Recovery &amp; Contaminant Elimination in Waste Streams of Increasing Concern</td>
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<td>Detection &amp; Fate of Health-Related Microorganisms in Water**</td>
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<td>Using Passive Sampling Techniques To Detect Organic Contaminants**</td>
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<td>Advances in Chemistry for Carbon Capture, Utilization &amp; Sequestration**</td>
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<td>Biofuels for Powering the World: Discovery to Application* (ENFL)</td>
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<td>Carbon Management: Recent Advances in Carbon Capture, Conversion, Utilization &amp; Storage* (ENFL)</td>
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<td>Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols &amp; Clouds* (PHYS)</td>
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<td>Pesticide Dose: Effects on the Environment &amp; Target &amp; Non-Target Organisms* (AGRO)</td>
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<td>Latest Trends in Environmental Fate &amp; Exposure Assessments: Filling in Knowledge &amp; Data Gaps across the Commodity Groups* (AGRO)</td>
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<td>Current Topics in Seed Treatment* (AGRO)</td>
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<td>Urban Agriculture: Turf, Ornamentals, Household Products &amp; Water Re-use* (AGRO)</td>
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<td>Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)</td>
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<td>Global Research Needs: Identifying &amp; Prioritizing Efforts To Sustain Environmental Quality* (AGRO)</td>
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<td>ACS Scholars: Rising Stars in Academe* (PRES)</td>
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<td>Environmental Fate, Transport &amp; Modeling of Agricultural Chemicals* (AGRO)</td>
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<td>Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications* (AGRO)</td>
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<td>Endangered Species Risk Assessment for Pesticides: Advances in Methods &amp; Process* (AGRO)</td>
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<td>Transforming University-Industry Partnerships for an Innovative Future* (PRES)</td>
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<td>Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis &amp; Ecological Effects* (AGRO)</td>
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<td>Pollinators &amp; Agrochemicals* (AGRO)</td>
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<td>Subsurface Geochemistry for Energy &amp; the Environment* (GEOC)</td>
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<td>Pesticides &amp; Hydrophobic Compounds in Sediment* (AGRO)</td>
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<td>Environmental Fate, Management &amp; Mitigation of Nitrogen in Agricultural Systems* (AGRO)</td>
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<td>Degradation of Halogenated Compounds in the Environment* (AGRO)</td>
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<td>Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage &amp; Monitoring Data* (AGRO)</td>
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<td>Recent Advances in the Analysis of Environmental Contaminants in Foods &amp; Feeds* (AGRO)</td>
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### Division of Environmental Chemistry (continued)

**D. Dionysiou, Program Chair**

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<td>Formulation Technologies for Improved Crop Protection* (AGRO)</td>
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<td>Computational Toxicology: From QSAR Models to Adverse Outcome Pathways* (CINF)</td>
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<td>Spray Application Technology* (AGRO)</td>
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<td>Data to Decisions: Software Solutions for Modern Analytical Workflows* (AGRO)</td>
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<td>Biomonitoring for Pesticide Exposures* (AGRO)</td>
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### Division of the History of Chemistry

**S. Rasmussen, Program Chair**

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<td>Edwin Land &amp; Instant Photography: Massachusetts’s First National Historic Chemical Landmark</td>
<td>Boston Convention &amp; Exhibition Center</td>
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<td>Memories of Henry Hill: His Legacy in Science &amp; in Professional Service**</td>
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<td>HIST Tutorial &amp; General Papers**</td>
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<td>HIST Award Symposium Honoring Christoph Meinel</td>
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<td>Professional Legacy of Henry Hill* (PROF)</td>
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<td>The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)</td>
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<td>Fifty Years of Innovation: The Legacy of the Westheimer Report* (MPPG)</td>
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<td>Henry A. Hill Centennial Symposium: Innovation in Polymer Science* (POLY)</td>
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### Division of Fluorine Chemistry

**V. Petrov, Program Chair**

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<td>Radiochemistry**</td>
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### Division of Geochemistry

**Y. Jun, Program Chair**

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<td>Subsurface Geochemistry for Energy &amp; the Environment**</td>
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<td>General Geochemistry Session</td>
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<td>Biogeochemical Cycling of Nutrients &amp; Contaminants in Physically Complex Environments</td>
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<td>Transformation &amp; Transport of Radionuclides in the Environment* (NUCL)</td>
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### Division of Industrial & Engineering Chemistry

**P. Smith, Program Chair**

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<td>Renaissance Boston Waterfront</td>
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<td>Industrial &amp; Engineering Fellow: Honoring Kenneth L. Nash</td>
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<td>Industrial &amp; Engineering Fellow: Honoring Henry C. (Hank) Foley</td>
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<td>Industrial &amp; Engineering Fellow: Honoring Gary M. Seabolt</td>
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<td>Industrial &amp; Engineering Chemistry Division Graduate Student Award Symposium</td>
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<td>Green Chemistry Makes a Difference: Pharmaceutical Industry/Academic Collaborations**</td>
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<td>General Papers</td>
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<tr>
<td>True Stories from Entrepreneurs: BRIC Edition* (SCHB)</td>
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### Division of Industrial & Engineering Chemistry (continued)

**P. Smith, Program Chair**

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<tr>
<td>Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)</td>
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<tr>
<td>Undergraduate Research Posters* (CHED)</td>
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<tr>
<td>Incorporating Green Chemistry Innovations &amp; Applications into the Classroom &amp; Outreach* (CHED)</td>
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<tr>
<td>The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)</td>
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<td>Starting Up &amp; Spinning Out: Commercializing Innovative Chemistry* (SCHB)</td>
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<td>Big Chemistry from Small Businesses* (SCHB)</td>
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<td>International Symposium on Mesoporous Zeolites* (ENFL)</td>
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### Division of Inorganic Chemistry

**S. Koch, N. Radu, Program Chairs**

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<tr>
<td>Building Innovative Solid-State Materials through Solution Chemistry</td>
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<td>Nanoscience</td>
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<tr>
<td>Environmental &amp; Energy-Related Inorganic Chemistry</td>
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<tr>
<td>Inorganic Chemistry Lectureship</td>
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<td>Industrial Inorganic Chemistry: Innovation from Discovery to Applications</td>
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<td>Molecular Water Oxidation Catalysis</td>
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<td>High-Energy Organometallic Complexes: Reactivity Driving New Synthesis &amp; Catalysis</td>
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<td>Metalloprotein Inhibitors: Drugs, Drug Candidates &amp; New Targets at the Interface of Medicinal &amp; Inorganic Chemistry</td>
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<td>Inorganic Nanoscience Award</td>
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<td>Inorganic Spectroscopy</td>
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<td>Transition-Metal-Catalyzed Olefin Polymerization: Toward Structure Control* (PMSE)</td>
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<td>2015 ACS Catalysis Lectureship* (CATL)</td>
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<td>Undergraduate Research Posters* (CHED)</td>
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<td>Innovation in Chemical Synthesis* (MPPG)</td>
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<td>International Symposium on Mesoporous Zeolites* (ENFL)</td>
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<tr>
<td>Polymer Concepts in Inorganic Chemistry Courses* (CHED)</td>
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*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
## Division of Medicinal Chemistry

**MEDI**

**Boston Convention & Exhibition Center**

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<td>Protein-Protein Interactions</td>
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<td>Ophthalmic Drug Discovery</td>
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<td>Emerging Antibody Drug Conjugates: Applications of Medicinal Chemistry</td>
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<td>Advances in Predictive Toxicology</td>
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<td>Strategies in the Design &amp; Characterization of Allosteric Inhibitors</td>
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<td>Cancer Immunotherapy: The Next Big Thing for Small Molecules</td>
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<td>Medicinal Chemistry Toolbox: Understanding the Roles of Inducible Pockets, Water &amp; Small Structural Changes</td>
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<td>Recent Advances in Heart Failure</td>
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<td>Integrated Approaches in Structure-Based Drug Design* (COMP)</td>
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<td>Advances in Oligonucleotide Therapeutics* (CARB)</td>
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<td>Innovation from Discovery to Application Plenary Session* (MPPG)</td>
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<td>Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits* (CHED)</td>
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<td>Innovation in Health &amp; Medicine* (MPPG)</td>
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<td>New Strategies &amp; Applications of Aminoglycosides* (CARB)</td>
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<td>The Future of Innovation Now* (MPPG)</td>
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## Division of Nuclear Chemistry & Technology

**NUCL**

**J. Terry, D. Hobart, Program Chairs**

**Seaport Hotel and World Trade Center**

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<td>Analytical Chemistry in Nuclear Technology</td>
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<td>Transformation &amp; Transport of Radionuclides in the Environment**</td>
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<td>General Topics in Nuclear &amp; Radiochemistry</td>
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## Division of Organic Chemistry

**ORG N**

**M. McIntosh, R. Broene, Program Chairs**

**Boston Convention & Exhibition Center**

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<td>Molecular Recognition &amp; Self-Assembly</td>
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<td>Asymmetric Reactions &amp; Syntheses</td>
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<td>Nanomaterials</td>
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<td>Peptides, Proteins &amp; Amino Acids</td>
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<td>Small Splash, Big Waves: Research at Primarily Undergraduate Institutions</td>
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<td>JOC/OL Lectureship Symposium</td>
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<td>E</td>
<td>Asymmetric Reactions &amp; Syntheses; Chemistry of Fullerenes, Carbon Nanotubes &amp; Graphene; Materials, Devices &amp; Switches; Nanomaterials; Physical Organic Magnetically Recyclable Nanocatalysts</td>
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### Division of Organic Chemistry (continued)

**M. McIntosh, R. Broene, Program Chairs**

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

**E. Sibert, Program Chair**

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<td>Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability &amp; Spectroscopic Signatures*</td>
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<tr>
<td>From Diradicals &amp; Polyradicals to Functionalized Materials: Theory Meets Experiment**</td>
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<td>Protein-Nanomaterial Interfaces &amp; Protein Coronas: Physical Properties, Biocompatibility &amp; Biological Impact**</td>
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<td>Structure &amp; Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies**</td>
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<td>Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols &amp; Clouds**</td>
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### Division of Physical Chemistry (continued)

**E. Sibert, Program Chair**

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<td>Electronic Structure Methods for Large Systems**</td>
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<td>Physical Chemistry of Clusters &amp; Nanoparticles DA</td>
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<td>Molecular Biophysics: Revealing the Interplay between Different Forces &amp; Effects in Biochemical Processes**</td>
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<td>Hydrophobicity, Ion Solvation &amp; Interfaces: Theory, Simulations &amp; Experiments</td>
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<td>Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage &amp; Materials* (ENVIR)</td>
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<td>Academic Innovations for Tomorrow’s Industries: GSSPC Symposium* (CHED)</td>
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<td>Innovation in Materials for Emerging Uses* (MPPG)</td>
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### Division of Polymer Chemistry (continued)

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

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<tr>
<td>Value of Basic Research in Solving Industrial Polymer Problems</td>
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<td>Henkel Award for Outstanding Graduate Research in Polymer Chemistry</td>
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<td>Henry A. Hill Centennial Symposium: Innovation in Polymer Science**</td>
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<td>Value of Basic Research to Industrial Polymer Science—A Senior Chemist’s Perspective</td>
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<td>Multicomponent &amp; Sequential Reactions in Polymer Science: Efficient Synthesis of Structurally Diverse Polymers</td>
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<td>Ionic Liquids in Polymer Design: From Energy to Health</td>
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<td>Herman Mark Young Scholars Award Symposium in Honor of Bradley Olsen</td>
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<td>Innovation from Discovery to Application Plenary Session* (MPPG)</td>
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<td>Professional Legacy of Henry Hill* (PROF)</td>
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<td>Memories of Henry Hill: His Legacy in Science &amp; in Professional Service* (HIST)</td>
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<td>The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector* (SCHB)</td>
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<td>From Raw to Varoom: The Science behind Getting a Car on the Road* (CHED)</td>
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### Division of Polymeric Materials: Science & Engineering

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

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### Division of Professional Relations

R. D. Libby, Program Chair

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## Division of Professional Relations (continued)

**R. D. Libby, Program Chair**

**Boston Convention & Exhibition Center**

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<td>Henry A. Hill Centennial Symposium: Innovation in Polymer Science* (POLY)</td>
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<td>Big Chemistry from Small Businesses* (SCHB)</td>
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## International Activities Committee

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

**Boston Convention & Exhibition Center**

<table>
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<th>Session</th>
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<tr>
<td>Opportunities for U.S./Cuba Collaboration in Chemistry, Chemical Engineering &amp; Chemistry Education**</td>
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<td>International Entrepreneurship: How To Start a Business &amp; Thrive in the Global Marketplace**</td>
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## Division of Small Chemical Businesses

**J. Sabol, Program Chair**

**Westin Boston Waterfront**

<table>
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<tbody>
<tr>
<td>Entrepreneurs’ Poster Session /DA</td>
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<td>Starting-Up &amp; Spinning-Out: Commercializing Innovative Chemistry** /DA</td>
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<td>Big Chemistry from Small Businesses** /DA</td>
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<td>ACS Scholars: Rising Stars in Industry* (PRES)</td>
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<td>GMOs &amp; the Entanglement of Intellectual Property Rights* (AGRO)</td>
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## Society Committee on Education

**G. Muller, Program Chair**

**Boston Convention & Exhibition Center**

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<td>What’s in Your Chemical Toolbox***</td>
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<td>High School Program* (CHED)</td>
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<td>Undergraduate Research Papers* (CHED)</td>
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<td>Incorporating Green Chemistry Innovations &amp; Applications into the Classroom &amp; Outreach* (CHED)</td>
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<td>Successful Student Chapters* (CHED)</td>
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## Women Chemists Committee

**A. Debaillie, K. Woznack, Program Chairs**

**Sheraton Boston Hotel**

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<td>Managing Transitions**</td>
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## Younger Chemists Committee

**A. Gavrilenko, T. Matos, Program Chairs**

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## Consultative Committee on Metrology in Chemistry & Biology

**W. May, R. Wielgosz, Program Chairs**

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<td>Chemistry &amp; the International System of Weights &amp; Measures</td>
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*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
How to Read the Technical Program

1. Search for the Division—listed in alphabetical order
2. Locate the day
3. Locate the session name
4. Locate the time or poster #
5. Locate the venue and room for each session

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

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

Picture Yourself in the ACS Booth

The ACS Booth is your opportunity to experience the world’s largest scientific society all on one carpet!

- Experience SciFinder from CAS, the world’s authority for chemical information
- Learn about the newest ACS Journals from ACS Publications, including Editors’ Choice
- Discuss how to achieve your career goals with ACS Career Navigator™
- Come to the Membership Benefits kiosk to receive a gift in thanks for your ACS membership
- Enter contests and receive giveaways, including tablets, gift cards, photos and more!

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.
### PRESIDENTIAL & CROSS-DIVISION PROGRAMMING

<table>
<thead>
<tr>
<th>Organizing Group</th>
<th>Acronym</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Presidential Events</td>
<td>PRES</td>
<td>TECH-70</td>
</tr>
<tr>
<td>Multidisciplinary Program Planning Group</td>
<td>MPPG</td>
<td>TECH-71</td>
</tr>
<tr>
<td>Academic Employment Initiative</td>
<td>AEI</td>
<td>TECH-72</td>
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</table>

### DIVISION PROGRAMMING

<table>
<thead>
<tr>
<th>Organizing Group</th>
<th>Acronym</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agricultural &amp; Food Chemistry</td>
<td>AGFD</td>
<td>TECH-74</td>
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<tr>
<td>Agrochemicals</td>
<td>AGRO</td>
<td>TECH-80</td>
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<td>TECH-95</td>
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<td>TECH-95</td>
</tr>
<tr>
<td>Business Development &amp; Management</td>
<td>BMGT</td>
<td>TECH-98</td>
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<td>Carbohydrate Chemistry</td>
<td>CARB</td>
<td>TECH-99</td>
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<tr>
<td>Catalysis Science and Technology</td>
<td>CATL</td>
<td>TECH-101</td>
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<tr>
<td>Cellulose &amp; Renewable Materials</td>
<td>CELL</td>
<td>TECH-110</td>
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<td>Chemical Education</td>
<td>CHED</td>
<td>TECH-110</td>
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<tr>
<td>Chemical Health &amp; Safety</td>
<td>CHAS</td>
<td>TECH-118</td>
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<tr>
<td>Chemical Information</td>
<td>CINF</td>
<td>TECH-119</td>
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<tr>
<td>Chemical Toxicology</td>
<td>TOXI</td>
<td>TECH-123</td>
</tr>
<tr>
<td>Chemistry &amp; the Law</td>
<td>CHAL</td>
<td>TECH-125</td>
</tr>
<tr>
<td>Colloid &amp; Surface Chemistry</td>
<td>COLL</td>
<td>TECH-126</td>
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<tr>
<td>Computers in Chemistry</td>
<td>COMP</td>
<td>TECH-136</td>
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<tr>
<td>Energy &amp; Fuels</td>
<td>ENFL</td>
<td>TECH-144</td>
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<td>TECH-166</td>
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<td>Industrial &amp; Engineering Chemistry</td>
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<td>TECH-169</td>
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### FULL TECHNICAL PROGRAM

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.

### COMMITTEE PROGRAMMING (In order of appearance)

<table>
<thead>
<tr>
<th>Organizing Group</th>
<th>Acronym</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Committee on Chemical Safety</td>
<td>CCS</td>
<td>TECH-241</td>
</tr>
<tr>
<td>Committee on Corporation Associates</td>
<td>CORP</td>
<td>TECH-242</td>
</tr>
<tr>
<td>Committee on Divisional Activities</td>
<td>DAC</td>
<td>TECH-242</td>
</tr>
<tr>
<td>Committee on Economic and Professional Affairs</td>
<td>CEPA</td>
<td>TECH-242</td>
</tr>
<tr>
<td>Committee on Environmental Improvement</td>
<td>CEI</td>
<td>TECH-242</td>
</tr>
<tr>
<td>Committee on Ethics</td>
<td>ETHC</td>
<td>TECH-242</td>
</tr>
<tr>
<td>Committee on Minority Affairs</td>
<td>CMA</td>
<td>TECH-243</td>
</tr>
<tr>
<td>Committee on Nomenclature, Terminology and Symbols</td>
<td>NTSC</td>
<td>TECH-243</td>
</tr>
<tr>
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<td>International Activities Committee</td>
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<td>Senior Chemists Committee</td>
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<td>Society Committee on Education</td>
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<td>Women Chemists Committee</td>
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<td>Consultative Committee on Metrology in Chemistry and Biology</td>
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Section A
Westin Boston Waterfront
Galleria
National Science Foundation's Centers for Chemical Innovation
Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB
S. Dasgupta, Organizer
3:00 - 6:00

PRES 11. Investigations on the emergence of peptides on the prebiotic earth. J. Fersht
PRES 12. Potential emergence of RNA from chimeric pre-RNA scaffolds. T.C. Effmyo, K. Kim, J.V. Gavette, B. Cafferty, C.L. Musset, N.V. Hud, R. Krishnamurthy
PRES 20. Alkanes to aromatic catalytic dehydroaromatization. A.M. Steffens, A.S. Goldman
PRES 23. Prebiotic phosphorylation of nucleosides by meteoritic minerals. M.A. Pasek
PRES 24. Controlled ring-opening polymerization of cyclic ester- acetals to polycarbosilanes and polyhydroxalkanoates. A. Neitzel, M. Petersen, E. Kokkoli, M.A. Hillmyer
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 30. Low-pressure homogeneous hydrogenation of CO to methanol under basic conditions. N.M. Rezayee, C.A. Huff, M.S. Sanford
PRES 31. Heterogeneous nucleation of ice on alcohol monolayers. Y. Qiu, V. Molinero
PRES 32. Optimizing and understanding photon absorption and charge transport of BIV4 oxahydrate nodules for solar water splitting. G.A. Galli, K. Choi
PRES 33. Theoretical and experimental study of the optoelectronic properties of tindacium nitride (TaN3) for photovoltaic chemical (PEC) water splitting. I. Narkeviciute
PRES 34. Oxidation chemistry facilitated by a hexacarboxamide cryptand. J. Staub
PRES 35. Discovery and characterization of transition metal phosphides as electrocatalysts and photocatalysts for the hydrogen evolution reaction. N.S. Lewis, R.E. Schraaf
PRES 36. Advances in heterogeneous tungsten catalysts for use in tandem alkane metathesis. P.E. Suess
PRES 38. Atom-efficient catalytic methods for reduction and oxidation of carbonates. T. Brewster
PRES 39. Chemical imaging and spectroscopy of single molecules with a tunable femtosecond laser coupled RF-STM. W. Cao
PRES 41. Mechanistic studies of Pd-catalyzed enantioselective hydrogenation. D. Blackmon
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. Mowassaghi, A.R. Narayan
PRES 45. Single molecule vibrational dynamics in time and frequency domain. N. Toida
PRES 46. Ultrastable pump-probe force microscopy 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 158

21st Century Chemistry Education: Formal and Informal
Cosponsored by AGRO, CARB, CHAS, CHED, CNF, COLL, ENFL, PROF and SCHB
G. M. Bodner, Organizer
I. Montes, Organizer, Presiding
1:30 Introductory Remarks.
1:40 PRES 48. A community for teachers of chemistry by teachers of chemistry. B.P. Sitzman
2:10 PRES 49. Young chemists in action: The benefits of informal chemical 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 presenting makes a difference for us and others as educators. L.E. Bloom
3:50 PRES 52. Teacher-tested, but student-blackbox online professional development for chemistry teachers. W. Hunter
4:20 PRES 53. Engaging researchers and students as partners in education and outreach. C.L. Alpert
4:50 Concluding Remarks.

Edwin Land and Instant Photography:
Massachusetts' First National Historic Chemical Landmark
Sponsored by HIST, Cosponsored by PRES
Professional Legacy of Henry Hill
Sponsored by PROF, Cosponsored by CEPa, CMa, ETHIC, HIST, ORAN, PMG, POLY, PRES 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
Sheraton Boston Hotel
Back Bay A

ACS Scholars: Rising Stars in Academe
Cosponsored by AGRO, CARB, CMAI, COLL, ENFL, ENVR, PROF, SCHB and YCC
A. Poggi, L. M. Watkins, Organizers
G. 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).
9:46 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.

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
TUESDAY MORNING

Section A
Westin Boston Waterfront

Transforming University-Industry Partnerships for an Innovative Future

Envisioning, Enabling and Executing
Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MED, PROF and SCHB

L. Graziano, Organizer
C. Ribes, Organizer, Presiding

8:30 Introductory Remarks.
8:50 PRES 69. Evolving concepts and changing landscape of chemistry education. M. Gutiérrez

10:05 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, ENVR, PROF, and SCHB

The Chemistry Enterprise in 2015
Sponsored by BMGT, Cosponsored by PRES, PROF and SCHB

True Stories from Entrepreneurs: BRIC Edition
Sponsored by SCHB, Cosponsored by CARB, COLL, I&EC, PRES, and PROF

Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais
Sponsored by YCC, Cosponsored by CHED, I&EC, PRES and PROF

MONDAY AFTERNOON

Section A
Sheraton Boston Hotel

ACS Scholars: Rising Stars in Industry
Cosponsored by AGRO, CARB, CHAS, 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 Ubierna (GSK-SmithKline)

3:40 PRES 68. ACS Scholar: Tashia Williams Amighiholizadeh, Ph.D., J.D. (Gilead Sciences, Inc.)

4:05 PRES 69. ACS Scholar: Dr. Jalonee L. White-Newcombe (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, I&EC, PRES and PROF

TUESDAY AFTERNOON

Section A
Westin Boston Waterfront

Transforming University-Industry Partnerships for an Innovative Future

Energizing and Education
Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MED, PROF and SCHB

L. Graziano, Organizer
C. Ribes, Organizer, Presiding

1:30 Introductory Remarks.

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


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, PROF, and SCHB

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace
Sponsored by IAC, Cosponsored by AGRO, AGRO, BMGT, CARB, CELL, INOR, MED, 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

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MONDAY MORNING
Section A
Boston Convention & Exhibition Center Room 102A/B
Innovation in Health and Medicine
Co-sponsored by BIOL, BIOT, MEDI and TOXI
R. D'Marchi, 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 crystallization. S. Kent
9:30 MPPG 5. Setting a course for biomedical innovation in the 21st century. A.D. Falkowitz
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

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-Sejo, 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-Sejo, 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
22. Design and development of novel synthetic methods for application toward the synthesis of natural products. R. Lamon-Bishop


57. From organofluorine chemistry to bioinorganic chemistry: A journey to bioinorganic chemistry. T. Cundari

66. Light-induced rotational dynamics in photoresponsive molecular rotor. A. Aylott. M.A. Garcia-Garibay

75. N,N-dimethylaminobenzyl boron ester functionalization into diarnines. K.A. McDann, A. Duans, T.B. Clark

84. Efficient synthesis of unimolecular architectures in water. J. Giannelis

91. From gas-phase to heterogeneous catalysts. K. Schwarz

98. Optical and electrical properties, and engineering. M. Gkikas

101. Theoretical insights of mechanistic details in graphene and hydrated ions. A. Aytan, S. Gurjat, A.G. Greymak


107. Materials design via supramolecular engineering: From folding polymers to assembling colloids. E. Bel, M. Mecklenburg

110. Carbon-rich architectures: Design, synthesis, and applications. D. Lehner, W. Dichtel

111. Multifunctional nanomaterials. M.B. Baker

115. Design and development of novel synthetic methods for application toward the synthesis of natural products. R. Lamon-Bishop

189. Physical mechanisms involved in viral infection and replication. D. Li

3.19. Quantitative proteomics of nitrosative post-translational modifications. T. Rhoads

10. Treating Tamoxifen resistant breast cancer by inhibiting protein degradation. J.A. Smith

20. Development of an isoto- pic approach for detailing related sequences. G. Quo, V.N. Rainhold


23. Observations of dynamic restructur- ing of nanorods gold during selective alcohol coupling reactions. B. Ziegler, M.L. Persson, R.J. Madix, C.M. Field

24. Innovation of peer learn- ing. H.N. Marashi


26. Advancing the technolo- gies for nanoparticles in living systems. G.B. Braun

27. Withdrawn.

28. Nanomaterials and devices for active interplay with the biological environment. A. Palloso


30. Withdrew.

31. Computational approaches to elucidate fundamental electron and energy transfer processes in complex supramolecular systems. L.A. Fedin

32. Dissecting the ion atmosphere surrounding nucleic acids. G.M. Giambasu, A.J. Olson, S. Ekins, J. Freundlich

33. Challenges in characterizing and predicting the activity of transition metal exchanged zeolites. F. Goeltl, P. Muslar, P. Uchupalanun, P. Sautet, I. Hermas

34. Calculation of protein-ligand binding affinities via a polarizable model. M.L. Arany, J.W. Ponder


36. Data-driven paradigm for encoding chemical intuition. E.O. Pyzer-Knapp

37. Nanomaterials: Possible ways for computational assessment and data mining towards rational design of new materials. B. Rasulev

38. Computational models design for sustainable energy and biomedical systems. S.V. Bambasvaro

39. Realistic and affordable ab initio cal- culations for electrochemistry. K. Schwarz

40. Modeling and design of large RNAs. S. Samarakovu, A.M. Pyle

41. New electronic structure theory methods and high-throughput computa- tional screening algorithms for catalytic processes. K.D. Vogiatz

42. Understanding single fission and other physical processes related to organic photovoltaics using theoretical models. S. Yost, M.P. Head-Gordon

43. Multifunctional nanomaterials at the water-energy nexus. N. Ach

44. Investigating and exploit- ing the interaction between graphene and hydrated systems. D.G. Dresen, J. Golovchenko

45. Green chemistry through electrocatalysis. A.B. Laurens

46. Pore scale microbial biogeography in sedimentary hydrocarbon- contaminated soils. A. Aksar, S. Ghoshal

47. Applications of organometallic complexes to organic transforma- tions: From tandem experiments and computational studies. K.D. Field, M. Emmert, A.S. Goldman


51. Band-edge modulation of p-Si(111) and integration of H2 catalyst with p-Si(111). J. See

52. Nano confinement effects on metal ions or nanoparticles catalysts. J. Shen

53. Advances in the use of gel permeation chromatography (GPC) to nanostructures: Purification, solvent change, and surface modification. Y. Shen, R. San, M.V. Gae, A. Polabge, A.B. Greymak


55. Paramagnetic transition metal complexes: From research to application and education. P.B. Tatschik

56. Stable luminescent metal-organic frameworks for sensing and light emitting applications. Q. Zhang


58. Synthesis of 18F-labeled inhibi- tor of indoleamine 2,3-dioxygenase for positron emission tomography imaging. N.M. Evdokimov, P. Clark, G. Flores, O. Witte, M.E. Jung, M. Phelps

59. Computer-aided design design and development: A Research program designed to produce novel research and enhance undergraduate education. M.J. Ferracane

60. Beyond morphine: Mu opioid/ NPP and mu opioid/NPFF bifunc- tional small molecules as anesthetics with reduced dependence and tolerance liabilities. V.B. Journigan


62. Withdrawn.

63. Amber Thaxton: Synthetic organic chemist. A.N. Thaxton

64. Heterogeneous catalysis: Synthesis and spectroscopy of supported metal oxide catalysts for natural gas upgrading. C.A. Carrero

65. Light-induced rotational dynamics in photoresponsive molecular rotor. A. Aytan, M.A. Garcia-Garibay

66. Signal transduction within supramolecular materials. M.B. Baker

67. Design and development of novel synthetic methods for applica- tion toward the synthesis of natural products. R. Lamon-Bishop

68. Mild palladium-catalyzed cyanation of (hetero)aryl halides and triflates in aqueous media. D.T. Cohn, S.L. Buchwald

69. Metalloinductive catalysis for stereoselective organic synthe- sis. X. Cui, X. Xu, L. Jin, F.X. Zhang

70. Theoretical insights of mechan- istic details and stereoselective organocatalysis by amino acid and cinchona alkaloid derivatives. Y. Lam

71. Development of cooperative Lewis acid catalysts for asymmetric Heintz reations, expedient library synthesis toward medical molecules, and development of bridged D–symmetric chiral anilide-acetamide catalysts for highly enantiomerically-switchable, intramolecular C(sp2)–H radical activation. K. Lang, S. Hong, D.W. MacMillan, F.X. Zhang

72. Trialkyphosphine-derived palladacy- cle as a catalyst in the selective cross-di- merization of two terminal alkynes. M.G. Giambasu, O.M. Gobbi, I. Smighnessy

73. Carbon-rich architectures: Design, synthesis, and applications. D. Lehner, W. Dichtel

74. Structure, morphology, and reversible mechanosteric progress of molecular gels derived from (R)-12- hydroxystearic acid as gelator. A.V. Mallia

75. Ambar Thaxton: Synthetic organic chemist. A.N. Thaxton

76. From organofluorine chemistry to bioinorganic chemistry: A journey to bioinorganic chemistry. T. Cundari

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 polyphos- phazene polymers. P.W. Peterson

78. Regio- and stereocontrolled allylic substitutions with organoacar- idates on α-substituted-β-, γ-unsubstituted esters and cyanohydrin phosphates. A. Picado, P. Dieter

79. From organofluorine chem- istry to bioinorganic chemistry: A journey to bioinorganic chemistry. T. Cundari

80. Inspiring diversity: Strategies for the classroom and the flask. R. Whittaker

81. Withdrawn.

82. Supramolecular approaches for improving reactivity and selec- tivity in transition metal catalyzed transformations. M. Young


84. Methane ene reaction simulation using the statistical temperature molecular dynamics algorithm. S.C. Bega

85. From gas-phase to hetero- geneous reaction: Applications in combustion to astrochemistry. B.B. Dani, R. Kaiser, KM. Ervin


87. Computational studies of proton transfer and proton-cou- pled proton transfer in chemical and biological systems. P. Goyal, Q. Cui, S. Harmes-Schiffer

88. New innovative ways for waste water cleaning. C. Janssen

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### SUNDAY MORNING

#### Section A
Boston Convention & Exhibition Center Room 212

**Phytonutrients: Thinking Beyond the “Essential” Nutrient Box**

B. Burton-Freeman, I. Edirisinghe, Organizers, Presiding

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<tr>
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<tr>
<td>8:00</td>
<td>Introductory Remarks</td>
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<tr>
<td>8:05</td>
<td><strong>AGFD 1.</strong> Chemistry and analysis of polyphenols in food and human samples. E. Richling, M. Schantz, D. Mueller</td>
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<td>9:05</td>
<td><strong>AGFD 3.</strong> Understanding factors that influence the bioavailability and kinetic profile of strawberry anthocyanins: A focus on meat timing and fasted-fed state status. A. Sandhu, L. Cisneros-Zevallos, F. Tomas-Barberan, Organizers</td>
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<td>10:05</td>
<td><strong>AGFD 11.</strong> Biological effects of anthocyanins from fruits. E. Richling, M. Schantz, M. Baum, T. Bakuradze, D. Mueller</td>
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<td>10:55</td>
<td><strong>AGFD 13.</strong> Optimized and validated method for the characterization and quantification of bioactive ellagitannins in pomegranate and other fruits and nuts. F. Tomas-Barberan, R. Garcia-Vilalta, K. Aaby, T. Koivumäki, A. Sandhu, S. Kupina, A. Shrikhande</td>
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#### Section B
Boston Convention & Exhibition Center Room 213

**Bioactive Compounds from Fruits & Vegetables**

C. Osorio Roa, F. Tomas-Barberan, Organizers, Presiding

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<td>8:00</td>
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<td>8:05</td>
<td><strong>AGFD 14.</strong> Olive oil authenticity and adulteration: Analytical tools and standards. R. Cantrill</td>
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<td>8:35</td>
<td><strong>AGFD 15.</strong> USP skim milk powder advisory group: The development of a toolbox of methods to detect food adulteration. R.L. Magaletta, J.C. Moore</td>
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<td>9:05</td>
<td><strong>AGFD 16.</strong> Development of field screening methods using surface enhanced Raman spectroscopy (SERS). L.G. Pogue, N.P. Sardesai, B.J. Yakes, S. Barcelo, M. Yamakawa, A. Peterson, A. Peterson</td>
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<td>9:35</td>
<td>Introductory Remarks</td>
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<td>9:45</td>
<td><strong>AGFD 17.</strong> Meat fraud and speciation: From vulnerability assessment to analytical methods. G. Cottenet</td>
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### SUNDAY AFTERNOON

#### Section A
Boston Convention & Exhibition Center Room 212

**Phytonutrients: Thinking Beyond the “Essential” Nutrient Box**

B. Burton-Freeman, I. Edirisinghe, Organizers, Presiding

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<tr>
<td>10:00</td>
<td>Introductory Remarks</td>
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<td>10:05</td>
<td><strong>AGFD 20.</strong> Is volunteer stratification necessary in clinical trials with phenolic phytochemicals? F. Tomas-Barberan</td>
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<td>1:30</td>
<td><strong>AGFD 42.</strong> Potential antimicrobial activity of protein hydrolysates from germinated black bean cotyledons. L. Lopez-Barrios</td>
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#### Section B
Boston Convention & Exhibition Center Room 213

**Bioactive Compounds from Fruits & Vegetables**

C. Osorio Roa, F. Tomas-Barberan, Organizers, Presiding

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<td>9:05</td>
<td>Introductory Remarks</td>
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<td>9:10</td>
<td><strong>AGFD 18.</strong> DNA-based species identification of seafood. A. Eischeid, S. Staszycki, S. Handy, F.S. Pry, J. Deeds</td>
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<td>10:45</td>
<td><strong>AGFD 19.</strong> Honey adulteration: Methods currently applied in the routine control of commercial samples, analytical challenges, legal and regulatory aspects. L. Efflein</td>
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### MONDAY MORNING

#### Section A
Boston Convention & Exhibition Center Room 212

**Complex Coacervation: Principles & Applications**

Financially supported by The Dow Chemical Company Co-sponsored by CCLJ

P. L. Dubin, S. L. Perry, Organizers, Presiding

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<td>8:00</td>
<td>Introductory Remarks</td>
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<tr>
<td>8:05</td>
<td><strong>AGFD 40.</strong> Complex coacervation: Principles and simple theories. R. de Vries</td>
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<tr>
<td>8:45</td>
<td><strong>AGFD 41.</strong> Polyelectrolyte complex-coacervate continuum. J.B. Schlenoff, O. Wang</td>
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<tr>
<td>9:15</td>
<td><strong>AGFD 42.</strong> Electrostatic complex between (bio)polyelectrolytes and nanoparticles. Effect of the chain persistence length over particle diameter ratio. F. Boué</td>
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Section B
Boston Convention & Exhibition Center Room 213
Bioactive Compounds from Fruits & Vegetables
L. Csíneros-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. Tocino
8:30 AGFD 48. Characterization of tomato volatiles by headspace-solid-phase micro extraction. G. Jayaparakasha, B. Pati
8:55 AGFD 49. Bioactive compounds 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. Susnov
10:30 AGFD 52. Preservation of anthocyanins in solid lipid nanoparticles: Optimization of microemulsion dilution method by Placket Burman and Box Behnken design. R. Ravanfar, A. Tamadon, M. Niakousari, M. Moien
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 carboxyl species: Will they be the next food safety issue? G. Ho
9:05 AGFD 55. Formation and reduction of furan in various food model systems. J. Heh, 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

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.
10:45 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
P. L. Dubin, Organizer, Presiding
1:15 Introductory Remarks.
1:20 AGFD 64. Artificial cells in picoliter droplets. W. Huck
1:50 AGFD 65. Biomimetic micro-compartamentalization by aqueous phase separation. C.D. Keating
2:50 Intermission.
3:25 AGFD 67. Design and construction of higher-order structure in function in coacervate-based protocols. S. Mann
3:45 AGFD 68. Biomimetic effects on actin cytoskeletal filament growth. S.L. Perry, P. McCall, S. Srivastava, M. McCall, S. Mann
4:45 AGFD 70. Coacervation of mussel-inspired zwitterionic adhesives. H. Waite, T. Keating

Section B
Boston Convention & Exhibition Center Room 213
Chemistry, Composition & Analysis of Dietary Supplements
M. Sucan, 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. Lee
1:25 AGFD 72. Reactions between polyphenolic dietary supplements and other biomolecules dictate bioactivity, bioavailability and analysis. S. Wang, L.L. Yu
1:45 AGFD 73. Rosemary: From nature to table. M. Jordan, C. Martinez-Conesa, S. Bahon, J. Sotomayor
2:05 AGFD 74. Simple UPLC-MS to measure the presence of pomegranate in juices. C. Mathon, A. Green, C.K. Larive
2:25 Intermission.
3:00 AGFD 76. Facile synthesis and characterization of curcumin metformin adduct: Potentially important gama-secretase inhibitor for Alzheimer disease. B. Dayal
3:20 AGFD 77. Coffee-based dietary supplements contain kauran diterpenoid glycosides inhibiting amine nucleotide translocase in mitochondria and reduce respiration. R. Lang, T. Fromme, A. Bousch, T. Lang, M. Kinigopoulos
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 poly cyclic aromatic hydrocarbons (PAHs) in edible vegetable oil. O.S. Olatunji, B.O. Osapu, O.S. Fatosi, B.J. Ximba
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. Pilati, K. Zhao, R.O. Juskels
3:35 AGFD 83. FDA update on acrylamide, furan, and other processing toxicants. L. Jackson
2:45 Intermission.
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‡ and TAGFD
3:45 E47. Use of nanomaterials in the design and fabrication of new functional materials. L. Chang, S.L. Perry
4:00 E49. Peptide complexation: From bulk coacervates to nanoscale assemblies. D. Pittel, L. Leon, K.O. Margossian, A. Tropnikova, M.V. Tirsch
Undergraduate Research Posters
Agricultural and Food Chemistry
Sponsored by MPPG, Cosponsored by AGFD and SCoCBE

MONTDAY EVENING
Section A
Boston Convention & Exhibition Center Hall C
Sci-Mix
B. Park, Organizer
8:00 - 10:00
26, 30, 57. See previous listings.
Chemical Innovation and Design (CID) Talks: The Future of Innovation Now
Sponsored by MPPG, Cosponsored by AGFD, AGRO, BIOT, MED, PMSE and SCBE

Technical program information known at press time.
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TUESDAY MORNING

Section A
Boston Convention & Exhibition Center Room 212

Complex Coacervation: Principles & Applications
Financially supported by The Dow Chemical Company
Cosponsored by COLLL

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. W. Trelill


9:05 AGFD 96. Self-assembled nanostructures from block copolymers for biomedical application. Y. Anraku

9:30 Intermission.

10:00 AGFD 97. Beyond elastin: New peptide oligomers that elicit aqueous coacervation. A. Chikoti

10:30 AGFD 98. Directing encapsulated stem cell fate via in situ forming, growth factor-loaded coacervate microparticle-embedded hydrogels. E. Alsbeg, O. Jeon


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. Scheiberle, Organizer
M. Granvogel, 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. Scheiberle

9:30 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
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 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 159. Effects of home-based preparation approaches in determining the release of bioactive 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 food, by inductively coupled plasma/atomic emission spectrometry. J. Hong, C. Liu, S. Chang, G. Lin, T. Huang


AGFD 162. Antimicrobial peptide sequences from soy protein for use in food safety. N. Xiang, Y. Lu, A. Bhuma, G. Narsimhan

AGFD 163. Flavonol glycosides in wild and cultivated berries of two major sub-species of sea buckthorn and influence of growth sites. X. Ma, D. 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 167. Withdrawn.

AGFD 168. Withdrawn.

AGFD 169. Withdrawn.

AGFD 170. Withdrawn.


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.G. Silva, T.B. Cesar, A.M. Nasser, J.A. Manthey, B. Elizabeth


AGFD 178. Development of lecithin emulsion gel to enhance the oral bioaccessibility of nobletin. Y. Ting, Y. Pan, G. Huang


AGFD 180. In-vitro digestion properties of Pickering emulsions stabilized by starch nanocrystals. R. Liang, Y. Jang, C. Yang


AGFD 184. Combination of pre-column fractionation and ultra-performance liquid chromatography with fluorescence detection for the sensitive quantification of 1-nitrosoimine, 2-nitrofluorene, and 1-nitropyrene in meat products. K. Deng, W. Chan


AGFD 186. Withdrawn.

AGFD 187. Saponins quantification in pigmented chickpeas cultivar. A.K. Milan, S.P. Serna SDakwar, J. Gutierrez

AGFD 188. Development and validation of analytical method of furan in seven different types of food matrices using UHPLC-MS/MS. Y. Sook, S. Jeong, H. Ker, G.K. Gu

AGFD 189. Analytical developments in food technology by establishment of a 14-C food technology lab and kitchen. M. Kothoff, B. Mockett

Section E
Boston Convention & Exhibition Center
Room 212

AGFD Division Award: Symposium in honor of Dr. Andrew Taylor
K. D. Debler, 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 complications 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 production and flavor perception. J. Le Guere

2:25 AGFD 143. Separation and concentration of trace high-impact odorants using multidimensional gas chromatography-mass spectrometry-spectrofluorometry with integrated preparative fraction collection. L. Jones, K. Chu, B. White, A. Ward

3:05 AGFD 144. Encapsulation, multimodal perception, and its applications. G. Renaveux


4:20 Concluding Remarks.

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**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**
Parameters impacting flavour profile and shelf-life of dairy ingredients. M. Troin, A. Cepea, B. Sues, P.R. Guiliet, J. Pfeter

**2:00** **AGFD 294**
Sensory and instrumental analysis of sweet potato fries. J.K. Parker, S. Lignou, J.S. Elmore, D.P. Balagiannis

**2:20** **AGFD 295**
1-p-Menthen-8-thiol, the grapefruit character impact volatile, is a thermally generated artifact in citrus juices. F. Jabapurwala, J. Lin, L. Jones, J. Addison, N. Hawkins, K. Ridgway

**1:40** **AGFD 293**
Kinetic analysis of exudates in citrus leaves as nonvolatile glycoconjugates. D. van Santen, C.W. Wood, J.S. Elmore, D.P. Balagiannis

**1:45** **AGFD 300**
Effect of growing environment on the characteristics of soybeans and reduce cross-contamination. S. Bai, A. Dunkel, K. Engel

**3:00** **AGFD 301**
Lipid-lowering activity of citrus polymethoxyflavones is mediated by down-regulation of lipogenic genes. Z. Chen, L. Lei

**3:25** **AGFD 302**
Citrus polymethoxyflavones and monodemethylated polymethoxyflavones inhibit adipogenesis in 3T3-L1 adipocytes. S. Lin, P. Chen, M. Pan, S. Li, C.H. Ho, C.Y. Lo

**11:15** **AGFD 290**

**3:45** **AGFD 304**
Polymeric flavonoids from aged orange peels. Extraction, formulation, and bioefficacy. Q. Huang, T. Song, X. Wu, Z. Gao, F. Xu, Y. Cao, H. Xiao

**3:50** **AGFD 306**

**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**

**2:10** **AGFD 308**
Effect of growing environment on the characteristics of soybeans for food uses. S.K. Chang, S. Meng

**2:30** **AGFD 309**

**2:35** **AGFD 310**
Mechanical characteristic of pigments in three guava (Psidium guajava) Colombian varieties. I. Gonzalez, A. Figueroa, F. Herneda, C. Osorio Roa

**2:50** **AGFD 311**
Fresh ginger vs. dry ginger. The impact of temperature on the bioactive components in ginger. S. Sang

**3:05** **AGFD 312**
Differentiating organic and conventional oregano using ultraperformance liquid chromatography mass spectrometry (UPLC-MS), headspace gas chromatography with flame ionization detection (headspace-GC-FID), and flow injection mass spectrometry (FIMS) fingerprints combined with multivariate date analysis. B. Gao, W. Lu, L.L. Yu

**Section D**
Boston Convention & Exhibition Center Room 211

**Chemistry and Bioactivities of Natural Polymethoxyflavonoids**

C. Ho, Organizer

S. Li, M. Pan, Organizers, Presiding

**1:00** **Introductory Remarks.**

**1:05** **AGFD 313**

**1:30** **AGFD 314**
Electrospun water soluble nanofibers for dehydration and storage of bacteriophage for decontamination of agricultural water. C. Ko, S.R. Nugen

**1:55** **AGFD 315**
Withdrawn.
Section B
Boston Park Plaza Hotel and Towers
Arlington Room
Combining Scientific Evidence for Health Policy and Regulation
Co-sponsored 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. Keizer
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. Haather
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.

SUNDAY AFTERNOON

Section C
Boston Park Plaza Hotel and Towers
White Hill Room
Pesticide Dose: Effects on the Environment and Target and Non-Target Organisms
Co-sponsored by ENVIR
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 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. Striebig
11:20 AGRO 20, Use of intermittent tenant sprayers for aggregate 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. Brindile, Organizer
H. B. Irig, C. Tu, 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 limits in Japan. A. Aski
10:10 Intermission.
10:25 AGRO 26, Conclusions and follow-up from 2014 IUPAC ACS MRL workshop. H.B. Irig
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. G. Sack

Hydrothermal Carbonization: Possibilities and Limits for Feedstocks, Processes and Applications

HTC Fundamentals and Sorption
Sponsored by ENVIR, Co-sponsored by AGRO
National Science Foundation’s Centers for Chemical Innovation
Sponsored by PRES. Co-sponsored by AGRO, CARB, COLL, ENFL, PROF and SCIBH
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 43. 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
2:45 AGRO 50. Occurrence and significance of pesticide-induced hormesis in insects. C. Cutler, R. Guedes
3:10 Intermission.
3:55 AGRO 61. Chemical hormesis on plant pathogenic fungi and oomy- cetes: 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
4:45 Discussion.

Section D
Boston Park Plaza Hotel and Towers
Whittier Room
Feeding the World Requires Pesticides and Maximum Residue Levels
H. B. Iriag, 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
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’ field in the pests and diseases by searching for existing solutions in other countries. F. Schueter
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-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 uplifted drain. T. Jindal, A. Kumar, A. Panjan, K. Gulati, S. Thakur
AGRO 63. Microagro 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 Ghagar 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

Section F
Boston Park Plaza Hotel and Towers
Terrace Room
Current Topics in Seed Treatment
Cosponsored by ACRYL 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
Pesticide Dose: Effects on the Environment and Target and Non-Target Organisms
Cosponsored by ENVR
S. O. Duke, K. R. Solomon, Organizers
1:00 - 5:00
AGRO 73. Microtransplantation of rat brain neurons into Xenopus laevis oocytes to study the effect of environmental tox- icants on endogenous voltage-sensitive ion channels. E. Murenzi, S.B. Summerton, A. Tolin, M.M. Morgan, J.M. Clark
AGRO 74. Effect of glyphosate formulations on two species with different leaf surface properties. A.R. Christensen, N. Caderring, H. Tescher, J. Streitig

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. Brenchow, S. Satter
AGRO 77. Withdrawn.

21st Century Chemistry Education: Formal and Informal
Sponsored by PRES, Cosponsored by AGRO, CARB, CHAS, CIED, CNF, COLT, ENFL, PROF and SOCED
AGRO 78. Hydrothermal Carbonization: Possibilities and Limits for Feedstocks, Processes and Applications
Sponsored by ENVR, Cosponsored by AGRO

National Science Foundation’s Centers for Chemical Innovation
Sponsored by PRES, Cosponsored by AGRO, CARB, COLT, ENFL, PROF and SOCED

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AGRO 117. Occurrence and formation of insecticide degradation products in urban environments. J. Richards, W. Jiang, J. Gan

AGRO 118. Uptake of triclozan and triclozanib by vegetables from soils and biosolids-amended soils. Q. Fu, S. Sangayarao, G. Qie, J. Yang

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 PRSC, Cosponsored by AGRO, CABS, CHAG, CHED, CNEF, COLLAB, ENFL, PROF and SOCED

ACS Scholars: Rising Stars in Academe
Sponsored by PRSC, Cosponsored by AGRO, CABS, CMA, COLLAB, ENFL, PROF, SCHB and YCC

Sensing of Environmentally Relevant Contaminants
Sponsored by ENVR, Cosponsored by AGRO

MONDAY AFTERNOON
Section A
Boston Park Plaza Hotel and Towers
Georgan 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. Lorsbach, Organizer
J. Green, T. C. Sparks, Organizers, Presiding
8:26 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
9:45 AGRO 80. Are pharmaceutical enhanced solubilization technologies useful in agriculture? R. Boucher
10:10 Intermission.
10:30 AGRO 81. Ultra-high resolution MS and label-free MALDI molecular imaging: A novel approach for the study of plant biosynthesis and metabolism. K.A. Kellerberger
10:55 AGRO 82. Visualization of small molecule distributions in plant, insect, and mammalian tissues by mass spectrometry imaging. N. Bjarnholt, B.W. Brooks
11:20 AGRO 83. RNA interference in agricultur: Today and tomorrow. R. Heidebroek
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 TOD
8:26 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. Rued, B.W. Brooks
8:55 AGRO 85. Formulating the identification of high priority research needs: A case example with pharmaceuticals and personal care products. B.W. Brooks, G. Anley, A. Boxall, M. Rued
9:45 Discussion.
10:10 Intermission.
10:30 Discussion.

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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. Peraringaninng, 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. Siwey, M. Burton, A.L. Roberts
9:45 AGRO 90. Withdrawn.
10:10 Intermission.
10:20 AGRO 91. Does the incorporation of vegetative filter strip mass balance and evapotranspiration processes affect the long-term pesticide environmental exposure assessments? R. Muñoz-Carpeta, G.A. Fox, O. Perez-Ovilia, A.M. Ritter
10:45 AGRO 92. Emerging contaminant soil fate and subsoil development for the USDA soil water assessment tool. J.L. Thibodeaux
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
Whitter Room
Advances in Pesticide Residue Analysis: Innovations that Lead to Novel Applications Cosponsored by ANYL and ENVR
K. Lynn, Organizer
L. Riter, 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 noncarcinogenic 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. Bleden
9:45 AGRO 97. Ultratrace 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
11:00 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. D. 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. Braveman, D. Kunkel, J. BARON, W.P. Bairey, K.D. Coleman
8:55 AGRO 102. Plant/plant allelopathy for herbicide and bioherbicide development and development. S.O. Duke
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

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. Peraringaninng, Organizers
8:00 - 12:00

AGRO 115. Encouraging the use of drift reduction technologies in the United States. C. Peck, F. Khan, A. Ovesen


AGRO 117. Occurrence and formation of insecticide degradation products in urban environments. J. Richards, W. Jiang, J. Gan

AGRO 118. Uptake of triclozan and triclozanib by vegetables from soils and biosolids-amended soils. Q. Fu, S. Sangayarao, G. Qie, J. Yang

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 PRSC, Cosponsored by AGRO, CARB, CMA, COLLAB, ENFL, ENVR, PROF, SCHB and YCC

ACS Scholars: Rising Stars in Academe
Sponsored by PRSC, Cosponsored by AGRO, CARB, CMA, COLLAB, ENFL, ENVR, PROF, SCHB and YCC

Sensing of Environmentally Relevant Contaminants
Sponsored by ENVR, Cosponsored by AGRO
AGRO for the 250th ACS National Meeting known at press time.

**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. Hoffmann, 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. Machner, C. Remensnyder, B. Selkew, T. Reemtsma

10:00 Award Presentation.


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. Hamper, 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 ENVIR

V. Forbes, N. Golden, T. Hawkes, M. F. Leggett, N. Poletika, Organizer, Presiding

T. Hawkes, Presiding

8:00 Introductory Remarks.

8:05 AGRO 163. Developing species maps from FESTIF’s aggregated species location data for EPW’s assessment of pesticides and endangered species. B. McEachery, A. Frank, D. Campagna, 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. Gooding, P. Whitting, B. McGaughey


10:10 Intermission.


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 ENVIR

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. Arikan, W. Mubry, C.P. Rice, S. Lansing


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


Section D

Boston Park Plaza Hotel and Towers

Whittier Room

GMOS and the Entanglement of Intellectual Property Rights

Cosponsored by CHAL, ENVIR and SCHB

A. Coates, Organizer, Presiding

8:25 Introductory Remarks.

8:30 AGRO 177. Scientific basis for GMOs. J.M. Van Emom

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. Keshen

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. Keshen

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

8:50 Introductory Remarks.

8:55 AGRO 184. Identifying the molecular basis of insecticide resistance in mosquitos vectors and agricultural pests. L. Grigoraki, J. Vontas


9:45 AGRO 186. Characterizing the physiological role of inward rectifying potassium channels in the insect nervous system. D. Swale

10:10 Intermission.


10:55 AGRO 188. Comparison of immune responses between body and head lice following bacterial challenge. J. Kim, K.S. Yoon, D.J. Pirollo, J.M. Clark, S. Loe


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 ENVIR

D. S. Aga, J. S. Wallace, Organizers

8:00 - 12:00


AGRO 193. Structure based prediction of substituted pyridine calixene exchange to soil aluminosilicates: Implications for antibiotics containing pyridine substructures. J. Sullivan, B. Stuyesant, 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 196. Phytohormone levels in coconut (Cocos nucifera) L. water at three different stages of maturity. R.R. Singh, V. Migo, D.S. Aga
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, Aphis malielloides 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. Cubert, V.R. Hebert, J. Sarto, 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. Overymer
3:10 Intermission.
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. Polietka, Organizers
N. Golden, M. F. Leggett, Organizers, Presiding
1:25 Introductory Remarks.
2:45 AGRO 220. Using targeted monitoring to evaluate mitigation strategies that reduce pesticide loading to streams. K. McLain, G. Tuttle, J. Hancock, M. Blascho
3:10 Intermission.
3:55 AGRO 222. Protecting endangered species from pesticides with stakeholder solutions. R. Marovich
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 ANHY and ENVR
D. S. Aga, J. S. Wallace, Organizers, Presiding
1:25 Reconvening Remarks.
1:30 AGRO 224. Stereospecific 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. S. Munoz, R. Aueroth
2:45 AGRO 227. Determination of antibiotics, estrogenic hormones, and UV filters in water, sediment, and crayfish from an urban watershed. K. He, A. Tinn, C. Wetyl, M.L. 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 metabolites of pharmaceutical and personal care products (PPCPs) in plants using plant cell cultures. J. Gan, X. Wu
4:30 AGRO 231. Plant Uptake of Pharmaceuticals from Soil Treated with Unine and Struvite. L. Su
5:20 Concluding Remarks.

Section D
Boston Park Plaza Hotel and Towers
Whitter Room

Immunoochemistry Summit XII: Immunooassays and Other Bioanalytical Techniques
Cosponsored by ANHY, 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. Van, J. Carpio, E. Fanth, K. Loffen, J. Molgo, R. Aranz
2:45 AGRO 236. Recombinant antibodies that distinguish between methylated and non-methylated derivatives of phencylthrene, a major polycyclic aromatic hydrocarbon present in crude oil. Y. Sun, M.Bradbury, G. Ansari, D.A. Blake
3:10 Interessions.
3:30 AGRO 237. Nanoboy based immunooassay for soluble epidermal growth factor detection using polypHR for signal enhancement: The rediscovery of polypHR? D. Li, Y. Cui, S.J. Gee, Y. Ying, B.D. Hammock
4:45 AGRO 240. Development and testing of genetically modified crop plants throughout their life cycle. L. Privile

Section E
Boston Park Plaza Hotel and Towers
Back Bay Room

Current Advances and Challenges of Arthropod Vector Control
L. J. Denson, D. Swale, Organizers, Presiding
1:50 Introductory Remarks.
2:20 AGRO 242. Identification of immunogenic tick saliva proteins secreted into the host during 24-48 hours after attachment. Z.M. Radiodicov, L. Lewis, T. Kim, L. Porter, A. Mulenga
2:45 AGRO 243. Withdrawn.
3:10 Intermission.
3:30 AGRO 244. Sabaddula 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. Rinekevich, Y. Du, J. Tolinski, A. Ueda, C. Wu, B. Zhov, 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. Totor, P.R. Carle, J.R. Bloomquist
4:55 Panel discussion an Concluding Remarks.

Section F
Boston Park Plaza Hotel and Towers
Terrace Room

Immunoochemistry Summit
XII: Immunooassays and Other Bioanalytical Techniques
Cosponsored by ANHY, 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 immunooassay. D. Li, C. Bever, J. Dong, J. Wang, Y. Cui, X. Liu, N. Vasyliova, B. Barych, Y. Wang, K. Ahn, H. Kim, S.J. Gee, B.D. Hammock

AGRO 205. Biological validation of enzyme-linked immunosorbent assays for detection of BiCry proteins in the environment. V.C. Albright, R. Helmich, 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


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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. Breatrner, R. Fell, T.O. Anderson

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Ericc Brillas and Professor Mehmet A. Ozturan

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, Cosporsored by AGRO, BMGT, CARB, CELL, INOR, MED, ORGN, POLY, PRES, PROF and SCHB

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry
Sponsored by SCHB, Cosporsored by AGRO, COLL, IEGC, PRES, PROF and YOC

Transforming University-Industry Partnerships for an Innovative Future

Energizing and Education
Sponsored by PRSS, Cosporsored by AGRO, CARB, CHAS, COLL, ENFL, ENVIR, MED, 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. Rierer, Organizers, Presiding

8:25 Introductory Remarks.

8:30 AGRO 247. 2015 Kenneth A. Spencer Award address: A career in crop protection development. T.P. Selby


9:45 AGRO 249. Synthesis and SAR studies of insecticidal pyridazin-3-yl amides, hydrazides, hydrazines, and diazaoxanes. M.C. Yap, A. Buyse, R. Hunter, M.H. Parker

10:10 Intermission.


11:20 AGRO 252. Total synthesis of indolet 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 use inform pesticide exposure assessments? Examples of the use of AgroTrak® and CA Pesticide Use Reporting data. C.M. Holmes, V. Sclater, 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


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. Barfoot, T. Xu, A.M. Ritter, C.M. Holmes


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. Ambrust, B. L. Brot, 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. Hannah, S. Christopher


9:45 AGRO 264. Slow-release, non-polluting, cost-effective fertilizer systems. G. McNeely, B. Green

10:10 Intermission.


10:55 AGRO 266. Discovery, mode of action and development of nitrapyrin as a nitrification inhibitor. C. Wojciech, J. Troth, R. Kaan

11:20 AGRO 267. Formulation innovations for nitrapyrin nitrification inhibitor for use with multiple fertilizer types. E. Scherder, C. Vogtweide, M. Li, L. Liu, B.L. Brot

11:45 AGRO 268. Management and mitigation of nitrates from nitrogen fertilizers in California. A.S. Gunasekara, B.A. Morad

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.


8:55 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 real time (DART) coupled to mass spectrometry. M. Busman

9:45 AGRO 272. Survey of glyphosate residues in honey, corn, and soy products. F.M. Ruble, E. Giao, L. Kamp

10:10 Intermission.

10:30 AGRO 273. Hologenated 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


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

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. Chackert, J. Owen

8:55 AGRO 277. Modeling compound loss from passive sampler sorbents. D. Rebbe, C. Thomas

9:20 AGRO 278. Investigating soil-water partition coefficients of organic compounds using frontal chromatography and polyparameter linear free energy relationships. P.M. Geach

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.


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. Rierer, T. K. Trullinger, Organizers

8:00 - 12:00

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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
AGRO 293. Renewable syntheses of agrochemicals and pharmaceuticals from biomass-derived platform chemical 5-chloromethylfurfural (CMF). F. Chang

AGRO 294. Development of a high-throughput screening system for the detection of PaOD, octopamine receptor antagonists and agonists from Peniplaneta americana. E. Norris, A. Gross, M. Kimber, L. Bartholomay, J.R. Coats


AGRO 296. Modeling the vibrational spectroscopy of amorphous carbonaceous materials using DFT. A. Brown, M.T. Tinkin, N.A. D奥斯, G. Tompson

AGRO 297. Prospecting of oil and deoiled cakes of Jatropha curcas L. with EPR spectroscopy of amorphous carbonaceous materials using DFT. R. Kalra


AGRO 301. Development of Neurotoxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by ONF, Cosponsored by AGRO, CINF, EWNR and MEDI

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehmet A. Oturan

A Symposium in Honor of Professor Mehmet A. Oturan and Professor Enric Brillas and Developing a scalable process for microbial degradation of PAHs: A new bioremediation process. B. A. Lorsbach, T. K. Trullinger, Selby and 2015 AGRO Award for the A Spencer Award in honor of Thomas Boston Park Plaza Hotel and Towers

Developing a More Efficient Pesticide Exposure Screening Informed by Fate, Usage, and Monitoring Data

Cosponsored by EWNR

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. Desmarais, P. Hendley


3:10 Intermission.


3:55 AGRO 313. Improved modeling approach to evaluate aquatic pesticide impact for products to impact surfaces 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

Degradation of Halogenated Compounds in the Environment

Cosponsored by EWNR

K. Lee, M. Ma, K. Myung, N. M. Satchivi, Organizers

1:00 - 5:00

AGRO 284. Anaerobic abiotic reduction of dichloroacetamide safeners in Fe(J)-amended, heterogeneous mineral systems. A. Rios, J.D. Sury


Section F

Boston Park Plaza Hotel and Towers

Development of More Efficient Pesticide Exposure Screening Informed by Fate, Usage, and Monitoring Data

Cosponsored by EWNR

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. Green
Wednesday Evening

Detection and Fate of Health-Related Microorganisms in Water
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. Lorsbach, T. K. Trulliger, Organizers, Presiding
8:50 Introductory Remarks.
8:55 AGRO 335. Lead generation: Revving up the engine of discovery. V.B. Hegde
9:45 AGRO 337. Design and synthesis of pyridine and pyrimidine derivatives as insecticides. M. Xu. T. Bridell
10:10 Intermission.
11:20 Concluding Remarks.

Section B
Boston Park Plaza Hotel and Towers
Arlington Room

Biomonitoring for Pesticide Exposures
Sponsored by ENVR
S. Hayes, J. N. Seiber, Organizers, Presiding
8:50 Introductory Remarks.
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
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. Beaton
11:45 Concluding Remarks.

Section C
Boston Park Plaza Hotel and Towers
White Hill Room

Degradation of Halogenated Compounds in the Environment
Sponsored by ENVR
K. Lee, M. Ma, K. Myung, N. M. Satchivi, Organizers, Presiding
8:50 Introductory Remarks.
8:55 AGRO 346. Combinatorial quantity and quality determine reductive dechlorination rates and extents. F. Loeffler, J. Yan
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. Kubick, C. Yang
11:20 Discussion.

Section D
Boston Park Plaza Hotel and Towers
Whittier Room

Spray Application Technology
Sponsored 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. Henny, C.F. Creach
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

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
**Section C**

**Boston Park Plaza Hotel and Towers**

**White Hill Room**

**Degradation of Halogenated Compounds in the Environment**

Co-sponsored by ENVR

K. Lee, M. Ma, K. Myung, N. M. Satchivi, Organizers, Presiding

1:00 Introductory Remarks.


1:30 AGRO 370. Degradation of organohalogenated alkylxides by the catalytic hemoglobin dehalogenase from Amphitryon ornata. R.A. Ghadiri, N.L. McComb, L. Carey


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 perchloroethylene and trichloroethene in chemostat reactors and a continuous flow column. L. Sempini


3:50 Discussion.

4:05 Concluding Remarks.

Section D

**Boston Park Plaza Hotel and Towers**

**Whitier Room**

**Spray Application Technology**

Co-sponsored by ENVR

P. L. Havens, Organizer

S. H. Jackson, G. Kruger, Organizers, Presiding

1:00 Introductory Remarks.

**SUNDAY MORNING**

**Section A**

**Renaissance Boston Waterfront**

**Pacific Bllm 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


9:30 ANYL 3. Trading bunless for cuvettes: 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. Quinty, M. Roca


11:00 Discussion.

**Section B**

**Renaissance Boston Waterfront**

**Pacific Bllm F**

**Analytical Chemistry Applications in Pharmaceutical Sciences**

J. F. Castner, Organizer, Presiding

8:25 Introductory Remarks.


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


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


11:45 Concluding Remarks.

**SUNDAY AFTERNOON**

**Section A**

**Renaissance Boston Waterfront**

**Pacific Bllm 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. Kimura, 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.

**Section B**

**Renaissance Boston Waterfront**

**Pacific Bllm F**

**Forced Degradations in Pharmaceutical Industry**

H. Yanabe, Organizer, Presiding

1:25 Introductory Remarks.

1:30 ANYL 18. Predictability of forced degradation studies for real world stability. S.W. Baertschi


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


4:15 ANYL 24. Reduction of false positives in the peryox radical based stress test. R. Harmon

4:40 Concluding Remarks.

**Section C**

**Renaissance Boston Waterfront**

**Pacific Bllm 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. AnML: A new analytical data standard. S.J. Chalk

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**SUNDAY EVENING**

Section A
Bostom Convention & Exhibition Center

Hall C

General Analytical Posters
D. C. Duckworth, Organizer

6:00 – 8:00

- **ANYL**
  - **21.** Determination of individual C18 and C20 long chain base GM1 Gangliosides in a heterogeneous GM1 standard: Two strategies compared. A. Gobbrri, R. Zhang, B. Willard, D. Imran, D.J. Anderson
  - **22.** Syntheses of lignin-derived dimers from thioacetalization followed by Raney nickel desulfurization and their uses as GC quantitation standards. F. Yue, F. Lu, R. Sun, J. Ralph

- **ANYL**
  - **23.** Determination of thermally induced isomerization of polyether containing electrodes using electrospray ion mobility time-of-flight mass spectrometry. P. Xiao, D. Song, H. Li

- **ANYL**
  - **25.** Performance attributes of HPLC columns and relations to the separation of biocides. M.J. O’Leary, F.G. Alden

- **ANYL**
  - **26.** Evaluation of an LC-ESI-MS method for detection of sugars released after the enzymatic degradation of wood. S. Galster, D. Fangru, R.G. Grether

- **ANYL**

- **ANYL**
  - **28.** Graphene-based sensor interface for DNA charge transfer. L. Lu

- **ANYL**
  - **29.** Imaging and sampling with nanoplates. L.A. Baker

- **ANYL**
  - **30.** High-throughput microfluidic method to profile the dynamical properties of cellular currents. C. Vyas, A. Lam, K. Long, B. Natarajan, H. Ma

- **ANYL**
  - **31.** Multiplexed, in-situ detection of protein binding on plasma microelectrode delivery to the semantic web. S.J. Chak, A. Williams

- **ANYL**
  - **32.** Before we can handle big data we need smarter data. P. Jones, D. Vandenbroucke

- **ANYL**
  - **33.** Utilization of multiple data points and data sources in the identification of unknowns. D. Hardy, V. Laski, J. Nelson, L. Devore

- **ANYL**
  - **34.** Laboratory informatics environments: Why unified platforms and integration now? G.A. McKibben, D. Hardy, R. Sasaki

Current Topics in Seed Treatment
Sponsored by AGRO, Cosponsored by ANYL and ENVR

**SUNDAY EVENING**

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
Renaissance Boston Waterfront
Pacific Bldm G

Analytical Developments in Protein-DNA Thermodynamic Analysis
G.L. Baveghems, Organizer, Presiding
9:05 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. Boveridge
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 ENWIR

MIDNIGHT AFTERNOON

Section A
Renaissance Boston Waterfront
Pacific Bldm H

Addressing Challenges in Spectroscopy
A. G. Cavagnato, 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
3:05 ANYL 159. Correlation of IR spectra with thin film structure at solid-water interfa- ces. K. Hinrichs, A. Koning, A. Fuchner
3:45 Intermission.

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Section C
Renaissance Boston Waterfront
Pacific Ballroom G

Advanced Analytical Techniques for Early Cancer Screening

C. Burton, Organizer, Presiding

1:15 Introductory Remarks.


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. Wirt


2:40 ANYL 213. Ultrasensitive microfluidic immunoassay for protein pro-inflammatory cytokines and C-reactive protein in serum using a hybrid ESI-MS interface. J. Zaia, C. Lin, M.E. McComb


4:15 ANYL 216. Withdrawn.

4:35 Concluding Remarks.

Section D
Renaissance Boston Waterfront
Pacific Ballroom H

ACS Award in Analytical Chemistry: Symposium in Honor of John R. Yates III

J. R. Yates, Organizer
C. E. Costello, Presiding

1:00 Introductory Remarks.

1:15 ANYL 217. Qualitative and quantitative determinations of disease-related post-translational modifications to proteins. C.E. Costello, J. Zaa, C. Lin, M.E. McComb

2:45 ANYL 211. Chemopreventive interrogation of small molecule inhibition in vivo. J.A. Marto


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. Bambarger

4:40 Concluding Remarks.

Academic Innovations for Tomorrow’s Industries: GSSPC Symposium

Sponsored by CHED, Cosponsored by ANYL, BIOT, BMGT, CORP, D2C1, ENVR, PHYSYS and POLY

Antibiotics, Pharmaceuticals, Personal Care Products: Fate, Treatment, Analysis, and Ecological Effects

Sponsored by AGRO, Cosponsored by ANYL and ENVR

Immunochimistry Summit XI: Immunoassays and Other Bioanalytical Techniques

Sponsored by ANYL, Cosponsored by ANYL and ENVR

WEDNESDAY MORNING

Section A
Renaissance Boston Waterfront
Atlantic Ballroom I

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

8:00 ANYL 224. Infrared imaging and multivariate curve resolution for the forensic examination of automotive paints. B.K. Lavin, M.D. Allen, K. Nohieda, M. Sanderson

8:30 ANYL 225. Strontium isotope ratios of hair for human provenancing. B. Tippie, T. Chai, L. Chesson, J. Ehinger


9:30 ANYL 227. Effect of environmental conditions on the stability of trace explosives. M. Najjar, E. Sisco, J. Lawrence

9:50 ANYL 228. DHS Chemical Forensics Program – REACTS. K. Brady, E. Durham

10:10 Intermission.

10:25 ANYL 229. Monitoring ppt levels of toxic contaminants with a field portable GC-PID. J.N. Driscoll, J.L. MacLaughlan


11:05 ANYL 231. Pairing glycoproteins and surface-enhanced Raman spectroscopy (SERS) for the detection of toxic lectins. V. Szlap, M. Styles, A. Campos, D. Sprouse, B. Wagh, C.L. Haynes, T.M. Reineke

WEDNESDAY AFTERNOON

Section A
Renaissance Boston Waterfront
Atlantic Ballroom I

Open Air Analytical Measurements for Forensics, Health and Homeland Security

A. Hall, B. Musselman, Organizers, Presiding

1:25 Introductory Remarks.


2:20 ANYL 249. Isobaric drug analyses using direct analysis in real time (DART) and hydrogen/deuterium exchange. W.D. Hoffmann, G.P. Jackson


3:30 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. Backes

3:50 ANYL 252. High pressure handheld mass spectrometry. K. Gregory


5:05 Concluding Remarks.

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Section B  Renaissance Boston Waterfront  Pacific Birm F  

**Technological Program**

**Thursday Morning**

**Section A**  Renaissance Boston Waterfront  Atlantic Birm 1  

**Challenges in Bioanalytical Chemistry**  J. Wang, Organizer, Presiding  

- 8:25 Introduction Remarks.  
- 8:30  ANYL 269. Microtechnologies to interrogate single cells. N.L. Albritton  
- 9:00  ANYL 270. Quantifying protein expression in single cells. S.R. Walter, S. Schubert, M. Manioso, D.R. Walt  
- 9:40  ANYL 272. Paramagnetic NMR probe to study RNA-protein binding. L.M. Seebald, C.M. DeMott, A. Shekhtman, M. Roijen  
- 10:00  ANYL 273. Cholesterol Regulation of Granule Exocytosis in Platelets. S.A. Finkelstaudt-Quinn, S.M. Gruba, C. Haynes, S. De  
- 10:20 Intermission.  
- 10:35  ANYL 274. Collection and content analysis of tear film. S. Phippy, V. Akov, O. Zeng  
- 11:55 Interim Remarks.  

**Section B**  Renaissance Boston Waterfront  Pacific Birm F  

**Nanotechnology for Analytical Sensing and Spectroscopy Based Applications**  

**Biological Applications**  R. Narayanan, Organizer  

- 9:00  ANYL 278. Direct aminoglycoside coated gold nanoparticles synthesis, Characterization and antibacterial susceptibility testing. S. Cockstein, T. Modi, R. Dakshinamurthy  
- 10:00  ANYL 280. DNA-functionalized metal oxide nanoparticles as highly sensitive and selective biosensors for arsenate and hydrogen peroxide. J. Liu, B. Liu  
- 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. Multi-purpose application of Sacha Inchi (Plukenetia volubilis L.) plant: Pancreas from the Andean region. B. Kumar, L.H. Cumbal, A. Debiq  

**New Developments and Applications of Electrochemistry**  D. C. Duckworth, S. H. Pratt, Organizers  

- 8:25 Introduction Remarks.  
- 8:30  ANYL 284. Up-regulation of quorum sensing molecules for early and rapid electrochemical detection of bacterial pathogens. H.J. Bismart, T.A. Webster, E.D. Goluch  
- 9:10  ANYL 286. DNA Mikado: Effects of mismatches and DNA bending upon thermal hybridization behavior on gold electrodes. G. Fleisch, K. Bia, M. Vix  
- 10:10  ANYL 289. Investigation on the electrochemistry of atom-thick graphene nanoelectrode. H. Luo  
- 10:30 Intermission.  

**Thursday Afternoon**

**Section A**  Renaissance Boston Waterfront  Atlantic Birm 1  

**Challenges in Bioanalytical Chemistry**  J. Wang, Organizer, Presiding  

- 1:55 Introduction Remarks.  
- 2:00  ANYL 294. Sensitive and selective detection of point mutations using single molecule arrays. B.P. Reghri, M.R. Hartman, D.R. Walt  
- 2:30  ANYL 295. Withdrawn.  
- 3:00  ANYL 297. Butyrylcholinesterase extraction efficiency comparison between protein-G agarose spin columns and protein-G magnetic beads. A. Indapurkar, P. Eangco, J. Knaack  
- 3:15  ANYL 298. Chemicalimines labels released from long spacer arm-func- tionalized 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 luminescence determi- nation of CO/H,S 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-en- coded DNA strategies. M. Marco  
- 4:45  ANYL 303. Magnetic beads-based chemicalimines assay enables ultrasensitive quantification of microRNA. Z. Li, H. Yang, N. He  
- 5:00 Concluding Remarks.  

**Section B**  Renaissance Boston Waterfront  Pacific Birm F  

**Nanotechnology for Analytical Sensing and Spectroscopy Based Applications**  

**Other Sensing and Spectroscopy**  R. Narayanan, Organizer  

- 1:30  ANYL 304. Aluminum plasmonic am- atas based on a modified nanosphere tem- plate 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. Galpothdeniya  
- 2:30  ANYL 306. Non-invasive implant- able 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. Bil, A. Abbas  
- 3:30  ANYL 308. Rapid, nanoscale chemire- sistive vapor sensors. K. Fu, B. Willis  
- 4:00  ANYL 309. Study of ligand-induced cell signaling through the use of dissipation monitoring of the OCM-D. J.Y. Chen, M. Garcia, L.S. Parm, J. Xi  
- 4:30  ANYL 310. Withdrawn  

**Data to Decisions: Software Solutions for Modern Analytical Workflows**  

Sponsored by AGRO, Cosponsored by ANYL and DVM  

**Structure Elucidation in Metabolism Studies: Plant, Animal, and Soil**  

Sponsored by AGRO, Cosponsored by ANYL and ENVR
Division of Biological Chemistry
G. Cresw and V. Bandarian, Program Chairs

SUNDAY MORNING
Section A
Boston Convention & Exhibition Center Room 253A
Young Investigator Symposium
C. M. Cresw, Organizer, Presiding
9:00 BIOL 1. Examining the molecular recognition properties of MshB deacetylase. X. Huang, M. Hemrick
9:40 BIOL 3. Molecular characterization of the blood brain barrier tight junctions. S. Nangia, F. Kudrjanhan
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 small GTPases. J. Zhao, T.J. Nelson, C.J. Stains

Advances in Oligonucleotide Therapeutics
Sponsored by CARB, Cosponsored by BIOL, MEDI and ORGN

SUNDAY AFTERNOON
Section A
Boston Convention & Exhibition Center Room 253A
Pfizer Award in Enzyme Chemistry
D. Mitchel, 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. Gamea-Todkova
2:30 BIOL 12. Culture independent approaches for the discovery of new bacterial metabolites. S.F. Brady
4:00 BIOL 14. Peptide heterocyclization: The defining modification for an emerging natural product class. D. Mitchell

Advances in Oligonucleotide Therapeutics
Sponsored by CARB, Cosponsored by BIOL, MEDI and ORGN

BIOL 15. Rationally designed protein domain mimics to inhibit recalcitrant protein-protein interactions. A. Modell, D. Rozokin, Y. Zhang, P. Aorea
BIOL 16. Expanded genetic systems deliver DNA aptamers against hepatic cellular 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 19. Small molecule drug conjugates targeted to cholecystokinin 2 receptor. J. Roy, C. Wayya, 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 22. Identity of cofactor bound to mycotoxin conjugate amidas (Mca) is influenced by expression and purification conditions. E. Kocabas, H. Liu, M. Hemrick
BIOL 25. Light-activated azide ligation within living animals. L. Shah, S.T. Laughin, L.S. Canco
BIOL 26. Photoactivatable produgs of kinase inhibitor vemurafenib. B. Pinchuk, R. Horbert, D. Alesi, P. Davies, C. Peter
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. Musian, S.L. Curti, M.J. Maroney
BIOL 31. Probing the catalytic charge relay system in alanine racemase enzyme with genetically encoded histidine mimetics. V. Shrama, Y. Wang, W. Liu

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 lycopene as an antimicrobial agent. H. Park, R. Park, V. Kim, J. Min
BIOL 37. Fluorescent mechanism-based probes for aerobic flavin-dependent enzyme activity. I. McCulloch, J. La Clair, M.J. Jarmolik, M.D. Burkat
BIOL 38. Redirecting small molecules for malaria: Inhibitors of enoyl-ACP reductase for Plasmodium falciparum (PFER). L. Talion, J.D. Dunnant, Q.G. Nguyen, J.A. McCormon, M.D. Burkat
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 E1 synthase 1 (MPEGSI). M. Goodman, R.N. Armstrong
BIOL 42. Examining liposome association and small molecule inhibition of fatty acid amide hydrolase (FAAH) by hydrogen/deuterium exchange mass spectrometry. B. Kochert, A. Makriniyi, J. Engen
BIOL 44. Role of a guanidination catalysis-phosphodiation pair in the transition state stabilization of glycerol 3-phosphate dehydrogenase-catalyzed hydrate transfer. A.C. Reyes, A. Koudeika, T.L. Amyes, J.P. Richard
BIOL 45. Synthesizing biologically relevant phosphonohydrides and analogs by chemoselective coupling of phosphoramidites with phosphonates. A. Hofer, G.S. Cremosnik, H. Jessen
BIOL 46. Biochemical and biophysical characterization of AzO2, a novel azo-dye suicide enzyme from Clostridium perfringens. J. Morrison, G.H. John
BIOL 47. Characterization of DhP1-C, a tRNA-dependent enzyme in dehydrobiosynthesis. E.C. Ulrich, D.J. Bougioukou, W.A. van der Donk

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BIOL 49. Acrylamide warheads for targeted drug design against bacterial glutaredoxins. D. Morris, R.B. Khattry, S. Bilinovich, T. Leeper

BIOL 50. Development of tripeptide-based nucleic acid binding binders. S. Barros, D.M. Chenoweth

BIOL 51. Assessing the role of protein flexibility in Helicobacter pylori HyPA nickel delivery. P. Baskas, R. Kuranian, M. Manneur

BIOL 52. Internal dynamics of methionyl-tRNA binding domains in the presence of DNA. S.M. Bilinovich, D.C. Williams

BIOL 53. In vivo quantification of MMA-13 using molecular beacon to realize early, sensitive, and long-lasting arthritis diagnosis. H. Yu, Y. Chen, B. Vornius, E. Darling, Q. Chen

BIOL 54. Withdrawn.

BIOL 55. Structure and aromatic substrate-strain interaction in the pyrulone peptidyl carrier protein PLT. M.J. Jaremko, D. Lee, M.D. Burkart

BIOL 56. Design and development of gencitabine-loaded liposomes for the treatment of pancreatic cancer. G. Tarsos

BIOL 57. Withdrawn.

BIOL 58. Two faces of Pai: Elucidating the two orientations of Pai protein in E. coli. B. D'arcy, J. Shaw, M. Pichichero, L. Vacca Michel

BIOL 59. Protein-DNA interactions in mammalian transcription by molecular dynamic simulations. A. Sebastian, J. An, D. Xiao, J. Lu

BIOL 60. Supramolecular organization of carotidial extracellular matrix. F. Horkay, I. Horakne-Szakaly, E. Dimitriadis, P.J. Basser


BIOL 62. Crystal contact deletion enables recovin to crystallize with a calcium ion bound in EF-hand 2 and 3. R.P. Kumar, M.J. Ramnarayanan, A. Kaur


BIOL 68. Fast chelators and fluorescent sensors reveal a functional role for mobile zinc in the follicar bell. 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 arginime-rich-GNGG nanospheres. K. Chang, L. Sun, T. Webster

BIOL 70. Targeting cancer cells with virus-like particles for photodynamic therapy. S.N. Crooke, A. Abid, N. Rohmer, S. Thomas, M.G. Finn

BIOL 71. Locating the estradiol binding pocket for the G-protein coupled estrogen receptor (GPER). A.R. Vadid, S. Macaspac, H. Ng

BIOL 72. Yeast three-system hybrid for evolving a copper “clickase” enzyme. L. Zhao, D.F. Doyle, M.G. Finn

BIOL 73. Aldehyde captureligation for synthesis of native peptides. H. Wu, M. Raj, P. Fosk, J. Su


BIOL 77. Development of cytostatic-targeting mass spectrometry platforms for the targeting of senescent proteins and the mitochondrial proteome: Enrichment of low abundance protein sets. D. Baki, E. Weeparana

BIOL 78. Identification, characterization, and quantitative analysis of DNA-protein cross-links induced by phosphomycin mustard. A. Grethel, N.Y. Tretyn

BIOL 79. Structural and functional characterization of histidine triad nucleotide binding protein 1 mutants associated with inherited peripheral neuropathy. R. Shah, K.M. Mace, B. Fries, C.R. Wagner

BIOL 80. Hemipereipheral groups interactions in proteins and the role of the dielectric constant of the medium. J. Cerda, A. Stockhausen, N. Wilkes, A. Lange, K. Silva

BIOL 81. Investigating the structure and function of PsPT and PpPT, phosphopentathionyl transfers from M. tuberculosis and M. ulcerans. C. Vickyer, N. Kissa, E. Casavant, S. Suan, 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 agrin 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 86. Elucidating the two orientations of vaccine candidate P6 from post-b Nicholas influenza virus, B. Kisselstein, C. Readbach, J. Shaull, M. Pichichero, L. Vacca Michel

BIOL 87. Antibacterial activity of dextran-coated nanoceria at various pH values. H. Yazici, E. Alpaslan, t. webster


BIOL 89. Effect of cholesterol on the interaction between the antimicrobial peptide jelleine-I and binary lipid mixtures. N. Andijani, A. Sundu-Meya, N. Phambu

BIOL 90. Heterologous construct of the nasso peptide, lariatin A. A. Adenj-Adele, J.W. Thomas


BIOL 92. Metabolic synthesis of clickable peptide for chemoelectrochemical detection of glutathionylation. K.T. Samarasinghe

BIOL 93. Conformational changes in feucilin induced by phosphomycin-erin-containing model membranes. A. Alshammari, A. Sundu-Meya, N. Phambu


BIOL 95. Computational models of the chemical evolution of complex metabolic systems. P.M. Schwartz, I.M. Kubala, P. Dutta, S.M. Barratt


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. Aziz, J.J. Guiraks, D. Bucella

BIOL 99. Unnatural amino acids with enhanced reactivity for in vivo covalent chemical capture. C.M. Joiner, M. Green, A.K. Maip

BIOL 100. Generic approach to purify recombinant proteins from E. coli using MBP and silk-binding peptides. S. Ranar-Kumar


BIOL 102. Nature of the low catalytic activity of monomeric mutants of triose-phosphate isomerase. E.V. Contreras, R.M. Bastida-Santoyo, M.E. Chavez-Cardenas

BIOL 103. Domain-specific targets for evolving a copper “clickase” enzyme. L. Zhao, D.F. Doyle, M.G. Finn

BIOL 104. RNA-gold platform: Metals, catalysis, and drugs. V. DeRose, M.M. Hau, J.D. White, A.D. Moghaddam, R. Cunningham, R. With, K. Plakos


BIOL 106. Finding homes for orphan enzymes. F.M. Raushel

Biochemical Bioprosthetics: Discovery and Regulation of New and Potential Products

Sponsored by AGRO, Co-sponsored by BIOL

Innovation in Health and Medicine

Sponsored by MPPQ, Co-sponsored by BIOL, BIOT, MED and TOX

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 110. Exploiting protein homeostasis for cancer therapy. R. Deshaies, J. Lu

9:00: BIOL 112. Small molecule antagonists of the deubiquitinating USP7 interfere with ubiquitin binding. I. Everts

9:30: BIOL 113. Investigating deubiquitination with DUB-specific probes. Z. Zhong

10:00: BIOL 114. Understanding how deubiquitinasises catalyse isopeptide bond cleavage. E.R. Strieter, L. Anderson


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 (mMoA) compounds in thera-peutics discovery. S.L. Schreiber


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 diagnosis and intra-operative imaging applications. L.O. Olson, N. Withana, M. Venkova, J. Sorger, M.S. Bogoy

Section A
Boston Convention & Exhibition Center Room 253A

Young Investigator Symposium
C. M. Chris, Organizer, Presiding


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 RhO catalyzed GTP hydrolysis via a strain-free transition state. R. Mott, V. Jin, E. Pellegino, M.W. Bowler, N.G. Richards, G. Blackburn, J.P. Wallo
BIOL 177. Crystallization of a heterocyclization domain in yersiniabactin biosynthesis. Y.K. Miah, D. Fruth, D.P. Dowling

BIOL 178. Crystallization of a kinase involved in 5-hydroxymethyldeoxyuridine modification in phag. C.A. Hunt, C. Guan, P. Weigelt, 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 asyline 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. Tow

BIOL 185. Role of hydrogen bonding between Ang2 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. Kovač, C. Maloy, A.D. Shemy

BIOL 187. Withdrawn.

BIOL 188. Engineering bacteriophage for the ultrasensitive detection of foodborne pathogens. T. Henkley, A. Jackson, S.D. Alcaine, S.R. Ngun

BIOL 189. Withdrawn.

BIOL 190. Withdrawn.


BIOL 192. Withdrawn.

BIOL 193. Improvement in production of gamma-aminoibutyric acid from glutamate using glutamate decarboxylase separated from Escherichia coli. D. Dinh, T. Kang, K. Won

BIOL 194. Softer side of chemistry: Tunable, fluorescent, multicolored, stable, bioactive, bioabsorbable protein and enzyme nanoparticles (nano-proteins). B. Stromer, C.V. Kumar


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. Nanotechnology sensing through synthetic biology. B. Saltape, U. Sekar

BIOL 198. Pneumococcal neunnaminidase substrates identified through chemoselective labeling. J.E. McCombs, J.J. Kohler


BIOL 200. Use of CF-2-fluorodeoxyglucose (FDG) to label antibody fragments for immune-PET of pancreatic cancer. M. Rashidian, H. Poiob


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. Momeau, C. Barratt

BIOL 205. Quantification of deubiquitinating enzyme activity in cancer cells using a protease-resistant, peptide based reporter. A.T. Melvin


BIOL 207. Substrate specificity of bacterial endo-β-N-acetylglucosaminidases. A. White, R. Johnson, G.C. Hoops

BIOL 208. Gene categorization: An algebraic topololgy perspective. A.M. Kabza, D. Ho, J. Lastimosa, R. Konkenda

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 bro-modomain inhibitors. J. Bradner

9:45 BIOL 210. Chemical- proteomic strategies to investigate reactive cysineines. E. Weerapana

10:30 BIOL 211. Transition state and inhibitors of DNA methyltransferase Dnmt1. O. Du, S. Gulab, A. Woodhouse, 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


1:45 BIOL 214. TYW1: A radical SAM enzyme bringing that catalyzes the the biosynthesis of all wyosine derivatives. A.P. Young, V. Bantilan

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


2:30 BIOL 217. Conformational restriction of the NPF motif to target EHD1 and endocytic recycling. A. Kamens, R. Eset, T. Corin, J. Dala, J. Kitzig

2:45 BIOL 218. New insights into the mechanism of biological nitrogen fixation. V. Hoek, D.R. Dean, L.C. Soekht, B.M. Hoffman

3:00 BIOL 219. Nanomechanical study of the interfacial enzymatic activity of cellulases. W. Du, J. Xi


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

4:00 BIOL 222. Unraveling the importance of home reox redox pathways toward controlling enzymatic activities. A. Bhagi, V. Lu

4:40 BIOL 223. Structure-activity relationship studies of Grancicadin A mutants enabled by facile reductive amination. B. Zieras, J. Gas


4:55 BIOL 225. Role of the highly-conserved intervening domain of NEMO in high-affinity binding to IKKÎ². R. Shafter, D. Petrossi, M. Finai, S.M. Cote, K.N. Allen, A. Whitby

MONDAY MORNING

Section A

Renaissance Boston Waterfront

Atlantic Blm 1

The Chemistry Enterprise in 2015

Cosponsored by PREG 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. Connell

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 Birm 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. Kranich
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. Manika, T. Subtbach
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. Grös Schmidt
4:45 Concluding Remarks.

TUESDAY MORNING
Academic Innovations for Tomorrow’s Industries: GSSPC Symposium
Sponsored by CHED. Cosponsored by ANYL‡, BIOT‡, BMGT, CORP‡, DACC, 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‡, DACC, 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. Roizner, Program Chair
OTHER SYMPOSIUM 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 INOR, Wednesday, Thursday)

SUNDAY MORNING
Section A
Seaport Hotel and World Trade Center
Beacon Hill 2/3
Fundamental and Applied Aspects of Glycoinformation
R. Naran, 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
9:50 CARB 4. Heparin nanoparticles for β amyloid binding and mitigation of β amyloid associated cytotoxicity. P. Wang, X. Huang
10:10 Intermission.
10:55 CARB 6. Carbohydrate based systems for liver targeted cancer therapy. R. Naran
11:45 CARB 8. Smart microarray platforms for understanding biochemical interactions. C.J. Biggs, M. Gibson
12:10 Intermission.
10:05 CARB 11. Recent advances in RNA Chemistry: From RNA chips to novel functional RNA structures. M.J. Damha
10:35 Intermission.
National Science Foundation’s Centers for Chemical Innovation
Sponsored by PRES, Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB

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. Arna, Presiding
9:00 Introductory Remarks.
9:05 CARB 9. Mammalian cell nuclei: A rich source of targets for synthetic nucleic acids. D.R. Corey
9:30 CARB 10. Expanding chemical diversity of therapeutic oligonucleotides for treatment of neurodegenerative disorders. A. Khvorova
10:00 CARB 11. Recent advances in RNA Chemistry: From RNA chips to novel functional RNA structures. M.J. Damha
10:30 Intermission.
National Science Foundation’s Centers for Chemical Innovation
Sponsored by PRES, Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB

21st Century Chemistry Education: Formal and Informal
Sponsored by PRES, Cosponsored by AGRO, CHAS, CHED, CNF, COLL, ENFL, PROF and SOQED
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, IMEC, IAC, PRES and PROF

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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 glycosphin-golipid immunostimulants. S. Kim
8:45 CARB 39, Immunostimulatory glycolipids: Polar opposites joined at the hip. J. Gervay-Hague
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. Benedito, L. Teyton
10:30 CARB 42, Design, synthesis, and evaluation of Th1 skewing α-Gal-Cer analogs. S.P. Van Calenberg
11:00 CARB 43, Aminocystic glycolipid mimetics are potent activators of NK cells and immune response. A. Liebarg
11:45 CARB 45, Glycolipid antigen-pre-sentation by CD1d and mechanism of NKT cell activation. D.M. Zajonc
5:15 Conclusion Remarks.

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

CARB 48, Synthetic chemistry of human syndecan-3 glycopeptides bearing two heparan sulfate glycan chains. W. Yang
CARB 50, Cellulose nanofiber prepared by persulfate oxidation of bagasse pulp. C. Du, H. Li, M. Liu
CARB 51, Synthetic glycolipids efficiently suppress CFTN non-sense mutations and are enhanced by Lactoferrin. V. Beljakov, M. Sholley, J. Schacht, D. Bedwell, S. Rowe, T. Baasov
CARB 53, Influence of the isoiochytane atio moitey on stereoselective synthesis of cis acid glycosides and subsequent diversification. A. Mandhapati, D. Cirich, R. Salla
CARB 54, Synthesis and properties of pentulose-RNA chimeric oligonu-cleotides. T.C. Ethimou, K. Krishnamurthy
CARB 55, Separation of lactose, lactulose and epilactose by a new HILIC column. M. Turcotte, S. Sakai, N. Nakajima, R. Benson
CARB 56,Withdrawn.

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 antiseense strand: Evaluation of gene silencing activ-
ity and stability. I. Zlatev, D.J. Foster, J. Liu, K. Charsse, B. Bringham, M.A. Maier, K.R. Rajeev, M. Egil, M. Manoharan
CARB 53, Positional trivalent of trigger GalNAc ligands on the gene silencing activ-
CARB 54, Effect of metabolically stable (E)- and (Z) - 5′-vinylphosphate on siRNA activity. R.G. Parmar, C. Thele, K. Charsse, 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-galactosylceramide. D. Chennamadhavan, A.R. Howell
CARB 56, α-Galactosylceramide analogs: A searchable data set of galactosyl induction levels. R.W. Franck
CARB 57, Cyclodeaddition way to O-glycosides: Vintage reactions for new tumor antigen mimetics. G. Natvi, R.W. Franck, B. Richich
CARB 58, Synthesis, characterization and binding studies of a biarylne based lectin mimic under physiological conditions. A.K. Addo-Mensah, M. Addo
CARB 60, Genome mining, functional expression and inhibition of arabino-olaganactan biosynthesis for therapeutic treatments of Nocardia infection. H. Chiu, Y. Chen
CARB 63, Chemical synthesis of human syndecan-3 glycopeptides bearing two heparan sulfate glycan chains. W. Yang
CARB 64, Chemical synthesis of isotope-labeled N- and O- glycopeptides for quantification of tumor associated glycopeptides. S. Ramadhan, W. Yang, A. Elisa, R. Goldstein, X. Huang
CARB 65, Cellulose nanofiber prepared by persulfate oxidation of bagasse pulp. C. Du, H. Li, M. Liu
CARB 66, Synthetic glycolipid mimetics efficiently suppress CFTN non-sense mutations and are enhanced by Lactoferrin. V. Beljakov, M. Sholley, J. Schacht, D. Bedwell, S. Rowe, T. Baasov
CARB 68, Influence of the isoiochytane atio moitey on stereoselective synthesis of cis acid glycosides and subsequent diversification. A. Mandhapati, D. Cirich, R. Salla
CARB 69, Synthesis and properties of pentulose-RNA chimeric oligonucleotides. T.C. Ethimou, K. Krishnamurthy
CARB 70, Separation of lactose, lactulose and epilactose by a new HILIC column. M. Turcotte, S. Sakai, N. Nakajma, R. Benson
CARB 71, Withdrawn.
CARB 72, Non antibacterial aminoglyco-side analogs as potentiators of ineffective antibiotics against multidrug resistant Pseudomonas aeruginosa. B. Gorityala, D. Fernandez, G. Guichati, G. Zhao, 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 synthe-
sis of (+)-Griseusin A. G. Liang, O. Zhang, G.A. O’Doherty

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

98. First synthesis of 2-ami-noacetly-2,3-dideoxy-D-glucose. T. Grone, Z. Witzczak, B. Brouer


100. Development of fluorescent saccharide sensors based on a 1,2,3-triazole ring. W. Zhai, J. S. Fossey


103. Targeting cancer cell metabolism using small-molecule modulators of reactive oxygen species. F. Nondorme


106. Substrate specificity for human alpha-1,6-fucosyltransferase (FucT) expressed in large scale from recombinant baculovirus infected SF9 insect cells. A. D. Caldeon Molina, L. Y. Liu, X. Wang, X. Li, P. G. Wang


108. Synthesis and positional effects of 2′-O-(2-methylaminoo)-2′-oxooxyl (2′-OMA) modification. C. S. Kuchinchi


110. Synthesis of novel aryl nucleosides. W. Dong, S. A. Woski

111. Novel chitosan-based avidin/biotin system for target-selective drug delivery. W. Li, D. Rammekkamp, Y. Meng


113. Antigenic activity of carbohydrate-based constructs Tn-PS A1 and Tn-PS B. H. P. Andreana

### WEDNESDAY AFTERNOON

**Section A**

**Seaport Hotel and World Trade Center**

**Waterfront 3**

**Carbohydrate Synthesis for Medicinal Chemistry and Biology**

G. A. D’Ohoertey, X. Y. Organizer, Presiding

1:45 CARB 120. Reagent controlled approaches to deoxy-sugar oligosaccharides. J. Liu, D. M. Gao, M. Gao


3:05 CARB 123. Synthetic approach towards the glicolasins and related C-glycoside natural products. D. Ray, G. A. D’Ohoertey

3:25 Intermission.

3:40 CARB 124. Directed evolution-based development of clustered carbohydrate antibiotics. J. Krauss

4:10 CARB 125. Explore the structure activity relationship of resin glycoside via the de novo synthesis of both enantiomers of Batatinone III. X. Liu, M. L. G. A. D’Ohoertey


### THURSDAY MORNING

**Section A**

**Seaport Hotel and World Trade Center**

**Waterfront 3**

**Carbohydrate Synthesis for Medicinal Chemistry and Biology**

G. A. D’Ohoertey, X. Y. Organizer, Presiding

9:00 CARB 113. De novo synthesis in carbohydrate medicinal chemistry. G. A. D’Ohoertey

9:30 CARB 114. Synthesis of diverse types of campeagel otsacchae-rides. C. Kimmam, D. M. Gao

9:50 CARB 115. Synthesis and bio- logical studies of amphiplkamycins. C. T. Chang

10:20 Intermission.

10:55 CARB 117. Chemical synthesis of bioactive natural molecules bearing 2-deoxy sugars. J. Zhu


11:45 CARB 119. Investigation of antitolic entirely carbohydrate constructs Tn-PS A1 and TF-PS B. R. Andreana

### SUNDAY MORNING

**Section A**

**Renaissance Boston Waterfront**

**Atlantic Blrm 3**

**Single Atom Catalysis**

A. M. Karim, Organizer, Presiding

Z. Wei, Presiding

8:00 CARB 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 CARB 4. CO oxidation by CuO supported Pt catalysts. A. Therrien, E. H. Sylvester

9:05 CARB 3. Anchoring single atoms for better catalysis. J. Liu

9:35 CARB 13. CO and NO oxidation on supported single Pt group catalysts. C. K. Narula, A. F. Lawrence, S. M. G. M. M. Bobst

10:05 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
Heterogeneous Catalysis for Environmental Applications
Photocatalysis for Energy and Environment
Sponsored by ENFL, Cosponsored by CATL
Innovative Chemistry & Electro catalysis for Low-carbon Energy & Fuels: Discovery to Application
CO$_2$ & Solar
Sponsored by ENFL, Cosponsored by CATL

**MONDAY MIDDAY**

**Section A**

_**Renaissance Boston Waterfront**_

**Atlantic Blrm 3**

**2015 ACS Catalysis Lecture**

**Supported 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[NP(N$_2$)$_3$]$_2$ catalysis for H$_2$ production. M. J. O. Hagan, A. P. Caradonna, 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 electron catalysis. S. Hammes-Schiffer

**10:20** CATL 78. Non-ingenious 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. Raugei

**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. Grisovska-Pargovska, 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. A. Gilbertson

**9:30** CATL 83. Ultrahigh-flux 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 H$_2$ without a change in overpotential with a bioinspired iron molecular electrocatalyst. J. Darmont, N. Kumar, S. Raugei, 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. Edaoudi, 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. Rosowsky

**8:40** CATL 88. Metal-organic frameworks as catalytic nanoreactors for sustainable energy applications. V. Stavila, K. Leong, P. Parthasarathi, K. Sale, R. Davis, M. Kent, M. Allendorf


**9:30** CATL 90. Metal-organic frameworks as heterogeneous solid acid catalysts for fixed-bed reactions. S. Ma

**9:55** Intermission.


**10:45** CATL 92. POMzites: A family of zeolitic polyoxometalate frameworks from a minimal building block library. L. Chen

**11:10** CATL 93. Inorganicmetallic catalyst design. L. Gagliardi, S. O. Gidley, O. K. Farha, J. T. Hupp, C. J. Cream

**11:35** CATL 94. MOF-mediated synthesis of highly active and stable catalysts for C1 chemistry. F. Kaptijn, T. A. Wezenek, X. Sun, M. Makkie, 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


**10:20** Intermission.

**10:35** CATL 98. Is there still life in the geometric model of sulfide catalysts? S. Solod, S. Miseo, J. E. Baumgartner, C. E. Klewer

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. Atominically precise gold and bimetal nanoclusters for nanocatalysis. R. Jin

9:00 CATL 103. Supported bimetallic AuPd clusters using Au$_n$Pd$_m$ clusters as precursors. K. Lee, A. Shirkhoda, Y. Hu, R. W. Scott

9:20 CATL 104. Withdraw


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 metals 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 shapes of AuCeO$_2$ catalysts for water-gas shift reaction. Y. He, B. Chen, X. Liang


Advances in Ceramic Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion Theory

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Biofuels for Powering the World: Discovery to Application
Hydrotreating, Upgrading and Gasification
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Heterogeneous Catalysis for Environmental Applications
Heterogeneous Catalysis for Energy and Environment
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Innovative Chemistry & Electrocatalysis for Low-carbon Energy & Fuels: Discovery to Application
Fuel Cells & ORR
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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 BIm 3

2015 ACS Catalysis Lecturehip
Cosponsored by INOR
M. Heim, E. S. Wedner, Organizers
M. Y. Darenbourg, Presiding

1:00 CATL 111. Amino acids on the outer coordination sphere of [Ni(NH₃)₄]²⁺ result in enhanced catalytic activity. W.J. Shaw, A. Dutta, A. Jain, S. Rauei, B. Ginoiska-Pangowska, J.A. Roberts


2:00 CATL 113. Bioinspired catalytic systems and technological applications of hydrogen. V. Arteo

2:30 CATL 114. Modified molecular N₅⁺Ni⁺ catalysts for photocatalytic proton reduction. M.R. Wasielewski, M. Majovsky, W. Han, B.T. Phelan

3:00 Intern. 3:15 CATL 115. Thermodynamic considerations in the design of molecular electrocatalysts for proton and CO₂ reduction. J.Y. Yang, C. Tsay, B. Livesey

3:45 CATL 116. Thermochemical and mechanistic insights into the selective reduction of CO₂ to formate using iron clusters. L.A. Berben, A. Tahori, M.D. Ral


Section B
Renaissance Boston Waterfront
Caspián

Role of the Outer Coordination Sphere on the Activity of Enzymes and Molecular Catalysts
B. Ginoiska-Pangowska, Organizer
M. O’Hagan, W. J. Shaw, Organizers, Presiding

1:00 CATL 118. Molecular H₂-evolving catalysts with proton relays: Design, mechanistic studies, and benchmarking of catalytic activity. V. Arteo


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. Lutz, W.J. Shaw


3:20 CATL 122. Nickel superoxide dismutase: The mechanism of superoxide disproportionation effected by the enzyme and metalloproteid based NiSOD mimics. J.M. Shearer


Section C
Renaissance Boston Waterfront
Atlantic BIm 2

Metal Organic Frameworks for Catalysis Applications
O. K. Farha, J. Gascon, Organizers
M. Edidinović, P. K. Thalapally, Organizers, Presiding

1:00 Introductory Remarks. 1:05 CATL 124. Metal-organic frameworks for sustainable catalysis. W. Lin

1:40 CATL 125. Porphyridine metal-organic frameworks for pho-toloredox catalysis. J. Zhang

2:05 CATL 126. Impacting functionality of biocatalysts by embedding enzymes into metal-organic frameworks by a de novo approach. C. Tsang

2:30 CATL 127. Withdraw. 2:45 Intern. 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


4:45 CATL 132. Impact of introduction of basic sites on adsorptive and catalytic properties of fcu metal organic frameworks. J.A. Navarro


5:45 CATL 134. Au-Pd bimetallic nanoparticle catalysts and their application in oxidative coupling. V. Yang

5:55 Concluding Remarks.

Section D
Renaissance Boston Waterfront
Pacific BIm 1

Catalyst Poster Session

6:30 - 8:30
Catalysis Poster Session

Concluding Remarks.

Section A
Westin Boston Waterfront
Galleria
Catalysis Poster Session
K. K. Ramanasamy, Organizer

6:30 - 8:30
Catalysis Poster Session

Concluding Remarks.

Section E
Renaissance Boston Waterfront
Section C

6:30 - 8:30
Catalysis Poster Session

Concluding Remarks.

Monday Evening

Section A
Westin Boston Waterfront
Galleria
Catalysis Poster Session
K. K. Ramanasamy, Organizer

6:30 - 8:30
Catalysis Poster Session

Concluding Remarks.

159. Porous cobalt oxide nanoparticles for electrocatalytic oxygen evolution reaction. J. Ryu, S. Park, J. Jang, H. Kim, J. Park, E. Hwang


162. Atomic layer-by-layer deposition of platinum on palladium octahedral for enhanced catalysts toward the oxygen reduction reaction. X. Wang, J. Park, L. Zhang, Y. Xia


165. Solid acid-catalyzed hydroygen transfer to breaking C-O bond in α-oxoaldehydes. X. Yue, W. Bai, B. Sun, Y. Wang, Z. Zong

166. Ruthenium catalyzed dehydrogenation and transfer hydrogenation reactions using dimethylamine borane as a hydrogen storage. S. Tanyildizi, I.A. Morkan, S. Gokalp

167. Stability of linker groups for immobilization of active catalytic molecules on catalytic supports. S. Kim, K. Koh, G. Kim, B. Lee, h. Lee


170. Rationalization of the interaction between surface species and MO (ZrO2, and Al2O3). Y. Chen, R. Banuma

171. Ordered mesoporous carbon spheres supported Pt nanoparticles for enhanced electrocatalytic activity and durability. L. Xu, C. Zhang, N. Shen, T. Sun, J. Chen, Y. Yan


175. Synthesis of mesoporous organosilicas containing 1,8-naphthalimides by the template-free sol-gel method: Their use as catalysts for the photodegradation of methylene blue. B. Castanheira, F.J. Trindade, E.F. Teliconi, M. Politi, S. Brochatchian


177. Adsorption of NO over a novel multifunctional catalyst. A.P. Cardenas, P. Rangsunvigit, P. Ngaotrakanwiwat


181. Enzymatic resolution of α,β-CHX (X = F, Cl)-ATP diastereomers by a protein kinase. F. Ni, A. Kung, C.E. McKenna, C. Zhang

182. Facile synthesis of hierarchical PS@Pd nanoparticles supported Cu(ll) complex: Studies of its aerobic oxidation catalytic applications and mechanic study using dodecyl big data function. H. Wang

183. CO reforming of CH4 to syngas over Ni/SSB-A/15 catalysts --- effects of Ni modification on catalytic performance. H. Liu, D. He

184. Synthesis characterization and photocatalytic studies of magnetic nanoparticle-silica-titania composites. R. Serrano Garcia


188. Oxidation energy storage. J. Hwang, F. J. Fox, S. Lee, K.O. Albrecht

189. Oxygen energy storage of photocatalytic degradation for acetic acid 7 by p-ZnO-n-TiO2, bilayer film catalyst. U. Sittongw, P. Rangsunvigit, P. Ngaotrakanwiwat

190. Influences of alkalinity and inorganic anions on the PA degradation during CeO2 catalytic oxidation. W. Qun, Y. Zhichao, X. He

191. Novel Ag@AgCl cubic cages modified with Cu(ll) catalyzer. Y. Pang, C. Chen, L. Ge

192. Activation of CO as a carbon source for carbonyl acid derivatives. J. Park, K. Stowers

193. CO adsorption induced inverse surface segregation of Pd on Au/Pd bimetallic surfaces and its effect on CO oxidation pathway. H. kim, G. Han, J. Shin, H. Han, S. Kim

194. Fabrication and characterization of aluminum-supported Pd, Rh, and Pt nanoparticles for hydrodeboromination application. K. Ke

195. Ring opening polymerization of Rac-lactide using zinc amine-bispholate complexes. Y. Liu, C.M. Kozak

Section A
Boston Convention & Exhibition Center
Hall C
Sci-Mix
K. K. Ramasamy, Organizer
8:00 - 10:00

218. Catalytic defunctionalization of amino acids to value-added amines, nitriles, or amides. D. De Vos, I. Claes, F. De Schouwer, J. Verduyckt, M. Janssen

219. Catalytic oxidation of low-concentration NO emissions. S. Y. Han, I. A. Morkan, S. Mohammed, M. Kim, G. Park, S. Lee

220. Synergism of Co3O4 with Bi2O3 to strengthen the catalytic performance for soot oxidation and NOx reduction in diesel exhaust. Z. Zhang, W. Li, Y. Guo, W. Li


222. Cascade engineered synthesis of ethyl benzyl acetoacetate over a novel multifunctional catalyst. G.D. Yadav, S.C. Patankar

223. From photocatalysis to micro/nanomotors: Light-controlled motion speed, direction, and swimming behaviors. M. Fou, C. Chen, Y. Li, L. Kong, L. Xu, J. Guan

224. Regeneration of Rh- and Pd-based automotive three way catalysts after simulated fuel shift off. Q. Zhang, R. Tamato, M. Debeer-Oremuttah,

225. Enhanced catalytic activity for NO oxidation over A or B site doping of hexagonal phase LaCo3O6; A combined experimental and theoretical study. H. Yin, C. Zhou, X. Liu, R. Chen, B. Shan
Section A
Renaissance Boston Waterfront
Caspian

Computational Catalysis
R. S. Assay, N. Kumar, Organizers, Presiding
8:00 CATL 242. Survival-of-the-most-transferable: Better density functionals from a combinatorial design strategy. N. Martinsson, 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
10:00 Intermission.
10:15 CATL 246. First principles analysis of metal and oxide-metal interfaces. J. Greeley, Z. Zhao, B. Liu, T.B. 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-Vidallo, D. Loffreda, M.T. Koper, P. Sautet

Section C
Renaissance Boston Waterfront
Atlantik 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. Randhorne, S.H. Overbury
9:30 CATL 251. Square pyramidal structure of oxo vanadium (V) and (IV) species over low coverage V0x/Ti0x anatase catalysts. L. Amaron, S. Rasmussen, H. Faeg, 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. Camero, I. Hermans, J. Grant
11:15 Concluding Remarks.

Section B
Renaissance Boston Waterfront
Caspian

Computational Catalysis
R. S. Assay, N. Kumar, Organizers, Presiding
8:00 CATL 242. Survival-of-the-most-transferable: Better density functionals from a combinatorial design strategy. N. Martinsson, M.P. Head-Gordon
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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.
10:30 CATL 257. Catalytic regioselective and regiodivergent functionalization of alyenes, allenes, amines, and silenes. J. Montgomery
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
9:20 CATL 265. AuPd binary alloy nanoparticles decorated carbon graphitic 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.
10:30 CATL 268. Cobalt oxide nanocubes for photocatalytic water oxidation. F. Jiao
11:10 CATL 270. Recent developments in nanocatalysts for fuel cell reactions. S. Guo

Section F
Renaissance Boston Waterfront
Pacific Blrm H
In-Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles
B. Roizard-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
9:45 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. M. Mistry, F. Behardt, C. Lumdea, J.A. Boscobicin, B. Roizard-Cuenya
12:25 Concluding Remarks.

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion
Theory & Powder Catalysts
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Innovative Chemistry & Electrocatalysis for Low-carbon Energy & Fuels: Discovery to Application
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Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions
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TUESDAY AFTERNOON
Section A
Renaissance Boston Waterfront
Atlantik Blrm 3
CO2 Reduction and Utilization
D. Pakhare, A. Raju, Organizers, Presiding
1:00 CATL 276. Reformer 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. Spyve
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.
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. Vidal, L.A. Curtis
1:30 CATL 287. O, and Ag/Alu 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.D. Jang, J.A. Larcher
3:55 CATL 293. Understanding the active CuO domains for methanol selective oxidation to methanol in zeolite: A computational study. Z. Zhao, L. Veela, F. Stuedi
4:15 CATL 294. Oxidation of carbon monoxide with a monovalent Zn ion embedding on zeolite: A mechanistic study. S. Wannaka, T. Mahom, M. Protob, J. Lintrnmal
4:10 CATL 301. Alkalii-doped manganese oxides as redox catalysts for oxidative dehydrogenation of ethane. L. Neal, S. Yiasut, J. Schranko, F. Li

Section E
Renaissance Boston Waterfront
Pacific Rim 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) aliphane nanoclays as iron dosage. E.G. Garrido, F. Oliveros, M.S. Unteta-Janartu
1:40 CATL 304. Metal oxides/met-alorganic-frameworks as efficient electrocatalysts for oxygen reduction/reaction evolution 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, W. K. Li, S. Ding
2:40 Intermission.
3:30 CATL 309. One-pot encapsulation of alloyed nanoparticles using metal organic framework as crystal lattice 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
3:10 CATL 311. Oxidized Ni-Y 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

Advances in Ceria Based Catalysis: Structural, Electronic and Chemical Properties Tailored for Chemical Conversion
Powder Catalysts
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WEDNESDAY MORNING

Section A
Renaissance Boston Waterfront
Atlantic Rim 3
CO2 Reduction and Utilization
D. Pakhare, A. Raju, Organizers, Presiding
9:00 CATL 314. Grain boundary–dependent CO2 and CO reduction catalysts. M. Kanan
9:40 CATL 316. Hydroxalite-like compounds derived highly effective Cu-based catalysts for CO2 hydrogenation to methanol. P. Gao, H. Wang, S. Xiao, Z. Zhang, W. Wei, Y. Sun
10:00 Intermission.
10:15 CATL 317. Dual function material for CO2 capture and conversion using renewable H2. M.A. Arellano, M.S. Dayar, R.J. Farnato
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. Dong, Q. Yuan, B. Brankovic
8:30 CATL 322. Toward a more accurate description of adsorption in Brunsted acid zeolites by combining static and dynamic molecular simulations. J. Van der Mynsbrugge, K. De Wispelaere, P. Cruyds, V. Van Speybroeck
9:00 CATL 323. Formic acid oxidation on platinum: A simple mechanistic study. K. Schwarz, R. Sundaramaran, T.P. Moffat, T. Allison
9:20 CATL 324. Elucidating the mechanism of hydroxymethane (HDO) of acetone on MoOx, B. Buesse, M. Shetty, Y. Raman-Leshkov, W.H. Green
9:40 CATL 325. Catalytic reduction of ketones and aldehydes with Ei(3)/Bi(2)Fe3O4 crystals, frustrated Lewis pairs. B. Givovska-Pangovska, A.H. Hackel, D.M. Carnaioni, G.R. Schenter, S. Kothmann, T. Autrey
10:10 Intermission.
10:25 CATL 326. Dynamic stereo-graphic map approach to substrate binding in organometallic chemistry. L. Cavallo, I. Falvani, R. Credendino
10:45 CATL 327. Oxidative addition of aryl chloride to mono-ligated and bi-ligated linear/bent Au and Pd complexes. S. Vamalenti, I. Falvani, A. Poater, L. Cavallo
11:05 CATL 328. Computational screening of natural enzymes for Monte-Baylis-Hillman activity. N. Colelli-Occu

Section C
Renaissance Boston Waterfront
Atlantic Rim 2
Catalysis by Mixed Oxides
M. Guerrero-Pérez, I. E. Wachs, Organizers, Presiding
8:30 CATL 331. Photocatalytic hydrogen production by reducible oxides. P. Fomasoni
9:00 CATL 332. Operando FTIR, NAP-XPS, and XAS studies of CoO4 and CeO2–CoO catalysts during preferential CO oxidation. G. Rupprecht, L. Lukashuk, K. Föttinger
10:00 Intermission.
10:15 CATL 334. Catalytic combustion of vinyl chloride on La0.5Na0.5MnO3 perovskite oxides. W. Li, Y. Guo
10:45 CATL 335. Withdrawn.

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Section D
Renaissance Boston Waterfront
Pacifie Blrm A
Cataltic 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
C. Dorado, C.A. Mullen, A. Bootang
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 napthenes.
H. Oj de Beeck, M. Dusselier, B.F. Sels
10:50 CATL 345. Investigation of the reaction kinetics of isolated Lewis acid sites on alanin.
S. Cao, C.T. Willams, S. Raghunath, J.R. Pagonabarraga
11:10 CATL 346. Systematic study of alkali promotion of alumina supported ruthenium for levulinic acid hydrogenation to g-valerolactone.
H. Luo, D. Consoli, W. Gunther, Y. Roman-LeShkoy
11:30 CATL 347. Direct conversion of levulinic acid to 2-methyltetrahydrofuran using discrete Ru and Rh N-triphos catalysts.
P. Miller, A. Panopoulos, 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. Stachowiak, 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
Section C
Renaissance Boston Waterfront
Atlantic Blrm 2

Energy Storage Applications of Ammonia: Synthesis, Storage, Charging and Utilization
B. David, M. Jones, Organizers, Presiding
8:40  CATL 404. Ammonia decomposition over La2O3 supported co catalyst at 450°C. V. Pottapatt, H. Habbabman.
10:00 Intermission.

Thursday Afternoon
Section A
Renaissance Boston Waterfront
Atlantic Blrm 3

General Catalysis
Heterogeneous
A. Raju, K. K. Ramasamy, Organizers, Presiding
12:30  CATL 414. Withdrawn.
1:50  CATL 417. Regulation of AI distribution in the framework of ZSM-5 via post-treat- ment for catalytic cracking of n-butane. J. Xiu, G. Jiang, Y. Zhang, J. Zhao, G. Xu, Y. Wang, Q. Sun, A. Duan, J. Liu, Y. Wei.
2:10 Intermission.
Section E
Renaissance Boston Waterfront
Pacific Ballroom A

In-Situ Methods for the Study of Model Catalysts: From Flat Surfaces to Nanoparticles

D. J. Stachowiak, Organizer
J. A. Boscozkinik, B. Roldan-Cuenya, Organizers, Presiding
1:00 Introductory Remarks.
1:05 CATL 452, Transition metal nanoparticles on metal oxide nanoparticles (TMn(Mnp/MOnp) as model catalysts: Prn/(Fe)Cr: J.C. Hemminger
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. Nelson, J. Buffton, J. Robbins
4:00 CATL 457, In-situ studies of redox-mediated reconstruction of Cu(111) during CO oxidation. R. Xu, K. Mudiyanselage, A. Babar, M.O. White, D.J. Stachowiak
4:20 Concluding Remarks.

Section F
Renaissance Boston Waterfront
Pacific Ballroom A

General Catalysis

P. Bhattacharya, N. Kumar, Organizers, Presiding
12:20 CATL 458, In-situ metamorphosis of cobalt phosphide (CoP) nanoparticles toward efficient and robust oxygen evolution catalysts. J. Ryu, J. Jang, H. Kim, S. Yoo
1:10 CATL 460, Withdrawn.
1:30 CATL 461, Synthesis of the uniform covering micro-and mesoporous composite material Y/ASA. Y. Yin, S. Ou, 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. Abdulfah, 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 electrolytists. B. Li, A. Atif, A. Badshah
2:40 CATL 464, Trace explosives detection using zinc oxide nanowires. Z. Caron, D. Mallin, M. Chaplin, 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. Rajapake

SUNDAY MORNING

Section A
Boston Convention & Exhibition Center
Room 253C

High School Program
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Financedly supported by ACS Education
K. Anderson, Organizer
S. B. Mitchell, Organizer, Presiding
8:00 Registration.
8:30 Introductory Remarks.
8:35 CATL 467, 1. Probing neurons and sequencing DNA: my adventures in simple pH chemistry. A.E. Cohen
9:15 CATL 468, 2. Work safely and have fun, too! E.M. Howson
10:05 Intermission.
10:45 CATL 471, 5. Periodic table: Highlights from the history of an icon. C.J. Guinta
11:05 CATL 472, 6. From discovery to practical application: Molecular spectroscopy in the high school chemistry curriculum. D. McGraw
11:25 CATL 473, 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.

SUNDAY AFTERNOON

Section C
Boston Convention & Exhibition Center
Room 207

Undergraduate Research Papers
Cosponsored by SOCED

C. V. Gauthier, J. V. Ruppel, N. Snyder, Organizer
J. R. Mieczkowski, Organizer, Presiding
8:30 Introductory Remarks.
8:35 CATL 474, 11. Inquiries in physical sciences: A bottom-up approach for incorporating next generation science standards (NGSS) in K-8 physical science education. T. Gupta, E. Meichels
8:55 CATL 476, 13. Understanding students’ misconceptions of acid-base chemistry. T. Mead, M.T. Danovksy
9:05 Intermission.
9:55 Intermission.
10:35 CATL 484, 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.

3:55 CHED 36. Teaching sustainable development in the chemistry classroom: The implications of focused ten-

sions for enacting a feminist chemis-
try curriculum. J. Bhattacharya

1:35 CHED 37. Promoting pro-environ-

mental behaviors in students and their families by connecting the chemis-

try classroom to blended learning experiences. P.L. Daubenmire

2:45 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 CHED

I. 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-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 SOCHED

J. R. Mieczkowski, 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 nanopar-

ticles for enhanced photodynamic therapy. S.V. Shuththanandan, M. Zhu, J. Jayakravamaran

1:45 CHED 44. Synthesis and character-

ization of water soluble zinically (II) complex for liver alcohol dehydroge-

nase. N.A. Bernier, J.R. Mieczkowski

1:55 CHED 45. Synthesis and charac-

terization of asymmetric water soluble zinically (II) complex for liver alcohol dehydrogenase. G.A. Van

Akin, N.A. Bernier, J.R. Mieczkowski

2:05 CHED 46. Light-activated inorganic-ester hybrid. M. Rotondaro, E.C. Glazer

2:15 CHED 47. Reactions of 1,2-bis[2,6-di-

isopropylphenyl]iminolacacenaphthene (dpp-BIAN) with vanadium chloride compounds. G. Pezca, N. Onsri,

N. Tsoachke, J.D. Gordon, C.D. Abney

2:25 Intermission.


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. Wiggin, J. Brennan

2:55 CHED 50. Synthesis and charac-

terization of diazxonon tetraclorau-


3:05 CHED 51. Determining the factors that dictate carbone retention vs. displacement in ligand addition to Co(NHC)(HC). J. Andjaba, C.A. Bradley

3:15 CHED 52. Voltage tuned acidity of catalyst surfaces for non-faradaic isomerization reactions. A. Yong, I.M. Kendrick, J.H. Duan, E.S. Smolkin

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 under-

graduate 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 labor-

atory. J.R. Knott, S.G. Timmons

2:35 Intermission.

2:45 CHED 56. Integrating technol-

ogy in classroom by developing and implementing interactive simulations in chemistry. T. Gupta, A. Mehta, G.T. Albing


3:25 CHED 58. Composition and mos-


3:45 Intermission.


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

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. Smith, 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. Calender, C.J. Foley, N. Leonard

CHED 65. Withdrawn.

CHED 66. Revised baccalaureate bi-

ological chemistry program to include informatics. M.J. D’Souza, R.J. Kashmar


CHED 68. Building interface chemistry cur-

riculum 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 enhance-

ment strategies: Implementation of economically self-sustained peer- leading (ESSP), PG/OIL, service learning, and live speakers in the classroom. A. Shukla, S. Shukla

CHED 70. Implementation of an undergraduate certificate in chem-

istry education: A peer-instruction program. E. Buginsky, D.M. York

CHED 71. Teacher quality in the chem-

istry program at the University of Maryland, Baltimore County. S. Mang, M.K. Perks, W.R. Lacourse

CHED 72. Shades of green chem-

istry. M. Yatin, D.L. Warner

CHED 73. Increasing student expo-

sure to chemical structures in Biochemistry and Medicinal Chemistry courses through test-enhanced learning. J. Ross, M. Hernick

CHED 74. Improving student under-

standing of lipids concepts in a biochemistry course using test-en-

hanced learning. S. Horn, M. Hernick
MONDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 253C

Citizens First: Using Real-World Contexts for Engaging Students in Learning Chemistry
Co-sponsored by CEI

P. L. Daubenmire, C. H. Middlecamp, Organizers, Presiding

8:30 Introductory Remarks.


9:15 chords 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.


10:05 chords 115. Understanding organic chemistry in the context of the production of hydrocarbon fuels in Brooklyn. P. Spatane

10:25 chords 116. General Chemistry assignment analyzing environmental contamination for the DePue, IL, National Superfund site. F. Geiger

10:45 Intermission.

10:55 chords 117. Drug detectives: Battling counterfeit drugs with wet chemistry and analytical techniques. C.H. Middlecamp


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
Co-sponsored by CEI

I. J. Levy, J. C. Warner, Organizers

8:30 Introductory Remarks.

8:40 chords 120. Intoxifying toxicity throughout the chemistry curriculum at South Dakota State University. D. E. Raynie, D. P. Cartette

9:00 chords 121. Teaching toxicity and environmental impact: A toxicology course for chemistry majors at Simmons College. A. S. Cannon, J. C. Warner

9:20 chords 122. Teaching toxicology in a laboratory safety program. D. G. Finster

9:40 Intermission.

10:00 chords 123. Incorporating principles of toxicology and environmental health into the chemistry curriculum at UBC Berkeley. M. J. Mulvihill

10:20 chords 124. Incorporating principles of toxicology and environmental health into the chemistry curriculum at UBC Berkeley. M. J. Mulvihill

10:40 chords 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

Co-sponsored by BMGT, CEI, ENWR, IC&G, MED, PROF, SCHIR and VCC

Financially supported by Green Chemistry Institute (GCI) Network of Early-Career Sustainable Scientists & Engineers (NESSIE)

A. Irani, M. Kipreos, Organizers

8:30 Introductory Remarks.

8:36 chords 126. Greener solutions program: A private/public partnership teaching students in advancing the design of safer chemistry. M. J. Mulvihill, M. Schwarzman


9:35 chords 128. Challenges and opportunities in green chemistry research academic institutions. S. O. Obare

10:05 chords 129. Green chemistry and entrepreneurship. J. C. Warner, J. Port

10:35 Intermission.

10:45 chords 130. Opportunities in government for students of green chemistry. N. D. Anastas

11:15 chords 131. Implementing green chemistry in the pharmaceutical industry: Challenges and opportunities. E. A. Peterson

11:45 chords 132. Green chemistry in action. S. Sullivan

12:15 Concluding Remarks.

21ST CENTURY CHEMISTRY EDUCATION: FORMAL AND INFORMAL

Co-sponsored by PRS, Co-sponsored by AGRO, CARB, CHAS, CHED, CNF, COFF, ENFL, PROF and SOCE.

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

Co-sponsored by VCC, Co-sponsored by CHED, IAC, PRS and PROF

MONDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253C

Citizens First: Using Real-World Contexts for Engaging Students in Learning Chemistry
Co-sponsored by CEI

P. L. Daubenmire, C. H. Middlecamp, Organizers, Presiding

1:30 Introductory Remarks.


**Section E**

**Boston Convention & Exhibition Center**

**Hall C**

**Undergraduate Research Posters**

**Chemical Education**

Consorted by SOCED

N. Di Fabio, J. Roberts, Organizers

**200 - 4:00**

**211.** Uncovering the genes involved in copper induced cell death pathway by applying Saccharomyces cerevisiae genomic library. B. Kumari, N. Gadura

**212.** Finding evolutionary relationships between New York City mosquitoes through DNA barcoding. O. Zagalo, T. Pierre-Louis, N. Gadura

**213.** Drug delivery: Encapsulated zeolite H-Y under simulated body conditions. N. Guthrie, S. Timchin, K. Bailey, O. Okun, A. Munsell

**Biotechnology**

Consorted by BIOT and SOCED

N. Di Fabio, J. Roberts, Organizers

**200 - 4:00**

**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. Cambaliza, D. Evans, J. Callahan, M. Cavallaro

**215.** Development and implementation of a novel organic chemistry lab curriculum: Evaluation of the reformed teaching method. W. Marmor, C. Ajottta, D. Saiado, T.G. Collison

**216.** Fischer esterification by microwave irradiation using various alcohols (or chemistry doesn’t have to stain). J. Cheng, S.C. Pitcher

**217.** Chemistry at the farmer’s market. R.L. Nispel, R. Morgan Theall, J. Pratt, E.J. Yezezki

**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


**220.** Mad Scientist Day Junior: Inspiring our future scientists. C.M. McCully, M.K. Triplet, J.A. Nikles

**221.** Reactivity of Cp*Co(I) equivalents towards E-E (= E = N, O, and S) bonds. K. Dalpion, C.A. Bradley

**222.** Synthesis and characterization of new XL N-heterocyclic carbenes (NHs) and their reactivity with base metals. G. Brown, Z.D. Call

**223.** Design of a greener kinetico-chemical experiment for general chemistry students utilizing an effluent acid. F. Nampayan, H. Shah, C. Weinrich

**224.** Determining the genetic pathways involved in cell death of copper treated Saccharomyces cerevisiae. H. Shah, N. Gadura

**225.** Screening a Saccharomyces cerevisiae genomic library to determine copper induced cell death pathways. R. Shao, N. Gadura

**226.** Determination of the ionization constant of carboxylic acids at 0°C using microscale freezing point depression measurements. U. Dewananun, P. Ingoyen, P.D. Svoronos

**227.** P-platinated nucleosides. R. Ciccariello, E. Holahan, S. Carson, T. Bogaczynsky, T. Lord, R.A. Stockland

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Section A  Boston Convention & Exhibition Center Hall C

Undergraduate Research Posters

Polymer Chemistry
Cosponsored by PMSE, POLY and SOCED

N. Di Fabio, J. Roberts, Organizers

1:00 - 4:00

Section B  Boston Convention & Exhibition Center Hall C

Successful Student Chapters
Cosponsored by SOCED

N. Di Fabio, Organizer

1:00 - 4:00

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 SCC1

Financially supported by IPC board

C. S. Rukes, Organizer, Presiding

4:00 Introductory Remarks.


4:40 CED 361, Making of the car: The building of the chassis and other parts. S. C. Rukes, A. Nydam

5:15 CED 362, Under the hood: What makes the engine work? S. C. Rukes, A. Nydam

5:40 CED 363, Getting rid of the excess heat: The cooling system. S. C. Rukes, D. Goodwin

6:05 Intermission.


7:30 CED 366, Extra features: Options to protect and beautify the car. S. C. Rukes

7:55 CED 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, 114. See previous listings.

468. 492. 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


369. University of Maryland, Baltimore County’s chemistry community. N. Steenrod, M. Shen, G. Blalack


371. Chemistry on the coast: Student activities at the University of New England. B.E. Boe, R. Joneau, M. Perry, A.E. Keirstead

372. Creating links and polymers: The ACS Student Affiliate Chapter at the University of Richmond. B. Zhang, D. Stevens, K. Jostoff, S. Howick, T. Bul, W. Case

373. Accomplishments of the UMD American Chemical Society student affiliates chapter. C. Ma, C. Tsui

374. Greening a student chapter. A. Goranov, S.L. Carterby


376. Wilkes University’s ACS Student Chapter: Educating the community about green chemistry principles. B.S. Clem, K.M. Kamis, A. Almousaw, C. Henkel

377. Northeastern University Student Affiliates of the American Chemical Society: Enriching the chemistry community in the greater Boston area. J. Conway, W. Timson

378. Saint Anselm College Chemistry Club: We work periodically. C.J. Muldoon, J. Cassidy, A. Scafidi, 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, B00L, B074, BM72, COPP2, DAC1, ENFL1, PHY5 and POLY1

Financially supported by UNN 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, Valpors, BASF, STREM Chemicals, UMN Department of Chemistry, L. M. Johnson, Organizer, Presiding

9:00 Introductory Remarks.

9:05 CED 379, Opening presentation: Building successful collaborations. C. Arnold

9:15 CED 380, Fundamental research to commercial products. R.H. Grubbs

9:50 CED 381, Toward the practical application and commercial translation of layer-by-layer assembly. P.T. Hammond

10:25 Intermission.

10:40 CED 382, From bench to market in the capital intensive energy market. D.G. Nocera


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. Bhattacharya, Organizer, Presiding

8:30 Introductory Remarks.

8:35 CED 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 CED 385, Team based learning reduces attrition in a first semester general chemistry course. L.L. Comford

17:00 Intermission.
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 CED 403. From discovery to application: Innovations in heterogeneous catalysis and implementation in undergraduate research and teaching.

A. C. Banerjee

8:55 CED 404. Computational chemistry in the undergraduate curriculum.

M. A. Boucher, D. A. Barr


M. Jee

9:35 CED 406. From discovery to application: Incorporating 50 years of the glass transition into a polymer chemistry course.

D. W. Holley

9:55 Intermission.


E. J. McIntire, H. W. Jakubowski, C. P. Schaller, K. J. Graham, R. A. Hutcheson

10:25 CED 408. Chemical education via biodiesel production.

M. B. Jacobs, T. C. Vogt, E. S. Ball, S. Alman, J. Zimmerman, S. M. Marusich, C. Faman, J. J. Holloway

10:45 CED 409. Inorganic molecular design: A two-credit advanced course designed to introduce an undergraduate 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, Co-sponsored by ACS, CII, CED and CINF.


D. Sun, L. E. Siclun, L. Dukeh

9:35 Intermission.

10:45 Section 4C.

396. Coordinated response to student deficiencies and their performance in “General Chemistry”.


10:05 CED 397. Student-driven interactive chemistry lab assessment tool to evaluate lab instructors and learners.

S. Burchett, J. L. Hayes


10:45 Intermission.

10:55 CED 399. Engaging students in learning analytical chemistry: Active learning through integrated labs, learning groups, and case studies.

R. E. Goacher

11:15 CED 400. Partnering with a local middle school to enhance science curriculum: A service learning opportunity.

F. Vyepe Castillo

11:35 CED 401. Engaging organic chemistry students with group activities.

C. Gabel, S. Gordan, S. Norris, N. Kuhl


M. Chatterjee

12:15 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Boston Convention & Exhibition Center
Room 253C

Academic Innovations for Tomorrow’s Industries: GSSPC Symposium

Co-sponsored by ANLYL, BIO3, BMOL, CED1, CORP1, DAC1, ENPL, PHYS2 and POLY1

Financially supported by U.S. National Science and Engineering, U.S. 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 Intermission.

1:35 CED 422. Well, how did I get here? The evolution of an organic chemistry experience.

N. E. Carpenter

1:55 CED 423. Active learning in a large organic chemistry class.

D. A. Canales

2:15 CED 424. Flipped classroom in undergraduate and post-baccalaureate premedical organic chemistry classes at Goucher College.

G. E. Greco

2:35 Intermission.

2:45 CED 425. Using ‘clickers’ to encode and decode conceptual knowledge in organic chemistry.

S. M. Graham

3:05 CED 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. Merril, P. J. Oro, J. A. Webb


L. I. Khalil, K. M. Chahine, B. R. Kasfarani

3:45 Intermission.
Section C
Boston Convention & Exhibition Center Room 207

General Papers
Tools
S. A. Fleming, Organizer
A. Gupta, Presiding
A. Rahman

8:30 Introductory Remarks.

8:35 CSED 442. Real-life real genres: Integrating research-based writing into an introductory quantitative chemistry lab sequence for majors. B. Abrams

8:55 CSED 443. Peer-assessment based learning in chemical education. A. Gupta

9:15 CSED 444. Student-generated content: Peerewis in undergraduate chemistry classrooms. A. Kay, J. Harty

9:35 Intermission.

9:45 CSED 446. Transforming learning pathways in the undergraduate chemistry laboratories. K. Hess

10:05 CSED 447. Entirely student-created wiki textbook to accompany a sophomore-level course in bio-organic chemistry. B. C. Goess


10:45 CSED 448. Improving student outcomes: Implementing study strategies. I. Sawchyn

11:05 CSED 449. Developing critical thinking skills using student group presentations in biochemistry. S. M. Tremain

11:25 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 CSED 474. Implementing an embedded chemistry research experience in an undergraduate Instrumental Analysis course. K. S. Wendling

8:25 CSED 475. Feasible screening method for antimicrobial activity of natural products for the interdisciplinary research project at an all liberal-arts college. H. Shin


9:05 Intermission.


9:35 CSED 478. Incorporating faculty research into upper-level chemistry courses when schedule and budget make it seem otherwise impossible. C. E. MacIntyre, D. H. Hamill, J. Cottrell

9:55 CSED 479. First physical chemistry lab: Monte Carlo calculations of dr. R. Riccardi, L. Pegram

10:15 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 CSED 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 CSED 461. Approaches to improve the teaching effectiveness of organic chemistry for biology majors. Z. Wang


2:40 CSED 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 CSED 464. Teaching organic chemistry for biology and environmental science majors. R. Swisher

3:30 CSED 465. Examining the nicotine-triggered dopamine response in pheochromocytoma rat cells (PC-12) in the organic chemistry laboratory: Engaging life science students in their home turf. J. Oscko, F. Yezpez Castillo, J. Utch

3:50 CSED 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 CSED 467. Attaining chemistry faculty diversity: A case study at a public, four-year liberal arts college. D. P. Pursell, P. Bell

1:55 CSED 468. Lighting the pathway to academic careers for Native Americans in STEM: Preliminary report. K. M. Hughes, S. E. Holthaus, M. J. Ondrechen

2:15 CSED 469. Comprehensive study of taking lab equipment in chemistry and other science laboratory classes to integrate students who are blind. C. A. Supalo

2:35 Intermission.

2:45 CSED 470. Chemistry camp for middle school girls. M. Levine, N. Seno, B. Rastam, S. Chaudhuri, W. Talbert

3:05 CSED 471. STEM educational enhancement in Oklahoma: Teaching chemistry to 4th-6th grade by high school students. A. Rahman


3:45 CSED 473. Development of technical chemistry language skills for non-native speakers. D. Ramella

4:05 Concluding Remarks.

SUNDAY MORNING
Combining Scientific Evidence for Health Policy and Regulation

Sponsored by AGRO, Cosponsored by CHAS and TJX

Section A
Seaport Hotel and World Trade Center Waterfront 1A/1B

Lab Safety 25 Years After Promulgation of the OSHA Laboratory Standard
Cosponsored by CC5

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? J. S. 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


2:35 CHAS 12. From accident analysis to accident prevention at UCLA. C. A. Merlic, J. Schroeder

2:55 Intermission.

3:10 CHAS 13. Impact of the OSHA Laboratory Standard on basic laboratory safety education for undergraduates. R. H. Hill
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. Wei, C. Perez, N. Keltbana

10:30 CHAS 6. DOE Energy Innovation Hub’s effort to influence laboratory safety among its funded research- ers. S. Rupkey, D. Hodge


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 CCS, CHED and CINF‡

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 AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF, SOCED and WCC

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 users. 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, CHED, COLL, ENFL, ENVIR, 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. Dunaivszla, W. Bukock, 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.

SUNDAY MORNING

Section A

Boston Convention & Exhibition Center
Room 104A

Substance Identifiers, Addressing the Challenges Presented by Chemically Modified Biopolymers: The Role of InChi & Related Technologies

S. R. Heller, K. Taylor, Organizers, Presiding

8:30 Introductory Remarks.
CINF

TECHNICAL PROGRAM

10:30 CINF 12. Chemical biology informatics approaches to identify and validate new therapeutic targets. P. Kutchukian
11:45 Closing Remarks.

Integrated Approaches in Structure-Based Drug Design
Sponsored by CINF and MEDI

Best in Class Computational Software by Integration
Sponsored by CINF and MEDI

SUNDAY AFTERNOON

Section A
Boston Convention & Exhibition Center Room 104B

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

Section B
Boston Convention & Exhibition Center Room 104B

Enabling Machines to “Read” the Chemical Literature: Techniques, Case Studies & Opportunities

10:05 CINF 22. Value of the Mediawiki platform for providing content to the chemistry community. A.J. Williams E. Champaign, P. Hunt, M.D. Segall
10:40 CINF 23. Chemical collaborations in the wiki realm. A. Mabbett
5:00 Concluding Remarks.

Guiding Compound Optimization
E. Davis, M. D. Segall, Organizers, Presiding
1:00 Introductory Remarks.
2:45 Intermission.
3:00 CINF 29. Visualization and manipulation of Matched Molecular Series for decision support. N. O’Boyle, R.A. Sayle
3:50 CINF 31. Interactive web-based tools for navigating the biologically relevant chemical space. O. Rabal, J. Oyarzabal
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. Mandley, C. Tudge
5:05 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal
Sponsored by PRES, Co-sponsored by AGRO, CARB, CHAS, CHED, CINF, COUL, ENFL, PROF and SOCED

Integrative Approaches in Structure-Based Drug Design
Sponsored by CINF, Co-sponsored by CINF and MEDI

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. War, Organizers, Presiding
8:30 Introductory Remarks.
8:35 CINF 48. What are the next steps in your synthesis? The Reaxys experience. J. Swiety Business
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
10:05 CINF 51. Analyzing success rates of supposedly “easy” reactions. R.A. Sayle


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.
10:00 CINF 55. SureCHEMBL: An open patent chemistry resource. G. Papadatos, M. D. Davis, N. Deelman, A. Hesey, J.P. O’Donning
10:25 CINF 56. Deuteron: Causes and consequences of automated extraction of patent-specified virtual deutered 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 community annotated chemical 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. Hilde, M. Rarey
8:55 CINF 61. New web based collabora- tive 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

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
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, A. W. A. War, Organizers, Presiding
1:00 CONF 65. SynTree, chemical synthesis on a P.C. - J. Figueras
2:00 CONF 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 Pittro, F. Huerta, M. Hutchings, H. Saller, P. Loew
2:30 CONF 68. Chematica - the Deep Blue of chemistry. - B. Grzybowski
3:00 CONF 69. Reaction mining with condensed graphs of reactions: Problems and perspectives. - A. Varnek
3:30 CONF 70. Assessment of optimal conditions for selective deprotection reactions resulted from analysis of large reaction database. - T.J. Madzhidov, A. Lin, I. Antipin, O. Kromchak, A. Varnek
4:00 CONF 71. Energy refinement of reactive molecular dynamics pathways. - L. Wang, R.T. McGibbon, V.S. Parde, T.J. Martinez

Section B
Boston Convention & Exhibition Center
Room 104B
ENABLING MACHINES TO “READ” THE CHEMICAL LITERATURE: TECHNIQUES, CASE STUDIES & OPPORTUNITIES
D. M. Lowe, Organizer, Presiding
1:30 CONF 72. Identifying chemical species in combustion models. - R.H. West
1:55 CONF 73. Text mining the chemical literature to find chemicals in context. - T. Wu, A.C. Hinton, D.R. Milward
2:20 CONF 74. Unlocking chemical information from tables and legacy articles. - D.M. Lowe, R.A. Sayle, A.J. Williams
2:45 Intermission.
3:00 CONF 75. Chemical structure identification and retrieval with OSRA. - I. Filippow, I. Welch
3:25 CONF 76. P-OSRA. Translating polymer images to text using extensions of open source software. - B. Reinstdater, H. Horn
3:50 CONF 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
1:05 Introductory Remarks.
1:05 CONF 78. Contributions of Jean-Claude Bradley to the vision and execution of Open Notebook Science. - A.J. Williams, A. Lang
1:25 CONF 79. Making it open: Putting cheminformatics in the hands of the public against the Ebola virus. - S. Ekis
1:45 CONF 80. Opening up and connect- ing up antimarial data: Progress with with caveats. - C. Southan
2:25 Intermission.
2:35 CONF 82. Promoting, supporting, and incentivizing openness in scientific research. - S. Bowman
2:55 CONF 83. OpenTox — an open community and framework supporting predictive toxicology and safety assessment. - B. Hardy
3:15 CONF 84. Toplist batchwise scheme reviewed in the era of Open Data. - L. Richter, G.F. Ecker
4:15 Intermission.
4:45 CONF 88. Open Spectral Database: Open data, open code, open concept. - S.J. Chalk
5:25 CONF 90. Changing landscape of scientific publishing: Open access, open data, and more. - C. Holfingworth
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.
94. 108. 119. 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 CONF 92. Force fields for biomolecular simulations. - A. Hagler
8:45 CONF 93. Paradigm which permits the parsing of information content arising from receptor-independent ligand activity models and receptor-depen- dant activity models. - A.J. Hopfinger
10:05 CONF 95. Molecular similarity approaches in chemoinformatics: Early history and bibliometric analysis. - P. Willett
10:45 Intermission.
11:00 CONF 96. Generic topographic mapping: Universal tool for chemical space analysis. - A. Varnek
11:30 CONF 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 COMSIC
J. N. Currano, Organizer
W. G. Town, Organizer, Presiding
9:00 Introductory Remarks.
9:05 CONF 98. Integrity, ethics, and trust in scientific research literature. - C. Leonard
10:05 CONF 100. Publishability. - M.G. Hicks
10:35 Intermission.
10:50 CONF 101. What is the role of peer review in protecting the integrity of scientific research? - N. Qin
11:50 CONF 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
Cosponsored by CHED, CINF, ACS, CINF and CNF

TUESDAY AFTERNOON
Section A
Boston Convention & Exhibition Center
Room 104A
HERMAN SKOLNIK AWARD SYMPOSIUM Cosponsored by COMP and MEDI
V. Shanmugasundaram, Organizer, Presiding
1:00 CONF 104. Enabling drug dis-covery by computational molecular design. - G. Schneider, P. Schneider
2:30 Intermission.
3:15 CONF 108. How many fingers does a compound have? The various ways to define molecular similarity. - E. Lounkine
4:15 CONF 110. Complexity and het-erogeneity 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 COMSIC
W. G. Town, Organizer
J. N. Currano, Organizer, Presiding
1:30 Introductory Remarks.
1:35 CONF 111. Toward a more reproducible corpus of scientific literature. - C. Benis
2:05 CONF 112. Extraordinary public access to scientific evidence in the FDA modified risk tobacco product process. - J.M. Solyst
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 AFTERNOON**

**Section A**

Boston Convention & Exhibition Center
Room 104A

**General Papers**

E. Davis, Organizer, Presiding

1:00 CINF 170. Experimental chemo-informatics study of tumour-ism 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. Aln, K. Birchall, C. Mpanathia, S. Knapp, A. Bender

2:00 CINF 172. HackAMol: An object-orien-ted Modern Perl library for molecular hacking on multiple scales. D. Riccardi


**SUNDAY AFTERNOON**

**Section A**

Westin Boston Waterfront
Habor Birm II

Founders Award Lecture & Symposium
A. P. Grollman, Organizer, Presiding

1:00 TOXI 6. Alflatoxins — another “A” in the library of naturally-occurring human carcinogens. T.W. Kensler, J.D. Groopman


2:00 TOXI 8. Somatic mutations in tumor DNA present in biological fluids as markers for the early detection of cancer. N. Papadopoulos


**MONDAY MORNING**

**Section A**

Westin Boston Waterfront
Habor Birm II

You ng Investigator Symposium
P. J. Beuning, Organizer, Presiding

8:00 TOXI 10. Replication bypass and muta-genesis of the CTG-trinucleotide repeat in Escherichia coli cells. N.J. Amato, O. Zhao, Y. Wang


8:30 TOXI 12. N’-nitrosonoronic acid 5’-hydroxylation causes DNA damage in rats. A.T. Zarth, P. Upadhyaya, J. Yang, S.S. Hecht


9:30 TOXI 16. Replicative bypass and muta-genic properties of O’-alkylthymidine lesions in E. coli. P. Wang, Q. Zhai, Y. Wang

9:45 Intermission.

10:00 TOXI 17. Biomonitoring the cooked meat carcinogen 2-amino-1-meth-ylyl-6-phenylimidazol(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. Wilkins, L. Le Marchand, R.J. Turesky


11:05 TOXI 21. Platelet biomarkers of metabolic disturbances in Friedreich’s ataxia. A. Worth, N. Snyder, I.A. Blair


11:35 TOXI 23. Synthesis and analysis of DNA lesions generated from oxidative damage at the C3’-position of deoxyri-bonucleotides. F.M. Bodi, P. Brinkhofs, W. Li, S. Ayoub, A.C. Bryant-Friedrich

**Innovation in Health and Medicine**

Sponsored by MIPS. CINF/TOXI/BIOT, BIOT, MEDI and TOXI

Global Research Needs: Identifying and Prioritizing Efforts to Sustain Environmental Quality
Sponsored by AGRO, Co-sponsored by ENVR and TOXI

**TUESDAY MORNING**

**Section A**

Westin Boston Waterfront
Habor Birm II

The Exposome
S. Balbo, Organizer, Presiding

8:00 TOXI 29. Exposome: A tool for untargeted discovery in the environ-mental health sciences. D. Balshaw

8:40 TOXI 30. Breath biomarkers to inves-tigate the human exposome. J. Piel

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 adduc-tomics approach for the investiga-tion of the exposome. S. Balbo

**TUESDAY AFTERNOON**

**Section A**

Westin Boston Waterfront
Habor Birm 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 modific-a-tions in gut microbiota. P.C. Dedon

2:20 Intermission.

2:45 TOXI 35. Biobarthromination of car-cinogens by gut microbes. S.J. Sturla

3:25 TOXI 36. Role of gut microi-borne in chemical toxicity and individual susceptibility. K. Lu

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WEDNESDAY MORNING

Section A
Westin Boston Waterfront
Harbor Bllm II

General Papers
A. C. Bryant-Friedrich, Organizer, Presiding

8:00 TOXI 109. Noninvasive measurement of carcinogen exposure by quantifying urinary DNA/DNA adducts using liquid chromatography coupled tandem mass spectrometry. W. Chan

8:20 TOXI 110. Miconium 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. Brudham, B. Schumacher


10:00 Intermission.


11:50 TOXI 120. Human DNA polymerase ε catalyzes correct and incorrect DNA synthesis with high catalytic efficiency. T. Spratt, A. Gowda, G. Moldovan

WEDNESDAY AFTERNOON

Section A
Westin Boston Waterfront
Harbor Bllm 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 Ilumina sequencing by polymerase engineering. M. He


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

TOXI/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. Pilla, 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. Pilla, 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


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 Endavors
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 earnest — in your searching: Or, what you

TUESDAY MORNING

Section A
Boston Convention & Exhibition Center Room 152

Developments in Pharmaceutical Patent Law
B. Tinque, Organizer, Presiding

9:00 CHAL 23. Pharmaceutical patent prosecution primer. B. Tinque

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, EMVR and SCOB

TUESDAY AFTERNOON

Section A
Boston Convention & Exhibition Center Room 152

Obtaining biomarker and diagnostic claims. S. Hasford

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. Karns

2:30 CHAL 30. Patenting of biologics in the biosimilar era. J. Veleta

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
TECHNICAL PROGRAM

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.
10:00 CHAL 34. Alternative protection strategies. L. Di Lorenzo, 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. Di Lorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

THURSDAY MORNING

Section A
Boston Convention & Exhibition Center Room 152
The Many Faces of CHAL: Where Chemistry Meets the Law
K. E. Blanco, Organizer, Presiding
9:00 CHAL 40. Divided infringement: Is any one person liable for infringing your patent claims? J.L. Blackbum
9:30 CHAL 41. Best practices for patenting chemical and material compositions. J.V. Buggs, A.C. Pama
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

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. Di Lorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen
1:45 CHAL 37. Foreign patent protection. L. Di Lorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen
2:30 CHAL 38. Enforcing IP rights. L. Di Lorenzo, J.L. Kennedy, J. Link, D. Lorentzen, M. Pobanz, M. Smith, T. Taylor, J. Wen

THURSDAY AFTERNOON

Section A
Boston Convention & Exhibition Center Room 152
The Many Faces of CHAL: Where Chemistry Meets the Law
K. E. Blanco, 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

SUNDAY MORNING

Section A
Boston Convention & Exhibition Center Room 107A
Basic Research in Colloids, Surfactants & Nanomaterials
R. Nagaranj, Organizer
8:30 COLL 11. Colloidal synthesis and characterization of size tunable luminescent ZnP2 nanocrystals. M. Ho, R.J. Esteses, U.A. Azachighe
8:50 COLL 12. 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 13. Palladium nanoparticle seed mediated growth of palladium nanoshell on silica core. K. Bandyopadhyay, R. Teh

Division of Colloid and Surface Chemistry
R. Nagaranj, Program Chair

OTHER SYMPOSIUM 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 Env, Tuesday, Wednesday)

BUSINESS MEETINGS:
Executive Committee Meeting, 4:00 PM: Saturday
Open Business Meeting, 5:30 PM: Sunday

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 Sponsorship

COLL 138. Adaptation of FTIR spectrometer to the external nanometer range for surface analysis studies. S.V. Shkol, T. Tague, G. Zachmann, X. Stamper

COLL 139. Atomically precise gold nanoparticles for the control of carbon dioxide reduction. M. Kim, W. Choi, K. Kwak, D. Lee


COLL 142. Photocatalytic performance of a trifold nanocomposite material for the hydrolysis of 2-chloroethyl sulfide (CEES). C.A. Zoto

COLL 143. Silver seeds and aromatic surfactants facilitate the growth of anisotropic metal nanoparticles. Gold triangular nanorods and ultrathin nanowires. Z. Qian, S. Park

COLL 144. Synthesis of metal sulfide nanoparticles in toluene at room temperature. L. Bian, K. Ring, J. Sidtside, P. Goulet

COLL 145. Quantifying the surface coverage of mercaptophenolacetic acid on nanocrystalline SnO
thin films. G.R. Soja, M.J. Awad


COLL 147. Nitin protection from degradation and controlled release via polyacrylic acid encapsulation. L.W. Place, S. Flocamo


COLL 150. Magneto-responsive hybrid colloidal architectures: Preparation, processing, and opal film formation. D. Scheid, M. Garretson

COLL 151. Synthesis and self-assembly of copper nanowires. S. Darmakkolla

COLL 152. Electron induced surface reactions of organometallic precursors. J. Spencer, R. Thoman, M. Barday, J.A. Brannaka, Y. Wu, O. Ingolfsson, L. McElwee-White, H. Fairbrother

COLL 153. Modification of nitin nanoparticles with self-assembled monolayers. R. Quinones, S. Garretson

COLL 154. Modification of zinc oxide nanoparticles with perfluoro phosphonic acids. R. Quinones, C. Piek

COLL 155. Proton coupled electron transfer through 2-2′-bipyrindyl molecular wire between graphene - gold nanoparticle junction. G.Y. Jacob, A. Patnak


COLL 158. Mechanistic study using a quartz crystal microbalance: Effect of spacer length on the antimicrobial activity of the bound peptide, Chrysophsin-1. T. Alexander, L.D. Lozeau, T.A. Camesano


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 165. GCM-D based mechanistic study of Alzheimer’s disease: Membrane-amyloid peptide interaction. E. Kamaloo, T.A. Camesano

COLL 166. 2D nanoparticle cluster formation in supercritical fluid CO2. J. Wang, G. Brown, C.M. Wai


COLL 168. Magneto-fluorescent core-shell supernanoparticles. O. Chen

COLL 169. DNA-polypeptide polyplexes. M.J. Luckeheide, J.A. Chabian, J. Leon, M.V. Tirtell

COLL 170. Upconversion of trapped charge carriers in coupled lead salt quantum dot solids. R.H. Gilmore, W.A. Tidela

COLL 171. Mechanisms of metal deposition on colloidal gold nanoparticle substrates. P. Straney, J. Milestone


COLL 174. Polymer of glycolic acid-biodegradable for highly stabilized liposomes. Y. Zhang, K.E. Uhrich

COLL 175. Withdrawn.

COLL 176. Study of the relationship between cationic degree and the performance of nanoparticle dispersion. J. Gong, B. Bai, T.P. Schuman


COLL 178. Preparation of modified poly(ethylene-co-acrylic acid) (PEAA) using ammonium with aliphatic chains as antibacterial polymer. H. Noh, J. Ryu, S. Oh

COLL 179. Interpenetrating network polymer gel for improving oil recovery. Y. Long, C. Chen, B. Bai

COLL 180. Tunable intermolecular interaction in N-methylfurfurylpyrimidylne (8-NMFP) mediated with assembly of gold nanoparticles. S. Subradhar, A. Patnak


COLL 182. Size-dependent cellular uptake of sub-10 nm zincteric gold nanoparticles. Y. Jia, D. Wang, 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. Mays

COLL 184. Understanding the assembly and aligning of semiconductive quantum rods on DNA origami. Y. Chen, T.L. Doane, M.M. Mays

COLL 185. Designing stable foams in the presence of alkane and brine for oil field operations. Y. Sansen, U. Sunyaphakhidchorn, A. Cherontang, B.J. Shau

COLL 186. Vitamin E-conjugated lipidic mixed micellar system as nanocontainer for the delivery of curcumin in cancer. O. Muddiniet, P. Jha, B. Ghoos, S. Biswas

COLL 187. Withdrawn.

COLL 188. Antibacterial efficacy of carbohydrate-conjugate nanoparticles. S.A. Wijesundera, B. Jayakody, S. Jayaram, J. Yi


COLL 190. Blockcopolymer based crosslink surfactant for preparation of polymer nanoparticles by minimulsion process. K. Kim, R.W. Zentel

COLL 191. Silica supported zirconia-zine for hydroamination of olefin. Evidences for the mechanism. B. Hamazou, J.M. Basset, J. Pellutet


COLL 193. Withdrawn.

COLL 194. Photoinitiated covalent surface functionalization for enhanced control over electroless deposition on silicon nitride. Y.D. Bandara, B.I. Karawatyena, J. Whelan, B. Veil, J.R. Dwyer


COLL 196. Photoinitiated crosslinked surface functionalization through surface-directed azo coupling. N. Marshall, T. Mikhalova, B. Taylor


COLL 198. Surface properties of xerogel materials with unusual patterns and tunable topography for anti fouling applications. J.F. Destino, Z. Jones, A. Craft, C.M. Gatley, M.R. Detty, F.V. Bright

COLL 199. Understanding 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.
COLL 218. Toward the synthesis of ordered mesoporous organosilicas with closed mesopores. A.S. Manchanda, M. Mandal, M. Kruk


COLL 220. Dynamic coupling at the Angstrom scale. F.Y. Pong, K.K. Dey, J. Breffke, E. Hatzie, A. Sun

COLL 221. Enhanced cell performance with control of ZnO buffer layer using nanoparticles of various morphology for inverted organic photovoltaic (OPV)s. S. Oh, S. On

COLL 222. Silver sulfadiazine-immobilized inorganic fillers: Preparation, characterization, and antimicrobial functions. R. Srivastava, V. Sun


COLL 225. Zwitterion amphiphilic magnetofluorescent nanoparticles. V.G. Demilio, 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. Scenninich


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 233. Tuning the detection capacity and specificity of polymer protected graphene nanoclusters using endonucleases. N.M. Robertson, M. Haiz, M. Rana, M. Balcigu, M.S. Yazay, M.V. Yigit

Monday Morning

Section A

Boston Convention & Exhibition Center Room 107A

30 Years of Langmuir: Looking Back & Forward

F. M. Wilkin, Organizer
R. M. Crooks, Organizer, Presiding
M. M. Santore, Presiding

8:30 - 9:00

COLL 246. Charge transport by tunneling through SAMs. G.M. Whitesides

9:00 - 9:30

COLL 247. Langing for Langmuir. C.J. Murphy

9:30 - 10:00

COLL 248. Adsorption at the bio/nano interface: DNA, liposomes, and inorganic nanoparticles. J. Liu

10:00 - 10:15

Section B

Section C

Boston Convention & Exhibition Center Room 107B

Surface Modification to Control Cell/Surface Interactions

H. Moehwald, Organizer
A. M. Peterson, Organizer, Presiding

8:30 - 9:00


8:50 - 9:00


9:10 - 9:20

COLL 254. Increasing the stability of semiconductor quantum dots in biological solutions through surface chemistry. R.P. Brown, M. Muth, Z. Rosenzweig

9:30 - 9:40

COLL 255. Lasting alteration of compositional membrane asymmetry by LiCoO2 nanoparticles. P. Geiger

9:50 - 10:00

Section E

Section D

Boston Convention & Exhibition Center Room 108

Basic Research in Colloids, Surfactants & Natural Materials

Particle Systems
R. Nagarajan, Organizer
M. C. Buzzo, Presiding

8:30 - 8:50

COLL 267. From phenomenon to formulation: Investigating excitants that enhance the stability of colloidal drug aggregates in biological milieu. C.K. McLaughin, A.N. Ganesh, B. Shiochi, M.S. Shiochi

9:10 - 9:20

COLL 268. Dispersant interactions at oil-water interface: Insights from molecular dynamics simulation. D. Yu, A. Sava, M.D. Reichert, A.K. Schulz

9:30 - 9:40

COLL 269. Star diblock copolymer concentration dictates the degree of dispersion of carbon black particles in nonpolar media: Bridging flocculation vs. steric stabilization. S.P. Ames, D.J. Gowney, O.O. Mykhayliuk

10:10 - 10:20


10:30 - 10:40


10:50 - 11:00

COLL 272. Anti-agglomeration Ni-yolk-ZrO2 structure with sub-10 nm Ni core: Preparation, characterization, and catalysis in steam reforming of methane reaction. J. Lin, H. Yin, K. Cao, C. Wu

11:10 - 11:20

COLL 273. Interface bonding effect between ternary sulfide solid solution and TiO2NPs composite by solvothermal synthesis. Z. Yao, F. Jia, Z. Jiang

11:30 - 11:40

COLL 274. Wetting of solids. W. De Yoreo

11:45 - 11:50

Collaborative Cosponsorship

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 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
10:05 Intermission.
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, EMVR, 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 AGRO, Cosponsored by COLL

Memories of Henry Hill: His Legacy in Science and in Professional Service
Sponsored by HST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES‡, PROF and SCHB

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. Mazur
3:00 COLL 293. Metal-organic framework works for gas separations: Using fundamental experimental studies and molecular modeling to highlight features of interest and optimized material. P.L. Liewellyn, G. Maurin
3:30 Intermission.
4:15 COLL 295. Zwittersurfases and zwitteroids. J.B. Schlenoff
4:45 COLL 296. Personal views on Langmuir as a reader, author, reviewer, editor, and EIC. F.M. Winn

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. Gunasekara, T. Gu, H. Free, L. Nyberg, K. Johnson, K. Hurley, A. Vartanian, L.M. Jacob, S.E. Lohse, M.D. Terrell, R.J. Harnes, C.J. Murphy, C.L. Haynes
2:20 COLL 298. Investigation of effects of adsorption and immobilization onto silica nanoparticles on antimicrobial activity of Cepocin P1 and Cepocin P1G. 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.J. Biggs, M. Gibson
3:20 COLL 301. Sequence-specific peptides for the molecular design of antibody drugs and biopharmaceuticals. K. Lau, P.B. Messersmith, D. Palmer
3:40 Intermission.
4:00 COLL 302. Metal surface nano-structuring to guide cell behaviour. S. Ulesiech, O. Baidakovska, 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. Drachul, R. Geryak, M. Chrasnatychy, R. Calabrese, S. Hartbaugh, N. Kelley-Loughman, D.L. Kaplan, M.O. Stone, V.V. Tsutuk
5:00 COLL 305. Surface charge density in PEMs and its influence on cell adhesion. C.J. Arias Ramos, T.C. Keller, J.B. Schlenoff

Section C
Boston Convention & Exhibition Center Room 107C
Biocatalytic Ligands at Interfaces: From Molecular Scale Characterization to Devices
Finanly supported by JPK Instruments and NT MT
G. Liu, T. Ye, Organizers
A. B. Subramaniam, Presiding
2:00 COLL 307. Protein structures at device interfaces. G. MacLaughlin, W. Shi, G.C. Walker
2:40 COLL 308. Characterization of protein and binding at model interfaces for optimization of activity. C.L. Berry, J.K. Tucker, M.L. Richter
3:45 Intermission.

Section D
Boston Convention & Exhibition Center Room 108
Basic Research in Colloids, Surfactants & Nanomaterials

Organizer
R. Nagaran, 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 metal Janus particles. H. Liu, K. Yue, W. Zhang, Z.S. Cheng
2:40 COLL 314. Small angle scattering of anisotropic nanoparticles and their assemblies. A. Stoica, B. Lee
3:00 COLL 315. Withdrawn.
3:20 COLL 316. Withdrawn.
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, G. 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

Section E
Boston Convention & Exhibition Center Room 109A
Colloid-Polymer Architectures & Mixtures
Colloids at Interfaces and in Melts
S. M. Bakol, Organizer
T. Kreer, Organizer, Presiding
2:00 COLL 323. Conformation, effective interactions, and assembly of polymer-coated nanoparticles at liquid interfaces. H. Delgado, K. Schwenk
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 micromechanics. A. Kuhnhold

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Section F
Boston Convention & Exhibition Center
Room 109B
Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships in Organopolysulfides. J. F. Wehn

2:00 \( \text{COLL, HIST, I&EC, POLY, PRES and PROF} \)

2:30 \( \text{COLL} \), AP-XPS and HERFD-XAS as complementary operando probes in electrocatalysis. AP-XPS and HERFD XAS as complementary operando probes in electrocatalysis. D. Friebel

3:00 \( \text{COLL} \), in operando tracking of surface electrochemical redox activity in solid oxide electrochemical cells using near infrared radiation imaging. A. Geller, M.G. Pomper, J. Orwulak, B.W. Eichhorn

3:30 Intermission.

4:45 \( \text{COLL} \), Vibrational sum frequency generation spectroscopy for probing the triple junction in heterogeneous catalysis. K. Geiger

4:15 \( \text{COLL} \), in operando studies of CuO and MoOx model surfaces for application as chemical warfare agent destruction catalysts. L. Trotchaud, A. Head, Y. Yu, O. Kaslioglu, M. Hart, B.W. Eichhorn, H. Blum

5:15 \( \text{COLL} \), Monitoring catalytic surface phenomena under reaction conditions and establishing structure-activity/selectivity relationships. I.E. Wachs, A. Chakrabarti, M. Zhu, S. Lwin, C. Katurakis, Y. Tang

ACS Scholars: Rising Stars in Industry
Sponsored by PSS, Co-sponsored by AGRF, CAP, CHAM, COLL, ENVR, PROF, SCBIE and YGC

Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-resolved Spectroscopies
Sponsored by PHSYS, Co-sponsored by COLL

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector
Sponsored by SCBIE, Co-sponsored by CMA, COLL, HIST, I&EC, POLY, PRES and PROF

Complex Covacvation: Principles & Applications
Sponsored by AGTF, Co-sponsored by COLL

Technological 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 107B
Surface Modification to Control Cell/Surface Interactions
H. Moehwald, Organizer
A. M. Peterson, Organizer, Presiding

38:00 \( \text{COLL} \), Cell surface engineering for translational medicine: From single cell modification to disease theranostics. B. Wang

8:40 \( \text{COLL} \), Investigating the impact of nanoconjugation on EGF-induced apoptosis. L. Wu, B.M. Reinhard

11:40 \( \text{COLL} \), Transferin-modified single walled carbon nanohorns for selective uptake into cancer cells. A. Pekkanen, M.R. DaVitt, T.E. Long, M.N. Rylander

9:30 \( \text{COLL} \), 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. Romanis, N. van Kampen, F. Sabri

9:50 \( \text{COLL} \), Impacts of surface modification induced by cold atmospheric plasma (CAP) on human mesenchymal stem cell (hMSC) differentiation. M. Wang, P. Faval, M. Keidar, T. Webster

10:10 \( \text{COLL} \), In-operando studies of supported heterogeneous catalysts during transformations of C=C and C-H bonds. R.G. Nuzzo

11:40 \( \text{COLL} \), Monitoring catalytic surface phenomena under reaction conditions and establishing structure-activity/selectivity relationships. I.E. Wachs, A. Chakrabarti, M. Zhu, S. Lwin, C. Katurakis, Y. Tang

ACS Scholars: Rising Stars in Industry
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Structure & Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-resolved Spectroscopies
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Coll/Comp Technical Program

Section A
Boston Convention & Exhibition Center Room 107A

Basic Research in Colloids, Surfactants & Nanomaterials
Biosensing and Biomedicine
N. Nagarajan, Organizer

M. Rutfus, Presiding

2:20 Coll. 515, Reactive amphiphilic polymer additives for self-decontamination of CWA simulants. J. Lundin, J.H. Wynne


3:00 Coll. 521, Nanometric hydro- 

carbon bronze reagents for the detection and neutralization of explosives. N.F. Materer, A.W. Appleyd

4:20 Coll. 522, Polymeric CoO nanoparticles for detection and high-sensitivity 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

4:30 Coll. 523, Hybrid platforms for improved bioassay detection limit. E. Bonyi, K. Asian

4:40 Coll. 524, Withdrawn.

3:20 Intermission.

3:30 Coll. 525, Rapid size and pH-de
dependent kinetics of silver nanopar

4:00 Coll. 529, Rhizosphere dissolu


5:00 Coll. 532, Bio-inspired silicon nanopar
ticles through biomolecular engineering. C. Zhao, D. Witcow, A. Mildbernd

Section B
Boston Convention & Exhibition Center Room 108

Basic Research in Colloids, Surfactants & Nanomaterials

Biosensing and Biomedicine

R. Nagarajan, Organizer

M. Rutfus, Presiding

2:00 Coll. 516, Reactive amphiphilic polymer additives for self-decontamination of CWA simulants. J. Lundin, J.H. Wynne


3:00 Coll. 521, Nanometric hydro- 

carbon bronze reagents for the detection and neutralization of explosives. N.F. Materer, A.W. Appleyd

4:20 Coll. 522, Polymeric CoO nanoparticles for detection and high-sensitivity 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

4:30 Coll. 523, Hybrid platforms for improved bioassay detection limit. E. Bonyi, K. Asian

4:40 Coll. 524, Withdrawn.

3:20 Intermission.

3:30 Coll. 525, Rapid size and pH-de
dependent kinetics of silver nanopar

4:00 Coll. 529, Rhizosphere dissolu


5:00 Coll. 532, Bio-inspired silicon nanopar
ticles through biomolecular engineering. C. Zhao, D. Witcow, A. Mildbernd

3:30 Introduction.

3:40 Coll. 526, Rapid size and pH-de
dependent kinetics of silver nanopar

4:00 Coll. 529, Rhizosphere disso-


5:00 Coll. 532, Bio-inspired silicon nanopar
ticles through biomolecular engineering. C. Zhao, D. Witcow, A. Mildbernd
### Sunday Afternoon

**Section A**
Boston Convention & Exhibition Center Room 157A

- **Accelerated Discovery of Chemical Compounds:** Design New Polymer-Inorganic Materials from Integration of Polymer Science, Materials Science, & Informatics
  - J. Cheng, Y. Tseng, Organizers
  - J. E. Rice, Organizer, Presiding

- **Application of Polymer Architecture:** S.G. Arujo

- **Simulation of Polymers:** A frustrating opportunity? J. Winter

- **Successes and Challenges in Polymer Materials:** Where are we now, and where can we be? G.M. Breneman, K. Wu, L. Schadler, C. Brinson, R. Rampasad, S. Kumar

**Section B**
Boston Convention & Exhibition Center Room 156A

- **Integrated Approaches in Structure-Based Drug Design:** V. Shanmugasundaram, F. F. Vajdos, Organizers, Presiding

**Section C**
Boston Convention & Exhibition Center Room 156C

- **Calculating pKa's & Redox Potentials Predicting Redox Potentials:** M. Coote, H. B. Schlegel, Organizers, Presiding

- **Computing Redox Potentials:** 2.00 G.P. Gurnya

**Section D**
Boston Convention & Exhibition Center Room 156B

- **Measuring "Success" of Molecular Modeling Efforts:** A. Rusinko, Organizer

### Sunday Evening

- **Panel Discussion:** Organized by E. S. Manas

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**COMP**

### MONDAY MORNING

#### Section A

**Boston Convention & Exhibition Center Room 157A**  
**Functional Polymers: Connecting Modeling and Experiment**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30 A.M.</td>
<td>Introductory Remarks.</td>
</tr>
<tr>
<td>8:40 A.M.</td>
<td>COMP 71. Functional polymers for water desalination. M. Chauchari, S.L. Rempe</td>
</tr>
<tr>
<td>9:10 A.M.</td>
<td>COMP 72. Transport of ions and penetrants through structured polymeric matrices: Interplay of structure and dynamics of polymers. V. Ganesan</td>
</tr>
<tr>
<td>9:40 A.M.</td>
<td>COMP 73. Simultaneous electron and ion conduction in block copolymers. N.P. Balsara, M. Bhattacharya, R. Das.</td>
</tr>
<tr>
<td>10:00 A.M.</td>
<td>COMP 74. Ion clusters in neutral-charge polymer blends and copolymers. M. Olvera de la Cruz</td>
</tr>
<tr>
<td>10:30 A.M.</td>
<td>COMP 75. Ionomer melt structure and dynamics: Connecting modeling and experimentation. M.J. Stevens</td>
</tr>
</tbody>
</table>

**Section B**

**Boston Convention & Exhibition Center Room 156A**  
**Molecular Dynamics Simulations in Drug Discovery**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00 A.M.</td>
<td>COMP 80. Using the Moveable Type sampling method to compute thermodynamic quantities for chemical and biological processes. K.M. Merz</td>
</tr>
<tr>
<td>10:15 A.M.</td>
<td>COMP 81. Free energy perturbation: Retrospective and prospective application to potency prediction. F.E.脱贫攻坚</td>
</tr>
<tr>
<td>11:45 A.M.</td>
<td>COMP 82. Rapid, accurate, and reproducible drug-protein binding affinity calculation. S. Wan, P.V. Coveney</td>
</tr>
</tbody>
</table>

**Section C**

**Boston Convention & Exhibition Center Room 156C**  
**Quantum Chemistry**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30 A.M.</td>
<td>COMP 83. FLUKE: An open-source QM/MM interface for simulations with polarizable receptor type fields. E.G. Kutz, G.A. Gineros</td>
</tr>
<tr>
<td>9:00 A.M.</td>
<td>COMP 84. Polarizable QM/MM based on the AMOEBA force field and linear-scaling DFT. J. Dedeoza, M.P. Head-Gordon, T.L. Head-Gordon, C. Skyllas.</td>
</tr>
<tr>
<td>9:30 A.M.</td>
<td>COMP 85. Accurate and efficient implementation of TD-DFT analytical frequencies within QM/MM and condensed-phase methods. G. Scalmani, M.J. Frisch</td>
</tr>
<tr>
<td>10:00 A.M.</td>
<td>COMP 86. QM/MM nonadiabatic dynamics of photoinduced proton-coupled electron transfer in solution. P. Goyal, C. Schwertfeger, A. Soudackov, S. Hammerschmidt</td>
</tr>
<tr>
<td>10:45 A.M.</td>
<td>COMP 87. Proton solvation in protic and aprotic solvents. E. Rosati, E. Knapp</td>
</tr>
</tbody>
</table>

**Section D**

**Boston Convention & Exhibition Center Room 156B**  
**Calculating pKa/s & Redox Potentials Methodological Advances**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Details</th>
</tr>
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<tbody>
<tr>
<td>8:30 A.M.</td>
<td>COMP 90. Pushing around protons and electrons: What could possibly go wrong? C.J. Cramer</td>
</tr>
<tr>
<td>9:00 A.M.</td>
<td>COMP 91. Solution-phase prediction of properties: Routes to predictive pKa’s. A.K. Wilson, A. Riojas, P. Patel, J. Wang</td>
</tr>
<tr>
<td>9:30 A.M.</td>
<td>COMP 92. Protonic ionic liquids: Effect of environment and solvent on proton transfer. E. Ilogorodia</td>
</tr>
</tbody>
</table>

#### 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**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30 P.M.</td>
<td>COMP 109. So we made all these polymers, now what do we do with the data? D.C. Webster</td>
</tr>
<tr>
<td>2:00 P.M.</td>
<td>COMP 110. Open source, semantically rich tools for polymer visualization and analytics. M.D. Hallwell</td>
</tr>
<tr>
<td>2:30 P.M.</td>
<td>COMP 111. WebFF: A smart force-field repository for soft materials. R.F. Heelan, H. Sun</td>
</tr>
<tr>
<td>3:00 P.M.</td>
<td>COMP 112. Virtual High Throughput Screening of Organic Photovoltaic Materials. M. Krompiec, L. Nansen, N. Blouin, O. Lezam</td>
</tr>
<tr>
<td>3:30 P.M.</td>
<td>COMP 113. Simulation-enabled genetic algorithm for polymer glass formation. D.S. Simmons, T. Patra, J. Hung, V. Manichandrasunderam</td>
</tr>
</tbody>
</table>

**Section B**

**Boston Convention & Exhibition Center Room 156A**  
**Molecular Dynamics Simulations in Drug Discovery**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Details</th>
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</thead>
</table>

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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](http://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 solvents
S.R. Kimura, H. Hsu, A. Ruzvelnos, W. Sherman, A. Favia
3:00 Intermission.
3:15 COMP 117. Molecular dynamics as a needed tool in pharmacophore and ligand design
A.E. Roitberg
3:45 COMP 118. Active site structure and dynamics in designed and evolved enzymes. G. Jimenez-Oses, S. Otsuna, K.N. Houk

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 electronic affinities. A. Heiden, J. Phillips, D. Zgid
3:00 Intermission.
3:45 COMP 125. Effect of impurities and grain boundaries on the electrical properties of MoS2 devices. A. Stroud, G.M. Leuty, C. Muratore, PA. Derosa, R. Berry
4:15 COMP 126. Density perturbation theory. M.C. Palenik, B.J. Dunlap
4:45 COMP 127. First principles united atom model for imidazolium based ionic liquids. G. Sen, J.G. McDonald, A. Yetzhaj

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. Rulisk, U. Ryde, M. Strmeć, M. Kyvat
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. Menucci

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. Detter
3:00 Intermission.
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. Eksenas, 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. Rebout, J. Maple, C. Wu, J. Xiang, D.S. Gerth, D. Lupyan, L. Wang, M. Dahlgren, D. DeLand
3:00 Intermission.
3:45 COMP 144. Atomic partial charges for fixed-charge force fields: Dealing with conformational dependence. C.J. Bayly
4:45 COMP 146. Conformational control of argylamide foldamers: Predicting oligomer structures in solution through molecular dynamics simulations. V. Papphristic, 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 SOGED
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
10:00 - 12:00
12:00 - 2:00
2:00 - 4:00
4:00 - 6:00

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. Swepe, Organizers, Presiding
8:30 Introductory Remarks.
8:40 COMP 147. Synergistic experimental and multiscale modeling approaches for optimizinganticancer drug nanocarriers. W. Jiang, X. Wang, J. Luo, S. Nangia
9:10 COMP 148. Computational studies of diblock star polymers and polyelectrolyte multilayers. T.L. Head-Gordon
10:10 Intermission.
10:30 COMP 150. Peptide-containing conjugates for triggered assembly and controlled delivery from collagen scaffolds. K.L. Kick
11:00 COMP 151. Coarse-grained simulations of star block-co-polymer aggregation and drug encapsulation. J.W. Pitera, W.C. Swepe
11:30 COMP 152. Protein stabilization in organic solvent via designed random copolymer. B. Panganbin, B. Qiao, M. Oliviera de la Cruz, E. Drockenmuller, T. Xu

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Computational Study of Water

**Applications of Thermodynamics of “Small Water”**

D. J. Sindhikara, Organizer

C. Dickson, Presiding

8:30 COMP 350. Quantifying the entropy of binding for water molecules to protein cavities by computing two-particle correlations. D.J. Huggins

9:00 COMP 351. Monte Carlo study of water oxygen-hydrogen correlations toward efficient calculation of solvation entropies and enthalpies in biomolecular systems. C. Velez Vega, D. Mikly, T. Kurtzman, V. Ananthanarayan, R.A. Pearse, J. Duca

10:00 COMP 352. Discrete solvent based method for the prediction of vibrational hydration sites. R. Betny


**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 density decomposition analysis for second-order Moller-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. Solving 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. Bleino, A. Bialard, V. Barone

**Computational Toxicology: From QSAR Models to Adverse Outcome Pathways**

Sponsored by ONF, Co-sponsored by AGRO, COMP, ENVR and MEDI

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. Tsvain, M.P. Head-Gordon

9:00 COMP 367. Development of an improved molecular dynamics force field for surface-adsorption simulations of maltodextrin disulfide (MS2). G.M. Leuty, R. Berry


10:00 Intermission.

10:15 COMP 369. Tuning the electronic structure of anatase through fluorination. D. Corradini, D. Dambournet, M. Salanne


**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. Krupka

9:00 COMP 373. Practical assessment of evaluating free energy differences between classical and QM Hamiltonians. C.I. Cave-Ayland, C. Skyllas, J. Essex


10:00 Intermission.

10:15 COMP 375. Molecular free energy calculation using the Movable Type method with conformer identification program. Z. Zheng, K.M. Marz

10:45 COMP 376. Free energy calculations with FEP++; Retrospective validation and prospective applications. W. Sherman


**Electronic Structure Methods**

**for Large Systems**

Correlated Wavefunction Approaches

Sponsored by PHYS, Co-sponsored by COMP

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. Dong, 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. Gut

2:30 COMP 386. Molecular dynamics studies of retirovin 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


**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. Avetisyan

2:00 COMP 391. Ab initio quantum mechanical calculations on -9 THC and important neurotransmitters: Implications for potential therapeutic interac-
tions. S.D. Baldwin

2:30 COMP 392. Withdrawn.

3:00 Intermission.

3:15 COMP 393. Solvation and primary structure effects on the deami-
ing of asparaginyl residues in peptides. J. Van der Mysnubre, S. Moors, V. Van Spybroeck, S. Catak


4:15 COMP 395. Automatic generation of detailed chemical models for chlori-nated hydrocarbons. F. Seyedsadd, R.H. West, R. Low, A. Sharratt, C. Giddiss


**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. Agutier-Irarraguirre, T. Hirzel, M.A. Forsythe, A. Asparu-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. Dehmomlale

3:00 Intermission.

Section E
Boston Convention & Exhibition Center Room 151B
Drug Discovery
Ligand-based Approaches
Y. Tseng, Organizer
E. Gianti, Presiding
1:00 COMP 403, Ligand deconstruction: Why some fragment binding positions are conserved and others are not. D. Kozakov, D. Hall, S. Jelveh, L. Luo, S.O. Ohana, E. Jones, M.P. Pollastr, K.N. Allen, A. Whitty, S. Vadas
2:00 COMP 404, Mix-and-match (Q) SAR modelability. A. Zakharov, O. Tarasova, V. Porokov, M.C. Nicolaus
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, Polymorphopharmacology modeling using deep learning approaches. O. Isayev, R. Politi, A. Topraka
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, Co-sponsored by COMP

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways
Sponsored by CINF, Co-sponsored by AGRO, COMP, ENFL, and MEDI

Molecular Biophysics: Revealing the Interplay Between Different Forces & Effects in Biochemical Processes
Macromolecular Interactions
Sponsored by PHYS, Co-sponsored 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. Snope, 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
10:00 10:15
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. Jaryamani, T.B. Martin, R. Krishnamoorthy, K. Mongocopa

Section B
Boston Convention & Exhibition Center Room 156A
Computational Study of Water
Water Models, Phenomena, & Applications
D. J. Sindhika, Organizer
C. H. Andrade, Presiding
8:30 COMP 415, Donor-acceptor interactions in the hydrogen-bond networks of hexagonal ice and liquid water. R. Khalilullin
9:00 COMP 416, Determining melting temperature of ice with the Effective Fragment Potential. C.H. Borca, L.V. Stojcenko
9:30 COMP 417, Molecular dynamics investigation of deeply supercooled water using a direct polarization model. L. Wang, C. Schwantes, T.J. Lane, J. Sellberg, 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. Saprai, 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
9:00 COMP 421, Computational study of Cr(dpda)(NiC5); Electronic structure and potential energy surface along the chromium chain. M. Spivak, V. Lopez, D. de Graa
9:30 COMP 422, Functional mimic approach toward rational design of biospinned iron molecular electrocatalyst for H2 oxidation. N. Kumar, J. Damon, M. Helm, S. Raugei
10:00 Intermission.
10:15 COMP 423, Establishing the zeolite SSS-13 as test system for quantum chemical methods. F. Goettl, P. Sautet, I. Hermans
10:45 COMP 424, Multiconfiguration pair-density functional theory: Applications for transition metal systems. R. Carlson, G. Li Manni, L. Gaggioli, D.G. Truhlar
11:00 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 recognition via symmetrical molecule-electrode coupling. W. Ding, M. Koept, C. Kronigmann, A. Batra, C.F. Negre, L. Venkataraman, W.B. Sudek, V.S. Batista, G.A. Schmuttenmaer, R.H. Crabtree
9:30 COMP 428, Why is the mercury electrode so good for CO2 reduction catalyzed by the Ni[cyclam]] complex? W. Ding, J. Ewchich, C.P. Kutik, 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. Mcke, Y. Xu, V. Meunier
10:30 COMP 430, Critical steps and structures in Pt(111) surface oxidation: A ReaxFF reactive field study. D. Tartauzi, 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
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. Westhoff, O. Botibouvy

THURSDAY AFTERNOON
Section A
Boston Convention & Exhibition Center Room 258B
Innovative Chemistry & Electrochemistry for Low-Carbon Energy & Fuels: Discovery to Application
H2 Generation
Sponsored by CINF

S. W. Lee, Y. Zhao, Organizers
F. Jiao, J. Sun, Organizers, Presiding
8:00 ENFL 437, Bimetallic Pt-M catalysts for aqueous phase reforming of glycerol. A.M. Karim, Z. Wei, D.L. King, Y. Wang
8:30 ENFL 438, Mechanistic studies and design descriptors for CO oxidation over transition-metal-substituted CeO2 nanoparticles. J.S. Elias, M. Reck, L. Giordano, M.N. Azzam, Y. Shao-Horn
9:00 ENFL 439, Manipulation of photo-generated electrons and holes in semiconductor photocatalysts for solar water splitting. J. Gong, P. Zhang
9:30 Intermission.
10:10 ENFL 441, Mesoporous crystalline silicon and evaluation of its hydrogen evolution performance. D. Wang
10:40 ENFL 442, Hydrogen production by plasma-induced decomposition in the presence of metal sulfide semiconductor catalysts. A. Wang, L. Zhao, Y. Wang
11:00 ENFL 443, Isothermal temperature and size-controlled activation of ruthenium-catalyzed ammonia borane hydrolization. C. Na, H. Ma
11:20 ENFL 444, 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. Katkaneni, C. Pett, Organizers, Presiding
8:30 Introductory Remarks.
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.
8:50 ENFL 16. Functional organic frameworks in non-powder forms. Y. Liu
9:20 ENFL 17. Porous polymers that rapidly remove organic contaminants from water. W. Dichtel, A. Altajae, 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

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 Tr-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.
11:20 ENFL 27. In situ low-energy electron microscopy of ceria inverse model catalysts. J. Plege

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
10:30 Intermission.
10:50 ENFL 31. Inorganic-organic hybrid tin and lead based perovskites: From chemistry to solar cells. M.G. Kanatzidis
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. Mukanora, 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. Boagton, Y. Elakasbi, M. Schaffter
9:05 ENFL 34. In-situ and ex-situ catalytic pyrolysis of miscanthus giganteus in PyGC-MS and with bench-scale spouted-bed reactor. D.P. Gamble, S. Du, G.M. Bolles, J. Yalal
9:45 ENFL 36. Catalytic cracking of soybean oil by different hierarchical zeolite containing mesoporous SiO2-Al2O3 using a Cure point pyrolyzer. A. Ishihara
10:05 Intermission.
10:50 ENFL 38. Steam cofeeding during vapor phase upgrading of biomass — mechanistic understanding through model compounds. D. Robichaud, T. Evans, C. Mukamura, M. R. Nimlos
11:30 Concluding Remarks.

National Science Foundation’s Centers for Chemical Innovation
Sponsored by PURES, Cosponsored by AGRO, CARB, CONL, ENFL, PROF and SCHB

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. Kanam
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 electrodissociation in dye-sensitized solar cells (DSSCs). Y.H. Hu

4:10 ENFL 46. Templating intermolecular reactivity on nanostructured surfaces for solar CO2 reduction. M.E. Louis, J. Jin, T. Fenton, G. Li
4:30 ENFL 47. Electrochemical CO2 conversion catalysts for integrated microalgae/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. Pett, O. M. Yaghi, Organizers
S. P. Katkaneni, J. H. Lee, Organizers, Presiding
1:30 Introductory Remarks.
3:50 Intermission.
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. Pett
4:15 ENFL 54. Carbonate eutectic promoted MgO based absorbents for CO2 removal at 300-450 °C. X.S. Li, R. Xing, K. Zhang, R. Dagle, D.L. King
4:35 Concluding Remarks.

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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
1:10 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
3:10 Intermission.
3:20 ENFL 59. Metal-organic frameworks from design strategies to applications. M. Edadaoui
3:35 ENFL 60. Nanopore controlled catalysis: Syntheses of core-shell MOF catalysts. G. Tsung
4:40 ENFL 62. Nanoporous materials for adsorption cooling applications. R. Motkuri, J. Jenks

Section D
Boston Convention & Exhibition Center Room 259B

Advances in Ceria Based Catalysis: Structural, Electronic & Chemical Properties Tailored for Chemical Conversion
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. Angeli, C. de Leonibus, J. Licona
3:10 Intermission.
4:30 ENFL 69. Taking advantage of oxygen transfer from ceria to metal catalysts. C. Chen, T.M. Ora, P. Fornasiero, R.J. Gorte

Section E
Boston Convention & Exhibition Center Room 260

Solar Energy and Solar Cells
Y.H. Hu, Organizer
R. T. Noodai, 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. Yan, 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 milimeter-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. Mukarate, M. R. Nimlos, Organizers
D. Robichaud, B. G. Trevyn, Organizers, Presiding

1:30 Introductory Remarks.
1:35 ENFL 77. Novel thermo-chemical biomass conversion with the recapturing biomass conversion reactor (RBRC). N. Parziale
2:05 ENFL 78. Hydrodeoxygenation of phenol over bulk nickel phosphides. Y. Wang, Z. Yu, T. Dong
3:05 Intermission.
3:20 ENFL 81. Integrated biofuel and nanomaterial production via pyrolysis of silver nitrate impregnated biomass. J. Xue, E. Zade, J.L. Goldfarb
4:10 ENFL 83. Production of hydrocar- bon-rich fuels by two-step hydrolysis of Scenedesmus/Desmodesmus sp. algae. W. Obed, P. Hatcher
4:30 Concluding Remarks.

Monday Morning

Section A
Boston Convention & Exhibition Center Room 258B

Innovative Chemistry Education: Formal and Informal
Sponsored by Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB
10:45 ENFL 96. CO2 hydrogenation to methanol over Cu2ZnZrO4 catalysts prepared by chemical reduction. X. Dong
11:05 ENFL 97. Advanced electrodi-alysis (ED) system for CO2 mineralization with chemical absorbents. J. Han, J. Chung, J. Son, D. Song
11:45 Concluding Remarks.

Section B
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. Sivakum, E. Leitiker, I. Pinnau
9:20 ENFL 101. Advanced molecu- lar sieve membranes. G. Song
9:50 Intermission.
10:00 ENFL 102. Tailoring the separation performance of zeolitic imidazolium- cationic metal nanocatalysts and evaluation for oxygen reduction reaction activ- ity. Y. Hamasaki, T. Fujikya, N. Nakashima

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
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. Senarayake, 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. Hennigson

2:00 ENFL 156. P2O5 - CeO2 novel thin film catalyst as PEMFC anode.
V. Matolin

D. Ginter, 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. Wess


4:40 ENFL 161. Faceting transition at the oxide-metal interface: The case of ceria on copper.
M. Aukica, T. Duchon, F. Dorcar, V. Stetsushvily, J. Beran, K. Vetruska, 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 biofuels from an algal feedstock.
P. Valsez

3:15 Intermission.

3:30 ENFL 165. Towards a model for predicting hydrothermal liquefaction of microalgae of varying composition.
J. T. Straathof, S. Low, Y. Lui, 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. Bhorac, A.L. Bootham

5:00 Concluding Remarks.

Section F

Boston Convention & Exhibition Center Room 261

Chemical Looping Innovation for Low-Carbon Energy

Z. Jiang, 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 carrier in chemical looping processes.
A. More, S. Bhanwar, G. Veser

2:55 ENFL 173. Pressurized carbonation experiments in the presence of steam in a spouted-bed reactor.
J. Yao, Z. Zhang, M. Sciacca, P. Fennell

3:30 ENFL 174. Development of CuO-FeOx mixed metal oxide carrier from lab scale to commercial scale: Bench scale fluidized bed tests and pilot scale (50 kW) chemical looping combustion tests with methane-air.

3:55 Intermission.

4:10 ENFL 175. Reaction of ceria with CO: from a gas phase to a catalyst.

5:00 Intermission.

S. W. Lee, Y. Shao, S. Ma, Organizer, Presiding

5:40 ENFL 177. Activity trends and design principles for multitransition-metal (oxy)hydroxide oxygen evolution catalysts.
S. W. Boettcher, M. Burke, L. Trotchoud, S. Zhou, L. Ennan, A. Smith, A. Batchelor, M. Kast

8:00 ENFL 178. From bulk to nanoscale: δ-MnO2 as a water oxidation catalyst.

8:50 ENFL 179. Controlled prepa- ration and electrode applications of manganese-based oxides with micro/nanostuctures.
J. Chen

9:20 Intermission.

9:30 ENFL 176. Self-healing oxygen evolving catalysis.
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 catalaists.
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(di-phenylphosphino)ethane.
A. Bloomfield, S.W. Sheehan, S.L. Colson, P.T. Anastas

X. Zhao, M. Yarney, M. Vennampalli, G. Liang, C.E. Webstar

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 relation- ship in layered cathode materials for sodium-ion batteries.
E. Lee, A. Gutierrez, M.D. Slater, J. Liu, Y. Kim, C.S. Johnson

9:35 ENFL 186. Olivine NaFePO4: cathode synthesized by a green aqueous electrochemical conver- sion route for sodium ion batteries.
Y. Fang, L. Xiao, A. Li, H. Yang, Y. Gao

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 mate- rials for high performance sodi- um-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. Pomerantsve

11:35 ENFL 190. Continuum-scale electrochemical modeling of a NaO2 battery.
S. Khaledi 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 Uio66- supported iridium complexes for ethylene hydrogenation and dimerization.

9:20 ENFL 193. Structural studies of small molecule adsorption in MOFs.
Z. Huyle, 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.

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.

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 CATAL
S. D. Semanayake, Z. Wu, Organizers, Presiding
8:50 ENFL 199. Computational modeling of nanostructured ceria for the rational design of catalytic materials. A. Bruix
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 CeO$_2$. W. Huang
11:40 ENFL 204. Extremely porous Pt-CeO$_2$ structures grown on carbon films for fuel cells applications. I. Matalinova, J. Lavkova, A. Park, Organizer
8:30 Introductory Remarks.
8:35 ENFL 205. Biomass economy: Challenges and opportuni- ties. M.A. Serio, M.A. Wojtowicz
9:10 ENFL 206. Molecular-level kinetic modeling in thermochemi- cal conversions: Software tools and their applications. M.T. Kean
9:45 ENFL 207. Poly cyclic aromatic mixtures, tar, and their phase behaviors: Their importance in fuel conversion processes. E. Suuberg
10:20 Intermission.
10:35 ENFL 208. High tempera- ture, 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. Takakera
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. Weiner
8:35 ENFL 173. Nanostructured metal oxides for chemical looping processes. O. Song, W. Liu, S. Cao, Z. Zhang, P. Fennell, A. Chestem, S. Scott, J. Dennis
9:05 ENFL 311. Investigation of multicycle performance of chemical looping gasification of biomass char using Fe-Ni bimetallic oxide carrier under different atmospheres. Z. Huang, F. He, D. Chen, S. Liu, K. Zhao, G. Wei, A. Zhang, Z. Zhao, H. Li
9:45 ENFL 415. Perovskite-structured redox catalyst for methanol partial oxidation with lattice oxygen. A. Mishra, N. Galinsky, F. Li
10:05 Intermission.
10:10 ENFL 310. Modelling the reduc- tion of Fe-based oxygen carriers for pressurised chemical-looping combustion of gaseous fuels. Z. Zhang, J. Yao, M. Booth-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. Bolis
11:10 ENFL 168. Studies on ethanol conversion for clean fuels. J. Zhang, X. Gao, P. Hu, Z. Zhong, J. Zhang, P. Li
11:30 ENFL 416. Carbon-hydrogen bond on the surface of nanosized hydrogenated graphene. Y. Zhang
11:50 Concluding Remarks.
Transforming University-Industry Partnerships for an Innovative Future
Envisioning, Enabling and Executing
Sponsored by ENFL, Cosponsored by ACED, ENFL, PHYS, POLY, ECS
12:00 ENFL 238. Pt-ReO$_2$nanoparticles for hybrid fuel cell application. H. Liu, Y. Xu, Y. Zhang, J. He, J.V. Blargan, Y. Xu, J. Belovich
12:45 ENFL 239. 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
14:00 ENFL 241. Roles of hollow silica and activated carbon on methane hydrate formation. R. Suessau, P. Rangaswigni, S. Kulprathipanja
15:20 ENFL 243. Preparation and photocatalytic activity of porous Bi$_2$O$_3$. A. Ishihara
16:00 ENFL 244. Modeling and optimization of electrocatalysts for the oxygen reduc- tion reaction with stacked carbon nanotubes and electrically driven molecule transport within a series of novel iono- mers. D. Wang, C.J. Comella
16:40 ENFL 245. Predicting the enthalpy and entropy of vaporization of gasoline using an enhanced vapor pressure acquisition system. S. Abernathy
17:20 ENFL 246. Novel large-scale synthesis of C/S nanocomposite with mixed conducting networks through spray drying approach for Li-ion batter- ies. I. Ma, Z. Fang, Y. Yan, Z. Yang, L. Gu, Y. Hu, H. Li, Z. Wang, X. Huang
18:00 ENFL 247. Sulfur precipitation and extraction in jet A. K. Greeno, A.J. Guenthrner, J. Reams, C. Lee, J.M. Maloy
18:40 ENFL 248. Shale gas fracturing fluids with polymer grafted silica with enhanced suspensibility. M.H. Bell, A. Viswanath, B.C. Berzowsicz
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ENFL 244. Chemoslective catalytic conversion of glycerol to methyl lactate in methanol over Sn-3 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 fungus that produces volatile organic compounds with fuel potentials. Y. Wang

ENFL 249. Extractants for adsorbed 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.D. Pyrz, S. Kim, C. Sun, 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 256. Detailed type analysis of petroleum samples by using comprehensive 2D gas chromatography/high-resolution mass spectrometry with field ionization. M. Ubukata, S.E. Rechenbach, 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 SiO2TiO2 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 ligandocellular 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 263. Evaluation on the potential with channel-type and cage-type metal-organic frameworks as absorbers in solid-phase microextraction. H. Huang

ENFL 264. Assembly and optimization of paper based microfluidic cells(MFCs) in an alkaline environment. V. Galvan, K. Domanov, S. Sotz, C. Tang, F.A. Gomez, J. Haan, M. Jalali Heravi

ENFL 265. Lignin deconstruction by oxidation: Model studies in conventional and ionic liquid solvents. Y.G. Yao, M.S. Meier, R. Pasce, M. Crocker

ENFL 266. Surface modification of activated carbon for the improvement of methane adsorption. K. Nimprapap

ENFL 267. Impact of municipal solid waste paper mix as a blending agent on enzymatic hydrolysis and acidification. F. Xu

ENFL 268. Comparative study of OMC, MCWONT, and Vulcan XC-72 as carbonaceous supports of Pt catalysts for direct alcohol fuel cell applications. D. Morales, F.I. Rodriguez

ENFL 269. Halogenation of natural gas components under mild conditions. A. Leichthaus, J. Bahrutsidis, J.D. Schuttefeld Christus, B. Nothern, I. Jansen


ENFL 273. Withdrawn.

ENFL 274. Preparation of electrochemically exfoliated graphene/MnO nanocomposites by an electrostatic self-assembly process for supercapacitor application. D. Shu

ENFL 275. Odd-symmetric memristor from asymmetric switches. P. Cheng, X.H. Hu

Section B

Boston Convention & Exhibition Center Room 259A

Porous Materials for Energy & Sustainability from Discovery to Application

Financially supported by KAUST & Framergy

D. Jiang, Organizer, Presiding

1:00 Introduction Remarks.

1:05 ENFL 276. Nanomaterials with controlled porosity for energy applications. F. Schueth

1:10 ENFL 277. Porous colloidal Pt superparticles. Y. Sun, Y. Hu, Y. Liu

2:20 ENFL 278. Synthesis of SAPO-18, SAPO-18/34 and SAPO-34 molecular sieves and their catalytic performance for methanol-to-olefins reactions. Y. Wang, S. Chen, V. Yang, Y. Gao, O. Zhang, F. Chen

2:40 ENFL 279. Nanoporous bimetallic catalyst for hydrogen evolution reaction. F. Jiao

3:00 Intermission.

3:15 ENFL 280. Synthesis and assembly of 10 inorganic semiconductor for solar energy conversion. X. Feng

3:30 ENFL 281. 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 282. Low-temperature nitrogen-doping and activation of soft-templated mesoporous carbon for CO2 capture. K. Huang, S. Cha, R.T. Mayes, S. Dai


5:10 ENFL 286. Waste-to-byproduct conversion of oil shale semicrude and ash to sorbent materials and zeolite precursors. A. Was, J.L. Goldfarb
Section B
Boston Convention & Exhibition Center Room 258C

Innovative Electrochemical Energy Storage

Advanced Characterizations & Electrolytes
J. Lu, Organizer
X. X., Organizer, Presiding
E. Pomerantz, 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 9-8 BM. T. Wu
9:05 ENFL 327. Ex-situ and in-situ characterizations of the Li removal from the anti-fluorite LiFeO\(_2\)/C. Z. Nan. J. Lu. Amine
9:25 ENFL 328. In situ transmission microscope observation of lithium hair growth. A. Kushima, K. So. J. Li
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. Aouz, C. Sun, J. Xie, W. Lu. Z. Chen
10:45 ENFL 331. Glycerol triester as co-solvent in Li-battery electrolyte for high voltage application. B. Roy, D. Kim, Y. Kang, J. Park, S. Do.
11:05 ENFL 332. Preparation and properties of proton and lithium conducting membranes from polymer brush nanoparticles. I. Zharov

Section C
Boston Convention & Exhibition Center Room 259A

International Symposium on Mesoporous Zeolites
Sponsored by CATL, ISEC and ANU
Financially supported by RVE Technology, Zeolyst International, Chevron, Quantachrome Instruments, W. P. Grace
J. Garcia Martinez, K. Li, Organizers
F. Schueth, Presiding
8:00 Introductory Remarks.
8:35 ENFL 335. Hierarchical zeolites: Increase in mesorsurface via “bottom-up” or “top-down” methods and its influence in catalytic cracking. E. Falabella Sousa-Aguiar
10:15 Intermission.

Section D
Boston Convention & Exhibition Center Room 259B

Advances in Analytical Methods for Petroleum Upstream Applications
C. F. Ovales, C. E. Rechsteiner, Organizers
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 GP performance in the real world: Multi lab studies for repeatability and reproducibility. C. E. Rechsteiner, J. Randle, 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. Penetre-Amauno
11:50 Concluding Remarks.

Section E
Boston Convention & Exhibition Center Room 250

Energy & Fuels Starch Award in Fuel Science: Symposium in Honor of Ripudaman Mahtra
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 selectivity during deactivation by oxidation or by changing space velocity at stable conditions over unpromoted and Ru promoted 25%Co/Al\(_2\)O\(_3\) catalysts. W. Ma, U. Grahm, G. Jacobs, B. Todic, D.B. Bulv, B.H. Davis
8:40 ENFL 348. 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 H\(_2\) with Ca(OH)\(_2\). A. Park, M. Storor, J.G. Chen
10:40 ENFL 351. Design and synthesis of materials for energy conversion and storage. Y.H. Hu
11:15 Concluding Remarks.

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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. Helebrandt, X. Wang, Organizers, Presiding
8:00 Introductory Remarks.
8:05 ENFL 314. Electrochemically-mediated Li-chalcogenation by 1,2,3,4-tetrahydro-6,7-dimethoxy-1,1,4,4-tetramethynaphthalene; in situ structural characterization and energy storage applications. E.V. Carino, J. Staszak-Jirkovsky, R.S. Assary, L.A. Curtiss, N. Markovic, F. Bruehwitt
8:45 ENFL 316. Electrochemical driven molecule transport modeling and optimization of electrodeposition desalination within a series of novel ionomers. D. Wang, C.J. Cornelius
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 FFC catalyst by vanadium trapping components. F. Ren, Q. Liu, Y. Zhu
10:55 ENFL 322. Mechanistic insight into coke formation by catalytic pyrolysis of biomass pyrolysis relevant model compounds. S. Du, D.P. Gamblin, J. Vals, G.M. Bolleux
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

WEDNESDAY AFTERNOON

Section A
Boston Convention & Exhibition Center Room 258B
Advances in Chemistry of Energy & Fuels
D. J. Helebrandt, 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. Swei, W.P. Liyanage, N. Akhsan, M. Nath
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 H\(_2\) 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. Rampf
2:45 ENFL 357. In-situ FTR investigation on semiconductor catalysis. B. Han, Y.H. Hu
3:05 Intermission.
3:20 ENFL 358. Engineering nanocrystals for oxygen reduction. S. Do
Section B
Boston Convention & Exhibition Center Room 258C
Innovative Electrochemical Energy Storage

Advanced Li-Ion Batteries
X. Li, 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
1:15 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. Yarar, E. Bicic, S. Akan Gursel
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 Li,MgO phases. D. Yeon, J. Song, J. Park
3:05 ENFL 367. Antiperovskite LiOCl oxide solid-state electrolyte films for Li-ion batteries. Y. Lu, Y. Zhao, H. Xu, Q. Jia
3:25 Intermission.
3:35 ENFL 368. New high energy and power chemistries in 3D mesostructured 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

Section C
Boston Convention & Exhibition Center Room 259A
International Symposium on Mesoporous Zeolites
Cosponsored by CATL, IFFC and INDR
Financially supported by Rive Technology, Zeolyst International, Chovan, Quantachrome Instruments, W. R. Grace
J. Garcia Martinez, K. Li, Organizers
E. Falabella Sousa-Aguir, Presiding
1:30 Introductory Remarks.
1:35 ENFL 372. Mesoporous zeolites and related materials for the conversion of biomass-based feedstocks. F. Schuett
2:45 ENFL 374. Modern view on zeolite stability: Integrity and application of zeolite catalysts in condensed aqueous phase. F. Pretorius, F. Jacobs, B. C. Sells
3:15 Intermission.
3:55 ENFL 376. Functionalization and mesoporosity control of zeolitic metal-organic frameworks. H. Zeng
4:55 Concluding Remarks.

Section D
Boston Convention & Exhibition Center Room 259B
Advances in Analytical Methods for Petroleum Upstream Applications
C. F. Ovales, C. E. Rechtestein, Organizers, Presiding
1:00 Introductory Remarks.
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. Jaine, L. Memb障碍
3:45 Intermission.
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 259C
Advanced in Chemistry and Bioenergy Storage, Utilization and Sequestration

Innovative Utilization Pathways for Natural Gas
Cosponsored by CATL
A. L. Boehm, A. Marchese, Organizers, Presiding
1:30 Introductory Remarks.
1:35 ENFL 385. Refining opportunity and crudes with a high iron concentration in FCC. F. Schuett
2:05 ENFL 386. Effect of Ni 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
4:55 Concluding Remarks.

Biological Inspiration for Environmental Sustainability: Biospired Approaches for Energy Conversion, Storage and Materials
Bioinspired Designs: From Molecules to Functional Materials
Sponsored by ENFL, Cosponsored by CEL, ENFL, ORGN and PHYS

ENFL TECHNICAL PROGRAM

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
8:45 ENFL 393. Upgrading inferior residue to produce light oil in a pretreating process. N. Gin, J. Gao, C. Wang, X. Gao, C. Xu
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. Boehm
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. Halthide, S. Ergas
10:55 ENFL 399. Comparison of the reduction products: Vinylene carbonate vs. Fluoroethylene carbonate. B.S. Subramanian, M. Nio, 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. Marcarinova

Advances in Chemistry for Carbon Capture, Utilization and Sequestration
Cosponsored by ENVR, Cosponsored by ENFL

Biological Inspiration for Environmental Sustainability: Biospired Approaches for Energy Conversion, Storage and Materials

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. Solovych
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.
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. Neked, E. Gilles, J. Duong, 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
5:10 ENFL 412. Multielectron electrochemical charge storage in 2D transition metal compounds. C.P. Rhodes, A. Zaleski, C. Ly, G. Cruz

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 Park Plaza Hotel and Towers
St. James Room
Designing Safer Chemicals
Cospersoned by CEI

A. Vourchokova, Organizer
P. T. Anastas, J. B. Zimmerman, Organizers, Presiding

9:00 ENVR 8. On the design of safer commercial chemicals: Past, present, and future perspectives. S. DeVito

Section C
Boston Park Plaza Hotel and Towers
Berkeley/Clarendon Room
Nano-Enabled Environmental Technologies
Cospersoned by CEI

D. Minakata, D. Kanath, M. Roulou

9:45 Intermmission.
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-Demesse, G. Sorial, Organizers, Presiding
1:30 ENV R 77. Electrochemical drinking water disinfection — are all problems solved? M.E. Bergmann, W. Schmidt, A. Grunert, T. Grimm
1:55 ENV R 78. Comparative study in treating disinfection by-products (DBPs) in biotricticking filters (BTFs) under different environmental conditions. B. Mezgebe, K. Palarsammy, G. Sorial, E. Sahle-Demesse
2:20 ENV R 79. Optimizing coagulation for treatment of high TOC surface water and minimizing disinfection byproduct formation potential. A. Waldorn, A. Manikonda, C. Bellona
2:45 ENV R 80. Modeling THM removals from a horizontal in-line diffused aeration system in pressurized water distribution pipes. M.R. Collins
3:00 Intermission.
3:50 ENV R 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. War
4:15 ENV R 83. Prioritizing environmental health and household demographic factors impacting biosand filter maintenance and diarrheal occurrences in Brazil. L.E. Voth-Gaadt, D. Onerth

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. Orlow, S. Zhao, Organizers, Presiding
1:30 Introductory Remarks.
1:35 ENV R 84. Effect of crystal defects on visible-light photocactivity. C. Huang
2:00 ENV R 85. Directed assembly of cuprous oxide nanocluster catalyst for CO2 reduction coupled to heterobinuclear light absorber in mesoporous silica. W. Kim, H.M. Fee
2:40 ENV R 87. Exploring tunability of catalysts for light induced reactions: Subnanometer particles and their interactions with support, reactants, and light. A. Orlow, Q. Wu, S. Zhao, Y. Li
3:20 Intermission.
4:00 ENV R 90. In-situ ATR-FTIR observation of selenate reduction by photocatalytic nano–metal oxides. A.W. Lounsbury, J.B. Zimmerman
4:20 ENV R 91. Supporting of TiO2 with metallic nanoparticles to improve the decomposition of paracetamol by photocatalysis: The effect of ultrasound. N.H. Ince
5:20 ENV R 94. Simultaneous photo-catalytic elimination of gaseous NO and SO2 in a BIO/ALO, wet scrubber system. C. Ha, L. Hui, 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 Professionals)
C. Coronella, K. Ro, Organizers
S. Chang, J. A. Libra, Organizers, Presiding
1:30 ENV R 95. Hydrothermal carbonization (HTC) of sewage sludge: Challenges and synergies for future waste water treatment. B. Wirth, L. Herklotz, U. Lüder
2:20 ENV R 97. Food waste as bioresource for hydrothermal carbonization and its products. S. Bae, S. Lee, S. Lee, Y. Hwang, S. Park
2:45 ENV R 98. Understanding the environmental impact of the hydrothermal carbonization of food wastes for energy generation using life cycle assessment. N.D. Borge, L. Li, J. Flora, K. Ro
3:10 Intermission.
4:25 ENV R 101. Economics of centralized 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, Environment and Environmental Protection
Energy/General
Cosponsored by ENFL
J. Mi, J. Song, Organizers, Presiding
1:30 ENV R 279. Giving new life to materials for energy, the environment, and medicine. A.M. Belcher
2:00 ENV R 280. Probing structure and dynamics of nanomaterials for energy applications. S. Corr
3:10 Intermission.
4:15 ENV R 285. Production of synthetic natural gas from catalytic syngas conversion using biomass waste. K. Kawamoto
4:55 ENV R 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
Prospects on CO2 Capture and Conversion
Sponsored by ENFL, Cosponsored by ENVR


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 ENV R 107. Influence of sea spray aerosols on cloud and climate. K.A. Prather

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Section C

Boston Park Plaza Hotel and Towers
Berkeley/Clarendon Room

Sensing of Environmentally Relevant Contaminants
Cosponsored by AGRO
Financially supported by AEEPS (Association of Environmental Engineering and Science Professors)
B. P. Chaplin, D. Jassby, Organizers, Presiding

8:00 Introductory Remarks.


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 Intermission.

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 pond and wetland sediment pore water. B. McAdams, Y. Chin, W. Arnold

11:25 ENVR 122, 2-Aminobenzothiazole imines as sensitive anion colorimetric sensors. Y.M. Hijji, H. Alarea

Section D

Boston Park Plaza Hotel and Towers
Beacon Hill Room

Advanced Materials and Technologies for Desalination and Wastewater Reuse
Financially supported by AEEPS (Association of Environmental Engineering and Science Professors)
J. Kim, Organizer

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, Biofuelling 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. Bates, F. Li

9:00 ENVR 126, Block copolymer functionalized thin-film composite membrane for antifouling and antimicrobial properties using atom-transfer radical polymerization. J. Lee, G. Ye, F. Perreault, M. Elimelech

9:20 ENVR 127, Withdrawn.


10:00 Intermission.


10:35 ENVR 130, In-situ and self-healing of water filtration membranes for wastewater reuse applica-


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 Introductory Remarks.


8:30 ENVR 135, First principles investigation of the hydrogen evolution reaction on nickel phosphides NiP2 and NiP3. R. Weiler, J.M. Martinez, A.M. Rappe

8:50 ENVR 136, Heterogeneous catalysis for sustainable energy: Atomically dispersed gold clasters for hydrogen production. N. Yli, M. Stephanopoulos

9:10 ENVR 137, Aromatic-hydroxyl interaction of a lignin model-compound on SBA-15, presenting pyrolysis temperatures. A. Savara, M. Kandathioka, M. Kidder, L.W. Gilt, Z. Wu

9:35 Intermission.

9:50 ENVR 138, Study of the mechanism for the formation of ionic and levulinic acids from HMF. E. Weitz, A. Das, T. Drake, P.C. Star

10:10 ENVR 139, Understanding and enhancing the selectivity of reductive lignin disassembly over doped porous metal oxides. C.M. Bent, J.A. Barrett, M.A. Churchill, B. Banth, H. Marusawen, K. Harta, 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. Guett, A. Love, P. Sautet, J. Hermans

10:50 ENVR 141, Study of NH3-SCR over Cu-zeolites: From straight channel zeolites to cage-type zeolites with DDR unit. R. Xu, B. Chen, Y. He, F. Jin

11:10 ENVR 142, Drawing bio-inspiration to design environmental catalysts. S. Liu, J.C. 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 Introductory Remarks.

8:05 ENVR 143, Organic reactions on a green avenue to added-value chemicals. C. Len

8:45 ENVR 144, Ionic liquids as solvents for metal extraction: Engineering Considerations. C. Janssen, M.N. Kobrak, M. Aguilar Martinez

9:05 ENVR 145, Using the waste materials to generate nanoparticles and electrosynpse the nanofillers. Z. Katircioglu, S. Dursun, M. Yazuv

9:25 ENVR 146, Controlling phosphorus as a preservation strategy for products with high organic load. T. Azimi, J.P. Thompson

9:45 Intermission.

10:00 ENVR 147, Nitrofuranic acid functionalized Anass待a gigantea bio-adsorbent: A potential means of waste water treatment in developing nations. A. Awedawi

10:20 ENVR 148, Removal of acid red 114 and basic blue 3 from aqueous solutions by activated carbon obtained from waste tissue. 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 disinfec-

10:50 ENVR 150, Lead removal from aqueous solution using pine wood biochar modified with chitosan. N.W. Bombuawala Dewage, T.E. Mitra

AC Scholars: Rising Stars in Academe
Cosponsored by FRESE, Cosponsored by AGRO, CARB, CMAL, COLL, ENFL, ENVR, PRO, SCHB and YCC

Carbon Management: Recent Advances in Carbon Capture, Conversion and Utilization and Storage

CO2 Conversion, Utilization and Storage
Sponsored by ENFL, Cosponsored by ENVR

Global Research Needs: Identifying and Prioritizing Efforts to Support 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, IMEC, MOD, PROH, SCHB and YCC

Chemical Processes Involving Atmosphericly 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
Cosponsored by AGRO, Sponsored by TOXI and ENVR

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
Stater 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/Inorganic
Cosponsored by CEI
R. de Fatima Peralta Muniz Moriera, D. D. Ionysios, D. Minalkata, 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-assisted 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-Peroxone process. D. Pro-Sandoval, R. Nu€ez-Salas, J. Rodriguez-Acosta, N. Marigna-Cabral


3:00 Intermission.

3:15 ENVR 154, Bromate formation from bromide oxidation by the UV/peroxymonosulfate process. D. Zhang, L. Ling, J. Fang, C. Shang

Cooperative Cosponsorship
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 CBE
D. Avisar, D. D. Dionysiou, D. Minakata, K. E. O’Shea, Organizers
T. H. Nguyen, V. Tarabara, Presiding
8:30 ENVR 210. Selective cell interactions and antibacterial behavior of functional fibrous membranes. S. Xu, B. S. Hisao, C. C. Han, B. T. Chu
9:00 ENVR 211. Human adenovirus removal by hollow fiber membranes: Effect of membrane fouling by suspended and dissolved matter. Z. Yin, V. Tarabara, I. Kagorporaki
9:30 ENVR 212. Withdrawn.
9:50 Introduction.
10:00 ENVR 213. 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. Vrouenrader, P. Sakaly
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) surrogates adsorption on polyamide water filtration membranes. A. Voza, B. M. Janzana, M. 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. Weinrich

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 AESAP (Association of Environmental Engineering and Science Professors)
S. Chang, C. Coronella, J. A. Libra, K. Ro, Organizers

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. Mashaware, L. Poyet, Organizers
Presiding
8:00 Introductory Remarks.
8:40 ENVR 227. Environmental fate of 14C-ringed labeled 2,4-dinitroanisole (ODAN) in anaerobic saturated soils. C. I. Olives, L. Abrel, R. Sierra-Avarez, J. Chozzar, J. Field
9:00 ENVR 228. Reductive transformation of explosives in soil with zero-valent iron-bearing biochar. S. Oh, Y. Soo
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
10:00 Intermission.
10:10 ENVR 231. Zerovolatent metals and vitamin B12 potential for remediation of persistent perfluorooalkyl acids in groundwater. L.S. Lee, S. Park, J.E. Zenobi
11:35 ENVR 235. NMR evaluation of cyclodextrin-perfluorinated surfactant-host-guest interactions. M.J.J. Weiss, K.E. O’Shea
11:55 Concluding Remarks.
Section B

Boston Park Plaza Hotel and Towers Plaza Ballroom

The Debate: How Do We Respond to Climate Change
Co-sponsored by CEI
C. W. Avery, L. E. Pence, Organizers, Presiding
3:30 Introductory Remarks.
3:35 Opening Statements.
3:45 ENV 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 Engineering Sustainable Stability: Bioinspired Approaches for Energy Conversion, Storage and Materials
Bioinspired Designs: From Molecules to Functional Materials Co-sponsored by CEI, ENVL, CRGN and PHYS
K. Rajeswar, V.I. Vuliev, Organizers, Presiding
1:30 Introductory Remarks.
2:15 ENV 268. Electrochemical conversion of CO2 to syngas with enzymes from the reverse TCA cycle. S.J. Elliott, B.L. P. Steindel
3:15 Intermision.
3:30 ENV 270. Protein-based hybrid catalysts for hydrogen production. G. Ghirlanda
4:50 ENV 272. Multivalency through dendritic building blocks: Fabrication of functionalizable hydrogels. R. Sanjal

Section D

Boston Park Plaza Hotel and Towers Beacon Hill Room

C. Ellen Gontier Awards Symposium
T. Anderson, Organizer, Presiding
1:30 Introductory Remarks.
2:00 ENV 274. Changes in physicochemical and transport properties of a reverse osmosis membrane exposed to chloraminated seawater. L. Valantino, T. Renkers, T. Maquin, J. Croue, B.J. Marinas
2:25 ENV 275. Polysulfone membranes modified with biosilanized perylene dyes and silver nanoparticles formed in situ to mitigate biofouling. L. Tang, K. Liu, K. Chen
2:50 Intermision.
3:30 ENV 277. Using in situ passive samplers to assess porewater concentrations in sediment beds influenced by groundwater flow. J. Appell, J.X. MacFarlane, P.M. Gashwer

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. Oulton
Membranes, Absorption and H202 Production Co-sponsored by AGRO
F.A. Montemuribu, I. S. Sardolin, Organizers
3:05 Introductory Remarks.
2:15 ENV 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 ENV 290. Development of reactive electrochemical membranes for water treatment application. B.P. Chapel, Y. Jing, L. Gao
3:15 Intermision.
3:50 ENV 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
4:30 ENV 305. Ecotoxicity of carbon nanotubes to algae, Dunaliella tertiolecta. M. Thakkar, S. Mtra, 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 in Control**
  - G. Wells, Organizer
  - J. Joonhong, H. Lee, Organizers

- **Microbial Conversion of Dissolved Methane to Methanol**

- **Removing nitrogen from wastewater treatment.**
  - R. Goel, A. Bhattacherjee

**Section B**  
Boston Park Plaza Hotel and Towers  
**Stuart Room**

- **Status and Trends of Biological and Persistent Organic Chemicals in the Great Lakes**
  - D. Dionysiou, J. J. Pagano, Organizers

- **The Great Debate: Investigating the roles of nitrogen and phosphorus in driving the growth and toxicity of cyanobacteria harmful algal blooms in western Lake Erie.**
  - T. Davis, T. Johnsen, M. Harke, G. Bullerjahn, S. Watson

- **Products of oxidation of microcystin-LR by ferrate(VI) as a function of reactant molar ratios and pH.**

- **Removal of cyanotoxins (microcystins and cylindrospermopsin) using UV-based processes.**
  - X. He, A.A. de la Cruz, D. Dionysiou

- **Sorption of human and veterinary antimicrobials in soils and sediments.**
  - S.A. Pagsuynog, J. Yap

- **Sediments as sinks of antimicrobials in rivers.**
  - S.A. Pagsuynog

**Section C**  
Boston Park Plaza Hotel and Towers  
**Berkeley/Clarendon Room**

- **Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials**
  - K. Rajeshwar, V. I. Valles, Organizers

- **Energy Storage, Solar Fuels, and Biofuels: Satisfying the Energy Needs While Decreasing the Carbon Footprint**
  - S.M. Uchimiya, J.J. Pignatello, J.C. White

- **Electrosynthesis of hybrid organic/inorganic photocathodes for solar fuel generation.**
  - D. Hunsar, K. Rajeshwar, C. Janaky

**Section D**  
Boston Park Plaza Hotel and Towers  
**Beacon Hill Room**

- **Resource Recovery and Contaminant Elimination in Waste Streams of Increasing Concern**

**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. Montenegro, I. S. Sardini, V. K. Sharma, Organizers

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, Co-sponsored by ANLY and ENVR

Pesticides and Hydrophobic Compounds in Sediment
Sponsored by AGRO, Cosponsored by ENVR

WEDNESDAY AFTERNOON

Section A

Boston Park Plaza Hotel and Towers

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. Weishaar, X. Li, V. Hanwood

1:20 ENVR 360. Development of CRAsphage as an improved indicator of human fecal pollution in the environment. E. Stachner, 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, J. M. Olson


3:00 ENVR 365. Removal of bacterial contaminants and antibiotic resistance genes by conventional wastewater treatment processes. J. Al-Jassar, O. O'Shea, B. Marashek, R. Zbor, V. Kamra

3:20 ENVR 366. Predicting the fate of waterborne viruses in surface water using photochemistry tools. M. J. Matte, D. V. Vone, 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, R. 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. Verteba, M. Inrata, A. Mercado, J. Hileleich

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 AESSP (Association of Environmental Engineering and Science Professors)

C. A. McDonough, Organizer

1:30 ENVR 369. Calibration of a novel passive sampler for the measurement of 34 polar organic contaminants in aquatic systems. J. Chahls, M. Hanson, C. S. Wong


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 sampling using sampling 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 polystyrene passive samplers. L. Fernandez, G. M. Ravetta, 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. G. Hombuckle

4:10 ENVR 377. HCBs 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


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
Cosponsored by CEI, ENFL, ORGN and PHYS

Introductory Remarks. T. H. Boyer, C. Huang, Organizers, Presiding

1:00 Introductory Remarks.


2:10 ENVR 381. Lithium recovery from low temperature geothermal brines through membrane distillation and manganese oxide sorption. J. Renew, J. Rijterowski, J. Wos


3:00 Introduction.


4:05 ENVR 385. Bioinspired adaptively reconﬁgurable material systems: A new paradigm for autonomous metal ion separation. N. Nan, Z. Zhao, J. Lu, X. He


4:55 Concluding Remarks.
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
Co-sponsored by AGRO
F. A. Montemurbo, I. S. Sardonil, V. K. Sharma,
M. Rodrigo, I. S. Sadornil, Presiding
1:30 Introductory Remarks.
1:35 ENVR 393. Heteroaggregation of nanoparticles with biocoll-
oids and geocoolloids. A. A. Keller
1:45 ENVR 394. Can carbon-based nanomaterials modulate the toxic activity of organic pollutants in the environ-
ment? D. Barcelo, J. Sanchez, M. Fare
V. Craver, M. Ayana, F. Solomon
2:55 ENVR 396. Uptake, distribution, and physiologial impacts of metal
oxide nanoparticles in mature crop
plants: Evidence for nanophototoxic-
ytic? J. Conway, S. Mazer, A. A. Keller
3:15 ENVR 397. Lithium nickel mangan-
ese cobalt oxide (NMC) nanoma-
terials: Interactions with biological systems. N. M. Hang, I. Gunsolus,
J. Rozich, H. A. Wayland, E. Maltby,
A. C. Mensch, K. Hurley, J. A. Pedersen,
R. L. Tanguay
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. Summer, E. Sahle-
Demessie, M. J. Kuperthief, G. Sorial
4:05 ENVR 399. Microbial aging of
fullerene C60 nanoparticles aggregate-
gates in water. S. Chae, D.E. Hunt,
C.K. Gunisich, M.R. Westman
4:25 ENVR 400. Tracking trace amounts (ppt) of silica nanoparticles in
complex fluids and seawage water
plants using DNA tracers. R.N. Grass,
D. Paunesku, P. Kaeg, W.J. Stark
4:45 ENVR 401. Influence of phytoplankton
on fate, transformations, and effects of
iron nanoparticles. A.S. Adeleye, A.A. Keller
5:00 ENVR 402. Evaluation of silver
nanoparticles – impregnated tex-
tiles across their life cycle. R.B. Reed,
M. Marco, T. Zaitkova, A. Barber,
J.E. Hutson, J.F. Ranville, R.L. Tanguay,
P.K. Waterhouse
5:25 ENVR 403. Preparation and charac-
terization of strawberry fruit extraction
loaded nano biodegradable chitosan
particles. R. Pulchra, C. Marques,
S. Brar, T. Rousis, M. Cledon, S. Sarma
Subsurface Geochemistry for
Energy & the Environment
Mineral Reactions in Subsurface
Energy and Waste Operations
Sponsored by GEOC, Co-sponsored by ENVR
Development of More Efficient
Pesticide Exposure Screening
Informed by Fate, Usage, and
Monitoring Data
Sponsored by AGRO, Co-sponsored by ENVR
Chemical Processes Involving
Atmospherically Relevant Trace
Gases, Aerosols & Clouds
Sponsored by PHSys, Co-sponsored by ENVR
Computational Toxicology: From QSAR
Models to Adverse Outcome Pathways
Sponsored by CNIF, Co-sponsored by
AGRO, COMP, ENVR and MEDI
 Degradation of Halogenated
Compounds in the Environment
Sponsored by AGRO, Co-sponsored by ENVR
Recent Advances in the Analysis
of Environmental Contaminants in
Feeds and Foods
Sponsored by AGRO, Co-sponsored by
ANLY and ENVR
Formulation Technologies for
Improved Crop Protection
Sponsored by AGRO, Co-sponsored by
ENVR and ORGN
WEDNESDAY EVENING
Section A
Boston Convention & Exhibition Center
Hall C
Advanced Materials and Technologies
for Desalination and Wastewater Reuse
Finan specifiedally supported by AEEC (Association of
Environmental Engineering and Science Professors)
J. Kim, Q. Li, Organizers
6:00 - 8:00
ENVR 412. Preparation of hydroxide
removal from brackish groundwater
by single-pass capacitive deioniza-
tion. W. Tung, P. Kovalsky, D. Waite
ENVR 413. Characterization of fouling poten-
tial through the use of fluorescent tech-
niques. L. Strahs, J. VanBriesen, K.L. Jones
ENVR 414. Aqueous synthesis of
polyvinyl alcohol-aldinate-mont-
morillonite nanocomposite parti-
cles for application in wastewater
purification. M. Bee, E. Kalivas,
J.C. Schwabacher, M.R. Hartings, D. Fox
ENVR 415. Adsorption of metal ions by mag-
netic carbon tubs. C. Chang, B. Wang
Section A
Boston Convention & Exhibition Center
Hall C
Advances in Chemistry for Carbon
Capture, Utilization and Sequestration
Sponsored by ENFL
P. Fennell, N. Florin, Organizers
M. Zhao, Organizer, Presiding
6:00 - 8:00
ENVR 416. Synthesis of a porphyrin
polymer with benzimidazole link-
ages for CO2 capture. V. Neti
ENVR 417. CPO-27-Ni incorporated
in nickel foam for efficient CO2
capture. Z. Liu, W. Han, K.L. Young
ENVR 418. Study of sorption kinetics of CO2,
CH4, and N2 on an organic molecular porous material (sacrificial)[EN]. J. Lee,
B. Min, H. Kim, Y. Park, D. Chun, J. Moon
ENVR 419. CO2 and H2S mixed gas
absorption in mixed aqueous solu-
tions of sulfone 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 antibiot-
ics and endocrine disrupting compounds
from aqueous solution by carbon
nanomaterials. X. Li, S. Chen, X. Quan
ENVR 421. On THM formation in direct elec-
trochemical drinking water disinfection.
M.E. Bergmann, J. Hartmann, T. Lourchouk
ENVR 422. Revealing the mecha-
nism and kinetics of UV-254 nm/ 
H2O2-based degradation of active
sunscreen ingredient PBSA.
W. Abdulrahim, X. Ho, D.D. Dionysios
Section A
Boston Convention & Exhibition Center
Hall C
Anaerobic Sewage Treatment: Dissolved
Methane and Nitrogen Control
P. Joohaon, H. Lee, G. Wells, Organizers
6:00 - 8:00
ENVR 423. Anaerobic digestion of
renovable materials for biogas
production: Experimental stage
G. O. Addelu
ENVR 424. Improved stability of meth-
ane-producing anaerobic biological reac-
tors through novel use of ion-exchange
fibers. Y. Tian, D. Brown, A. SenKupla
ENVR 425. Tale of two cities (Boston
and Detroit). S. Simopolous, J. Welch,
C. Darrash, S. McDailon, G. Dougherty
Section A
Boston Convention & Exhibition Center
Hall C
Assessing Transformation
Products by Non-Target and
Targeted Screening: The
New Frontier in Environmental
Chemistry and Engineering
Finanly supported by AEEC (Association of
Environmental Engineering and Science Professors)
S. A: Snyder, J. Drews, T. Letzlet, Organizer
6:00 - 8:00
ENVR 426. Withdrawn
ENVR 427. Suspected-target screening strategy to investigate degradation
by ozonation or photolysis of urban
micropolitants in wastewaters. A. Tado,
B. Mathon, J. Choubet, J. Chovelon,
M. Coquery, C. Mege, T. Brezowskiz
ENVR 428. Widening the analytical perspective – polarid extended
separations for the detection of trace
organic compounds in environmental
samples. B. Biber, J. Drews, T. Letzlet
ENVR 429. Biofiltration: An advanced
treatment process for removal of
EDCs and PPCPs. Z. Zhang, S. Gugno,
L.B. Aks, J.E. Dykaan, R.P. Raczko
ENVR 430. Characterization and determina-
tion 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
eficiency during algae-mediated transfor-
mation of estrogens and other emerging
chemicals. Y. Zhang, K. Girimes, L.M. Golosi
ENVR 432. Fate of six neonicotinoids during
full-scale wastewater treatment and
passage through an engineered wetland.
A. Sadana, 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 GE, ENFL, ORNL, and PNNL
K. Rajeshwar, V.I. Veliv, Organizers
6:00 - 8:00
ENVR 443, Glucose entrapped in titania under mild environmental conditions. Z. Yu, P. Huang, X. Wang

Section A
Boston Convention & Exhibition Center
Hall C

Emerging Electrochemical Water Remediation Technologies: A Symposium in Honor of Professor Enric Brillas and Professor Mehran A. Oturan
Cosponsored by AGRO
F. A. Monterrubio, I. S. Sardonil, V. K. Sharma, Organizers
6:00 - 8:00
ENVR 445, Degradation of anthyper- sensitive drug hydrochlorothiazide in water: electro-oxidation with BDD: Application of method to pharmaceuticals tablets. R. Salazar, N. Contreras
ENVR 446, Electrochemical degrada- tion of the anthyper-sensitive losar- tan in neutral aqueous medium by electro-oxidation with BDD electrode. C.A. Salazar, N. Contreras, H.D. Marolla, J. Yanez, R. Salazar
ENVR 447, Withdrawn.
ENVR 448, Electrochemical treatment of petrochemical industry effluent using TiO\textsubscript{2}O\textsubscript{3}-TaO\textsubscript{2} and BDD. S. Souza Leitao Castro, D. Ribeiro da Silva, C. Martinez-Huitle
ENVR 450, Electrolysis enhanced activated carbon catalyzing peroxymonosulfate for the degradation of Acid Orange 7 in simulated water at ambient temperature. J. Li, L. Yang, M. Chen, H. Zhang
ENVR 452, Electrochemical and photoelectrochemical dechlorination of tetracyclines and quinolones on Ti/TiO\textsubscript{2} electrode. P. Moreira, P. Koina, C. Borris

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 454, Graphene as passive sampler material for PFCs/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 concentration in environmental waters. L. Liu, J.M. Pettibone, M.R. Winchester, V.A. Hackley
ENVR 456, Effects of ultra-violet light on silver nanoparticle mobility and dissolu- tion. A. Mittman, J. Fortner, K.D. Pannel
ENVR 457, Shape-controlled synthe- siS of CuO/ZnO composites and their photocatalytic performance. L. Tan, J. Li, M. Yang, H. Gao

ENVR 458, Cu\textsubscript{x} transformation(s) in water: Elucidating and connecting critical oxidation/ reduction pathway and products. J. Wu
ENVR 459, Quantum dot dissolution kinetics monitored with SEC-ICP-MS. P. Maruyama, A. Larose-Cassan, C. Martinez-Huitle
ENVR 460, Monitoring the environ- mental effects of CeO\textsubscript{2} and ZnO nanoparticles through the life cycle of Daphnia pulex and cucumber (Cucumis sativus) plants. L. Zhao, Y. Sun, J.L. Garda-Toresde, J.R. Peralta-Vide, J. Hernandez-Vezcas, J. Hong, S. Malamud, A. Servin, M. Duarte-Garande
ENVR 461, Effects of nano- and microscale microplastics on the transformation and Daphnia bioaccumulation of phenan- threne in fresh water. Y. Ma, P. J.

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. Sakho, I. Irgibayova
ENVR 463, Study of the redox and properties of NOM with different origin and pre-treatments. S. Orsetti, E. Subitanga, 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 technolo- gies. Y. Kim, H. Kwon, J. Kim, S. Choi
ENVR 466, Effect of pH on the activa- tion 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 TiO\textsubscript{2}, on rotating corrugated aluminum drum. R. Baustia, W. Anderson, S. Paspuyon
ENVR 468, Dissolved organic matter mediated photolysis of 17-ethylyl- estradiol. M.M. Freiberg, S.N. Eiselt
ENVR 469, Changes in redox properties of humic acid upon sorption to alumina. S. Orsetti, E. Subitanga, 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 473, Solubility and kinetic studies on the adsorption of humic acid fractions onto clay miner- als. M. Khalaf, M. Elsayed, J. Fortner, K.D. Pennell
ENVR 474, Lead extraction from wastewater streams using dithi- ylphosphatoethyl functionalized mesoporous silica. G. Gunathilake, M. Hameleers, S. Huang, M. Matanaphiy\
ENVR 475, New porous MgO-ZnO sorbent to capture CO\textsubscript{2} at 473 K. J. Zha, Y. Li, Y. Wang
ENVR 476, Interaction of tetracy-cline antibiotics with nanocar- bonics. M. Juffer, E.E. Morita
ENVR 477, Derivationization of chlorinated phenols (CPs) for their detection and analysis by Nuclear Magnetic Resonance Spectroscopy. S. Hector, C.A. Valdez
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 Enterobacter Globulus extract as an insect repellant. S. Bomkamati
ENVR 481, Non-destructive screening of collagen content in archaeologi- cal bone samples using handheld Raman spectroscopy. B.J. Vesper, M.D. Colvard, G.A. Cordell, W.J. Pesto
ENVR 482, Degradation of polychlorinated biphenyls using magnesia-carbon with Ethanol/Ethyl Lactate solvent system and its potential applications for contaminated soil. K.M. Alfaro, D.E. Richardson, C. Clausen, C. Yestrebysk
ENVR 483, Using an artificial oil platform to study the dissolution rates of various PAHs in water. T. Ang, D. Xing

ENVR 484, Solid phase extraction of naproxen in environmental samples using molecularly imprinted polymer sorbents. R. Wiss, E. Ehrlich
ENVR 485, Analysis of continuous-flow column and batch bottle microcosm perchloroethylene biodegradation treatability studies. 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. Sajew, K. Baliu, T. Dietmoson, T. Morris, K. Meadows, B.G. Loganathan
ENVR 487, Photo-enhanced biodegrada- tion of a test substance using artificial sunlight with a ready biodegrada- tion test design. S.P. McLaughlin, T. Timmons, A. Griffith, K. Makkinai
ENVR 488, Triumpheta semilimbata mucilage a promising natural floculant for wastewater treatment. L.G. Romero, A. Aroya, J. Valverde, J. Jimenez, P. Rojas, A. Acuña
ENVR 490, Effects of environmental contam- inants on the weathering of stone cultural properties in South Korea. J. Jung, M. Jung, B. Shorn, K. Yoo, Y. Phee, H. Lim
ENVR 491, Evaluating the operation of an enhanced aeration system for conducting vapor pressure measurements on volatile organic compounds (VOCs). S. Abernathy
ENVR 492, New technique for pph level mercury on seawater. J.N. Driscoll, J.L. MacEachen
ENVR 493, Emissions changes of nitrous oxide from soil native shrub forest in Brazil shifted to urban plantation. C. Witches, T. Tavares, S. Oliva, D. Vasconcellos, C. Carvalho
ENVR 494, Illicit drugs in the air of three Northern European cities. A. Szymanska, C. Barlow, K.N. J. Rejki, C. Johansson, D.C. Green, P. Pantelides
Section A

Boston Convention & Exhibition Center

Hall C

Green Chemistry and the Environment

Co-sponsored by YCC

A. M. Balu, R. Luque, S. O. Obare, Organizers

6:00 - 8:00


818. 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

819. Crystallographic determination of Mn2+-exchanged site in zeolite Y (FAU; Si/Al = 1.56). D. Moon, S. Seo, J. Seo, H. Lee, H. Kim, C. Lee, W. Lim


821. Investigation of the thermal behavior of magnesium ammonium phosphate hexahydrate. M.V. Ramlogan, A. Rouff

822. Assessing quality of herbal medicines contaminated by heavy metals. F. Hassanei-Sadi

823. 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

824. Sustainable and hydrolysis- free dyeing process for polyacrylic acid using nonaqueous medium. S. Xu, J. Chen, B. Wang, Y. Yang


Section A

Boston Convention & Exhibition Center

Hall C

Heterogeneous Catalysis for Environmental Applications

Co-sponsored by CATL

S. Zhao, A. Oroz, A. Savara, Organizer

6:00 - 8:00

826. Withdrawn.

827. Application of Fe2O3 activated persulfate oxidation for the degrada- tion of PM2.5 in sediments. C. Hung, C. Chen, C. Chen, J. Huan, C. Dong

828. Heterogeneous catalytic conversion of biomass-derived vici- diols to epoxides. Y. Kim, B. Baek, C. Song, Y. Yun, D. Wu, Y. Kim, J. Han, J. Yi

829. 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

Co-sponsored by AGRO

Finacially supported by AEESP (Association of Environmental Engineering and Science Professors)

S. Chang, J. A. Libra, C. Cornella, K. Ro, Organizers

6:00 - 8:00

830. Withdrawn.


832. 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

Co-sponsored by Boston University, Division of Materials Science & Engineering

J. L. Goldfarb, K. Doudr, K. D. Hirstovski, Organizer

6:00 - 8:00

833. Aerogel catalysts for direct remediation of NH4+ malodor in air. H. Chen, W. Han, Z. Liu, K.L. Yeung

834. Nanometal oxides as potential remediating materials in remediating heavy metals in water samples. M. Qiu, E.E. Molja

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

Co-sponsored 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

835. Desemorphination of perflu- rooctanoic acid by palladium doped nanoscale zerovalent iron conjugated with persulfate and peroxy- monosulfate. W.A. Lawal, H. Choi


838. Comparative study on the catalytic degradation of paracetamol by Pt2+TiO2 and TiO2, induced advanced oxidation processes. A. Ziyian Yavas


840. Oxidation of three selected emerging contaminants by persul- fate coupled with UV irradiation. J. Benitez, F. Real, J. Acero, F. Casas

841. Evaluation of sensitizing effect of methyl red in the photo- catalytic degradation of diclofenac under natural sunlight. J. Diaz-Angulo, M. Mueses, F. Machuca-Martinez


845. Degradation of commercial drugs with a solar flat plate reactor by means of supported TiO2 - based photocatalyst. J.A. Colina-Marquez, F. Machuca-Martinez, M.A. Mueses


849. Enhanced degradation rate of emerging contaminants using luminent materials promoted visible light active photocatalyst. D. Sacco, D. Samnno, V. Vaiano, P. Ciaramboli


853. Comparative study for the removal and destruction of penta- chloro phenol using activated magne- sium treatment systems. A. Garbou, PM. Cole, C. Clausen, C. Yeobstal


855. Occurrence of glyphosate in agricultural farm drainage waters. B.G. Loganathan, P. Yerrani, 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. Masharie, L. Royer, Organizers
6:00 - 8:00
ENVR 556. Sulfamethazine adsorption isotherms and kinetics with hyper-crosslinked polymer MN250 at varying ionic strengths. M. E. Grippett
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 AESSP (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. Renow
ENVR 560. Screening the effects of lignin 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 AESSP (Association of Environmental Engineering and Science Professors)
B. P. Chaplin, D. Jassby, Organizers
6:00 - 8:00
ENVR 561. Ratiometric Culli® sensor: Design and synthesis of a Zn(II)-chelator to minimize interference with Culli® 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 AESSP (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 biomagnification. A. Joyce, R.M. Burgess

7:00 - 8:00
ENVR 564. Non-granular graphic carbon passive samplers. P. Benedetti, E. Guerrieri, C. Cresceni
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
Trenton 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. Zhdamar, V. Belosludkov, V. Kawaize
8:20
ENVR 567. Withdrawn.
8:40
ENVR 568. Analysis of nitroamines in amine-based CO2 capture. M. Combs, J. Thompson, K. Liu
9:00
9:20
9:40 Intermission.
9:55
ENVR 571. CO2 capture using metal hydroxide-biochar nano-composites. A. Creamer, B. Gao
10:15
10:35
ENVR 573. Minimizing nitroamine 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. Valleurin
11:15

Section C
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 AESSP (Association of Environmental Engineering and Science Professors)
T. H. Boyer, C. Huang, Organizers, Presiding
8:00 Introductory Remarks.
8:05
8:30
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
10:35
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. Lasere-Casanova, Organizers
B. Lau, W. Yan, Organizers, Presiding
8:00 Introductory Remarks.
8:05
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.
10:05
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
11:40

Section D
Boston Park Plaza Hotel and Towers
Tremont Room
Contaminant Elimination in Waste Streams of Increasing Concern
Financially supported by AGRO
F. H. Quina, J. Byun, H.A. Patel, D. Thirion, Organizers
9:40
ENVR 589. Detection and quantification of engineered metal nanoparticles in municipal wastewater and biosolids. M. Maddi, F. Piccapietra, N. Tufenkji, S. Ghosal
11:25
ENVR 590. Particles and VOC emissions properties from recent gasoline DI and DFI diesel vehicles. H. Yamada, S. Inomata, H. Tani moto
11:45
ENVR 591. 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. Oturana
Photo-Assisted Processes
Cosponsored by AGRO
F. A. Monterrubio, I. S. Sardonil, V. K. Sharma, Organizers
M. A. Oturan, H. Zhang, Presiding
8:00 Environ.
8:20
8:40
ENVR 593. Copper recovery combined with electrochemical reduction in a photoelectrochemical device. G. He, L. Hu, W. Pan, Y. Hou
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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. Streliau, J.A. Sohli, W. Arnold, R. Penn
2:20 GEOC 10. Iron Keggin-ion as a prenucleation cluster to fencyr-
drite. M.D. Nyman, O. Sardeghi
2:20 GEOC 11. Orientational ordering of car-
bonates lead to superstructure in vaterite: Modeling and experiment. J. Wang
2:50 GEOC 12. Understanding the con-
nection between composition, structure, and reactivity in amorphous precur-
3:20 Intermission.

MONDAY EVENING
Section A
Boston Convention & Exhibition Center
Hall C
Sci-Mix
Y. Jun, Organizer
8:00 - 10:00
GEOC 17. Fecal steroids and the 15th-century demise of Norse Vikings. T.J. Barraso, G. de Wet, L. Castafieda, R.S. Bradley
GEOC 18. Debris plastics are sources of chemical contaminations in coast and open sea. K. Saido, B. Kwon, S. Chung, A. Okabe, K. Koizumi, K. Kogure, N. Ogawa, D.M. Kari
GEOC 19. Comparing the solubility products of layered MeII(II)-Al(III)-
hydroxides based on sorption studies with NiII, ZnII, CoII, FeII, and MnII. L. Bhattacharya, E. Ezinge
GEOC 20. Role of pH and ionic strength in the structure and morphology of smec-
tite-natural organic matter composite materials. H. Aergsberg, B. Ferguson, R.J. Kirkpatrick, B. Areu, G.M. Bowers
GEOC 21. Impacts of sulfuric acid on chemical speciation of arsenic(III) and copper(II) bound to layer-structured minerals. S.P. Hyun, H. Moon, K. Kwon

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. D. Duckworth
8:00 GEOC 34. Molecular-level interactions of organic ligands with iron oxide mineral/ water interfaces studied using sum frequency generation (SFG). A.L. Mittin
9:00 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 competi-
tions at small molecule - mineral inter-
facces. D. Wu, X. Guo, H. Sun, A. Navotzky
10:00 Intermission.
10:20 GEOC 37. U(VI) and Sr(II) seque-
stration in aqueous minerals. The importance of confined pore spaces. D. Singer, H. Guo, J.A. Davis
10:50 GEOC 38. Metal reactivity in aban-
donned uranium mine waters. J.M. Cerrato, T. Zanmato, J. Blake, A. Al, A. Breney, K. Atyushkova, M. Spilde, J. Lezdec-Pachec
11:40 GEOC 40. Spectroscopic evidence for Cr3+/Fe3+ electron transfer at clay mineral edge and basal sites. M. Bishop, H. Dong, M. Penetrak, 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
Cospresented by ENVR
Y. Jun, C.A. Peters, Organizers, Presiding
1:30 Introductory Remarks.
2:55 GEOC 43. What if? Evaluating geochemical changes to shallow ground water under simulated carbon dioxide leakage conditions. A. Stitchler, J. McGuy, A. Wunsch
3:35 Intermission.
3:55 GEOC 44. Rare earth element geochemistry of kerogen samples from the Orange Basin. A. Karamalidis, A. Fatemi, J. Wilson
Sponsored by NUGL, Cospresented by GEOC
5:10 GEOC 48. Molecular-scale behavior at organo-mineral interfaces under supercritical CO2 and brine conditions: Implications for geologic carbon sequestration in carbonate reservoirs. S. Wang, T. Tokunaga, J. Wan
5:30 GEOC 49. Geochemical alter-
ations of carbonate fractures. H. Deng, J.P. Fitts, C.A. Peters
6:10 GEOC 50. Probing particle-based crystal growth via dynamic force spectroscopy. X. Zhang, J. Liu, K.M. Rosso, J.D. De Voreto, M.H. Engelhard, T.C. Droubay, M. Bowden
10:10 Intermission.
10:30 GEOC 51. Effects of sulfate and phosphate on scCO2 saturated brine bi-
obile interactions: Wettability changes under geologic CO2 sequestration (GEOC) & the Enviro21, 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
11:30 GEOC 53. Geochemical alter-
ations of carbonate fractures. H. Deng, J.P. Fitts, C.A. Peters

WEDNESDAY AFTERNOON
Section A
Seaport Hotel and World Trade Center
Beacon Hill 1
Subsurface Geochemistry for Energy & the Environment
Radionuclides in the Environment
Cospresented by ENVR
Y. Jun, Organizer
C. A. Peters, Organizer, Presiding
H. Deng, Presiding
1:30 GEOC 55. Evaluating the effects of seal/freeze fluid productions on re-
duced water chemistry and seal formation permeability. A. Hakala, C. Loredo, A. Paulant, V. Marion, C. Joseph, P. Schueumann, S.W. Hedges, G. Guthrie
2:10 GEOC 56. Contaminant mobilization from seal during hydrofrack-
ing 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. Akinbar, S. Sultana
3:30 Intermission.
3:50 GEOC 58. Pyrite-hydraulic fractur-
ing fluid interaction: Hydrolysis and catalysis of azomet. N. Consolazio, G. Lowry, A. Karamalidis
4:10 GEOC 59. Carbonation of wollastonite in a shale matrix. Z. Tao, J.P. Fitts, A. Claren
4:30 GEOC 60. Characterization of con-
centrated shale gas produced water treated with different water treatment technologies. E. Jang, E. Chung
4:50 GEOC 61. Two modes of iodine release from iodine-apatite in aqueous solution: Diffusion and dissolution. Z. Zhang, J. Wang
THURSDAY MORNING

Section A
Seaport Hotel and World Trade Center
Beacon Hill 1

General Geochemistry Session
Y. Jun, Organizer, Presiding
8:30 GECO 63. Biological redox cycling of iron in nontronite and its potential application in nitrate removal. L. Zhao, H. Dong, R. Kukkadapu
8:50 GECO 64. Reduction of hexavalent chromium and (CobaltII)-EDTA by thermophilic methanogen Methanothermobacter thermautotrophicus. R. Singh, H. Dong, D. Liu, L. Zhao, A. Marts, E. Fanquer, D. Tieney, C. Almquist, B. Briggs
9:40 Intermission.
10:00 GECO 66. Variations of soil n-alkanes 8D and glycol dialkyl glycerol tetraethers (GDGTs) distributions along an altitudinal transect from southwest China. C. Wang, M.T. Hton, G. Hoke, C. Gazonne, J. Liu
10:20 GECO 67. Model study of the feedbacks between lightning activity and atmospheric temperature and composition changes. L. Kolesnees
11:00 GECO 69. Variation of anion concentration in aerosol at Mt. Kinabalu, Sabah, Malaysia. H. Katsura
11:20 GECO 70. Spatial assessment of soil contamination from informal E-waste recycling site in Agbogbloshie, 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.

MONDAY MORNING

8:55 GECO 72. Radium adsorption to iron bearing minerals in variable salinity waters. M.A. Chen, B.D. Kocar
9:15 GECO 73. Aquiferal sulfide decreases transport of ferrihydrite colloids in anoxic porous media due to production of elemental sulfur. P. Liao, S. Yuan
9:55 Intermission.
11:15 GECO 78. Terrestrial carbon sequestration depends on Ca biogeochemistry and forest growth. W.C. Shortle, K.T. Smith
11:35 Concluding Remarks

MONDAY EVENING

Section A
Boston Convention & Exhibition Center
Hall C

Sci-Mix
S. C. Rasmussen, Organizer
8:00 - 10:00

HIST 17. Aspirin: Incorporating the history of chemistry in the community college classroom. G. Perkins

TUESDAY MORNING

50th Years of Innovation: The Legacy of the Westheimer Report

50 years of Innovation: The Legacy of the Westheimer Report

Henry A. Hill Centennial Symposium: Innovation in Polymer Science

Section A
Boston Convention & Exhibition Center
Room 50

HIST Award Symposium
Honoring Christoph Meinel
G. D. Patterson, Organizer
A. J. Rocke, Organizer, Presiding
1:00 HIST 19. Quiet revolution revisited: Theory vs. practice in nineteenth-century German chemistry. A.J. Rocke
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 Delacre (1862-1938). B. van Tiggeleen
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

Division of the History of Chemistry
S. Rasmussen, Program Chair

OTHER SYMPOSIUM 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

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. Rabinch
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, 1853 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
4:15 HIST 15. Early history of polyimide: 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

TUESDAY AFTERNOON

Section A
Boston Convention & Exhibition Center
Room 50

HIST Award Symposium
Honoring Christoph Meinel
G. D. Patterson, Organizer
A. J. Rocke, Organizer, Presiding
1:00 HIST 19. Quiet revolution revisited: Theory vs. practice in nineteenth-century German chemistry. A.J. Rocke
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Henry A. Hill Centennial Symposium: Innovation in Polymer Science
Sponsored by POLY, Cosponsored by HIST, PMSE, PRES and PROF

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

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Section B
Renaissance Boston Waterfront
Pacific Bllm 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 TALSPEAK 9. Investigation of CF terolomers in response to changing regulations, from molecules to application. J.M. Smith
8:55 TALSPEAK 10. Molecular recognition, bioseparations, screening, and diagnostics; A career in L.R. Willson
9:15 TALSPEAK 11. Effect of promoter type and amount on Fischer-Tropsch synthesis using iron catalysts on carbon supports. D. Dadyburj
9:55 Intermission.
10:10 TALSPEAK 13. Spectroelectrochemical sensor for technetium applicable to Hanford and other DOE sites. S.A. Bryan
10:30 TALSPEAK 14. On the road to a new large-scale sweet sorghum industry in rural America. G. Eggerton
10:50 TALSPEAK 15. Broadening the graduate student experiences — research internships with national laboratories and industry. P.K. Dorhout
11:10 TALSPEAK 16. Entrepreneurship, scientific outreach, and responsibility: It all works together. B.J. Steusand
11:30 TALSPEAK 17. ACS, career, and diversity. N.E. Jackson
11:50 Concluding Remarks.

SUNDAY AFTERNOON
Section A
Renaissance Boston Waterfront
Pacific Bllm 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 TALSPEAK 1. My time with Professor Nash: Reflections of a junior scientist. J. Braley
8:30 TALSPEAK 2. Game of second chances: A decade’s worth of separations. P.R. Zalupski
9:50 Intermission.
10:35 TALSPEAK 6. Studies of the protonation and complexation with Ln(III) of 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 TALSPEAK 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 TALSPEAK 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 Bllm C
Industrial & Engineering Fellow: Symposium in Honor of Henry G. (Hank) Foley
M. Strano, Organizer, Presiding
1:00 Introductory Remarks.
1:05 TALSPEAK 26. From nanoporous carbon membranes to carbon nanotubes and monolayer graphene barriers. M. Strano
1:45 TALSPEAK 28. In celebration of nice guys. M. Acharya
2:05 TALSPEAK 29. Clean green energy from coal via biotechnology. P. Dhurjati
2:25 TALSPEAK 30. Catalysis — an indispensable tool. S. Sengupta
2:45 Intermission.
3:00 TALSPEAK 31. Carbon molecule sieve membranes: Enabling large scale energy efficient separations. W. Koros
3:40 TALSPEAK 33. New approaches to developing high performance ultrafiltration membranes. A.L. Zydney
4:00 TALSPEAK 34. Ionic liquids from phase behavior to applications. M.B. Shiflett
4:20 TALSPEAK 35. Membrane fouling due to chemically-driven transport. D. Velegoll
4:40 Concluding Remarks.

MONDAY MORNING
Section A
Renaissance Boston Waterfront
Pacific Bllm D
Industrial & Engineering Fellow: Symposium in Honor of Gary M. Seabold
E. Frank, Organizer, Presiding
1:00 Introductory Remarks.
1:10 TALSPEAK 43. Industrial applications of polymer self assembly and association. J. Klier
1:50 TALSPEAK 44. Kinetic study of Pd-catalyzed hydrogenation of N-benzyl-4-fluorophenol. A. Varma, H. Huong
2:30 TALSPEAK 45. Surface characterization of alpha alumina catalyst carriers. D. Gough, N. Wickramaratne, P. Nguyen
3:10 TALSPEAK 46. 2015 American Chemical Society Industrial and Engineering Chemistry Division Applied Chemical Technology Fellow Award presentation. G.M. Seabold
3:50 Concluding Remarks.

Section B
Renaissance Boston Waterfront
Pacific Bllm C
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 TALSPEAK 36. Novel supported complexants for uranyl recovery from acidic solutions. S. Alexandratos, X. Zhu
9:45 Intermission.
10:05 TALSPEAK 39. Withdrawn.
10:30 TALSPEAK 40. Recent results of development and demonstration of the sodium bimuthate process for the oxidation and separation of americium from the lanthanides in engineering-scale equipment. J. Law, B.J. Mincher, R. Tilton, T. Nann, N. Schmitt
11:30 TALSPEAK 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, COL, IEC, IAM, IVES, and PROF
Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits
Sponsored by OHCED, Cosponsored by BRIC, CEI, ENVR, IEC, MED, PROF, SCHB and YCC

MONDAY AFTERNOON
Section A
Renaissance Boston Waterfront
Pacific Bllm D
Industrial & Engineering Fellow: Symposium in Honor of Gary M. Seabold
E. Frank, Organizer, Presiding
1:00 Introductory Remarks.
1:10 TALSPEAK 43. Industrial applications of polymer self assembly and association. J. Klier
1:50 TALSPEAK 44. Kinetic study of Pd-catalyzed hydrogenation of N-benzyl-4-fluorophenol. A. Varma, H. Huong
2:30 TALSPEAK 45. Surface characterization of alpha alumina catalyst carriers. D. Gough, N. Wickramaratne, P. Nguyen
3:10 TALSPEAK 46. 2015 American Chemical Society Industrial and Engineering Chemistry Division Applied Chemical Technology Fellow Award presentation. G.M. Seabold
3:50 Concluding Remarks.

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**TUESDAY MORNING**

**Section A**
Renaissance Boston Waterfront
Pacific Blrm D

**Industrial and Engineering Chemistry Division Graduate Student Award Symposium**
P. Savage, Organizer

8:00 - 10:00

**Monday Evening**

**TUESDAY AFTERNOON**

**Section A**
Renaissance Boston Waterfront
Pacific Blrm D

**Green Chemistry Makes a Difference: Pharmaceutical Industry/Academic Collaborations**
M. E. Kopach, Organizer, Presiding

10:00 I&EC 54. Continuous flow multistep synthesis. T.F. Jamison

1:00 I&EC 55. Grignard reaction past, present and future: Development of greener more sustainable processes. M.E. Kopach, T. Braden, M.D. Johnon, 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


**Starting-Up & Spinning-Out: Commercializing Innovative Chemistry**

Organizer: M. E. Kopach, Organizer, Presiding

3:00 - 6:00

8:15 I&EC 47. Amidine-modified mesoporous silica for uranium adsorption under seawater conditions. G. Gunathilake, M. Jaroniec, J. Garka, S. Dai

8:55 I&EC 48. Multiphase reaction studies in stirred tank and trickle-bed reactors. S. Lee, A. Varna


9:35 I&EC 50. Vapor phase ethanol carbonylation over supported Rh based catalysts. S. Yacob, S. Park, B.A. Kiös, D.G. Barton, J.M. Nottenstein

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 adsorbent for biologics purification. J. Wang, S.M. Husson

10:45 I&EC 53. Mechanistic insights into the electrochemical reduction of CO, CO on nanostructured Ag surfaces. J. Rosen, T. Jiao

11:05 Closing Remarks.

**Starting-Up & Spinning-Out: Commercializing Innovative Chemistry**

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

8:00 - 10:00

8:00 I&EC 60. Withdrawn.

8:00 I&EC 61. Removal of synthetic dye acid 186 from water by activated carbon. A.M. Turkay

8:15 I&EC 62. Comparative analysis of depen- dence of etching conditions (solution concentration, temperature and time) of track-etched membranes on ion beam fluence. D. Orazbayeva, Y. Koshman

8:30 I&EC 63. Investigation on the physicochemical properties of poplar lignin carbon precursors before and after melt rheology. G. Sun, A.J. Ragauskas

8:45 I&EC 64. Synthesis and characterization of CMc/Te-Eu nanocomposites with photoluminescence. W. Liang, J. Ye, J. Xiong

8:50 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

9:00 I&EC 66. Activity coefficients of RbF in urea -water and forma- mide-water mixtures. M. Hu

9:15 I&EC 67. Size dependence of optical properties of gold nanoparticle. H. Dong, J. Liu, J. Zhao, Y. Song


9:45 I&EC 69. Simulation of drilling pressure profile in directional drilling and user program development. W. Panichp, B. Prupark, K. Samanord

9:50 I&EC 70. Study on removal of nickel ions in the mint wastewater during coagulation enhanced by pre-oxi- dation and pH adjustment. W. Gun, W. Tan, X. He, Z. Yang, S. Chen, B. Chai

10:05 I&EC 71. Effective radiative cooling and optimized heat dissipation for high power electronic devices. T. Helao, T.N. Eyassu, C. Lin

10:20 I&EC 72. Bioinspired ultrathin polyamide coating skin layer on PDMS for enhanced hydrocarbon gas recovery. M. Fang, J. Li

10:30 I&EC 73. CFD modeling for fluid flow and mass transfer in spacer-filled cham- bers for pervaporation. T. Wang, J. Li

10:45 I&EC 74. Pervaporation performance of Octavinyl-POLS cross-linked PDMS membranes for ethanol-water separation. X. Zhan, S. Ma, Y. Xia

11:00 I&EC 75. Pervaporation performance of cycloexatin filled PDMS membranes for ethanol recovery from aqueous solution. X. Zhan, S. Ma, Y. Xia

11:15 I&EC 76. New computer controlled platforms for discovery and self-opti- mization bespoke flow systems. L. Porwol, A. Henson, V. Sans, L. Cronin

11:30 I&EC 77. Modularity and automation of multistep reactions combining 3D printing technology with continuous flow processes. V. Dragne, P. Kitson, V. Sans, L. Cronin


12:00 I&EC 79. High performance membranes for organic solvent nanofiltration via surface modification of P84® substrate followed by cross-linking. X. Li, J. Li


12:30 I&EC 81. Distillate flux enhancement in direct contact membrane distillation modules with inserting carbon-fi- ber spacers under countercur- rent-flow operations. G. Ho, P. Lin


13:10 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, G. Xu

13:25 I&EC 85. Modeling and NMR spec- tronoscopy tools for understanding coalescence efficiency and partitioning in polymer latexes for coatings applications. S. Arumugam, K. Bashah, J. Sparks, S. Antar, B. Rowe, J.R. El


14:00 I&EC 87. Withdrawn.

14:45 Intermission.

**Wednesday Morning**

**Section A**
Renaissance Boston Waterfront
Pacific Blrm H

**General Papers**
P. M. Smith, Organizer

J.A. Ritter, Presiding


8:50 I&EC 87. Analyzing refractory unit kinetic models by reaction network visualization. S. He, Z. Hou, C. Bennett, S.R. Horton, M.T. Klein, Q. Shi, S. Zhao


9:30 I&EC 89. Potassium fertilizers from ultraplasticsyntes. D. Ciceri, C.G. Estrada, T. Skorina, A. Allanone

9:50 Intermission.

10:05 I&EC 90. Comparison of boron fixation on different resins. H.T. Nguyen


10:45 I&EC 92. Developing workflows for continuous crystallisation processes within the pharmaceutical industry. T. McElone, A.J. Florence


**Big Chemistry from Small Businesses**

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

**International Symposium on Mesoporous Zeolites**

Sponsored by EUNL, Cosponsored by CATL, I&EC and NOR

**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. Perovskite membrane for the efficient recovery of ionic liquid from mixed lignocellulosic feedstock processing. J. Sun, S. Shi, T. Dutta, B.A. Simmons, S. Singh


2:00 I&EC 97. Methane oxidation on iron-based oxygen carrier with chemical looping redox reaction. L. Qin, Z. Cheng, J. Fan, M. Guo, D. Xu, B. Kopechek, N. Deshpande, L. Fan

2:20 I&EC 98. Withdrawn.

2:40 Intermission.
INOR Division of Inorganic Chemistry
N. Radu and S. Koch, Program Chairs

OTHER SYMPOSSA 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 pyrone and isodione-based BF2, fluorophores. C.J. Ziegler, L. Crandall, I. Tamgho
9:20 INOR 2. Polyporphosphazenes: Polymeric organophosphorus compounds with luminescent properties. J. Gaffet, 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 n system. T. Kupfer, H. Braunschweig
11:10 INOR 7. Stabilization of reactive main group species by coordination to carboxyl-,carboxylated carbones. T.W. Hudnall, A. Leidt, K.M. Mealancon, A.J. Torres
12:10 INOR 10. Pyridyl-functionalized 3H-1,2,3,4-triazaphospholes: Synthesis, coordination chemistry, and application in homogeneous catalysis. J. Skior, C. Mueller

Section B
Boston Convention & Exhibition Center Room 162B

Solid-State Inorganic Chemistry
C. G. Lugnar, Organizer
V. Poldavets, Organizer, Presiding
A. Choudhury, Presiding
8:30 Introductory Remarks.
8:35 INOR 23. TIs, and Ti5 layered materials: Intercalation and/or substitution to enhance the thermo-electric properties. A. Maignan
9:15 INOR 24. Magnetic anisotropy in new misfit layer compounds. S.M. Clarke, G.E. Freeman
10:15 Intermission.
11:10 INOR 29. Formation of transition metal oxides with high aspect-ratio geometry by high pressure CVD. Y. Liu, V. Gopalakrishnan, J.V. Badling

Section D
Boston Convention & Exhibition Center Room 190C

Environmental and Energy-Related Inorganic Chemistry
S. A. Koch, Organizer
F. N. Castellano, Presiding
8:20 INOR 32. Enhancements to electrocatalytic reduction of CO2 by cobalt phthalocyanine upon immobilization in polyvinylpyridine membrane. W.W. Kramer, I.M. Farrier, C.C. McKinney
8:40 INOR 33. Electrocatlytic reduction of carbon dioxide to carbon monoxide by manganese carbonyl complexes containing shenanthrene-7-ligands: Catalytic turnover even in the absence of Brønsted acids. B. Dhakal, D.A. Kurtz, R.J. Hultma, G.A. Felton
9:00 INOR 34. Stoichiometric production and delivery of chlorine to substrates. A. Stasney, A.E. Norton, J.A. Krause, W.B. Conrick
9:40 INOR 36. Photochemical upconversion beyond the molecule. F.N. Castellano
10:00 Intermission.
10:10 INOR 37. Electrocatlytic reduction of CO2 with manganese catalyst supported by pendant Brønsted-Lowry acid ligands. K. Ngo, R.P. Narayanan, B. Mahanti, B.R. Reed, S. Greysman, J.J. Routchard

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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. Pinzaru, R. Rudharia, M. Patra, S. Ferrari, G. Gasser
8:20 INOR 46. Small peptides-Re(CO) conjugates synthesis using new lysine linkage approach. K. Chanawanno, V. Kondeti, J.A. Caporoso, T. Leeper, R.S. Hertick, C.J. Ziegler
8:40 INOR 47. Lanthanide ion dependent DNAzymes: In vitro selection and metal binding studies. J. Liu, P. Huang
9:00 INOR 48. Facile synthesis and biological evaluation of metalloacenyl derivatives. J. Hess, M. Patra, A. Leonidova, V. Pinzaru, S. Ferrari, G. Gasser
9:20 INOR 49. 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 50. Rationally designed glucose-platinum(II) conjugates for actively targeting cancer cells. M. Patra, T.C. Johnstone, K. Suntharalingam, S.J. Lippard
10:00 Intermission,
10:30 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. Pluta, A. Alvarez, R. Ramos, R. Moclo, E. Castellano
10:50 INOR 51. Upconverting lipid vesicles for the red light activation of anticancer metallo drugs. S. Bonnet
11:10 INOR 52. Versatile and remarkably stable Mr-based MR imaging probe. Application to targeted thrombus imaging. E. Gale, I. Atanassova, F. Blasi, P. Caravan
11:30 INOR 53. In silico guided design and synthesis of new high reactivity Gold(III) derivatives. E. Borone, 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. Lugnar, Organizer
A. Hall, Presiding
8:00 INOR 55. Graphite-conjugated pyrazines as molecularly-tunable electrocatalysts. T. Fukushima, Y. Suenrudranath
8:20 INOR 56. Electrocatalytic CO2 reduction at ordered nanoporous metal-organic thin films. A. Hall, Y. Yoon, Y. Suenrudranath
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
9:40 INOR 60. Imparting architecture control over colloidal nanocrystal frameworks for energy storage devices. T.E. Williams, A.W. Wills, B. Heims
10:00 Intermission,
10:10 INOR 61. Experimental and theoretical investigation of LiFeO2 – tunnel: Fe2+/Fe3+ cathode for Li-ion batteries. V. Poltavets, B.J. Holliday, J.E. Vernia
10:50 INOR 63. Synthesis of mesoporous metal oxides via aerosol-assisted self-assembly pyrolysis for energy storage. M. Sheehan, M. Ruddin, C. Tsang
11:10 INOR 64. Band edge control of crystalline silicon by chemical functionalization of the surface. N.T. Pymale, A.A. Ramachandran, A.N. Lim, B.S. Brunschwig, 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. Fayed, L.I. Halalai
11:50 INOR 66. New iron-based polynuclear compounds as cathode material for rechargeable alkaline-ion batteries. H. Yaghoobnejad Asli, A. Choudhury
Section G
Boston Convention & Exhibition Center Room 160A
Coordination Chemistry: Synthesis and Characterization
D. C. Crans, Organizer
A. DeBettencourt Dias, C. Thomas, Presiding
8:50 INOR 68. Examining the interaction and redox activity of novel polynuclear iron complexes with carbohydrates: Synthetic, structure, electrochemical, and spectroscopic investigation of their interactions with monosaccharides. C.D. Stewart, H. Arman, G.T. Muse
9:30 INOR 70. Isolation and characterization of a µ1-tricarbonyl nitride in four different oxidation states. B. Lin, T. Betley
9:50 INOR 71. Synthesis and reactivity of tri-iron-III-Fe clusters. J. Liu, B. Tito, T. Betley
10:50 INOR 74. Coordination chemistry of mid-to-late first-row transition-metal complexes with tris(2-pyridyl)phosphine (PPh3) and its oxide (OPP3). K. Supra, C. Farfani, D. Bettle, N.A. Piao, W.S. Kassel
11:10 INOR 88. Class I mixed-valent dirhenium complexes. Y. Yan, T. Maque, J.P. Donahue, S. Sproules
Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control
Tutorial
Sponsored by PMSE, Cosponsored by INOR‡
SUNDAY AFTERNOON
Section A
Boston Convention & Exhibition Center Room 160B
Inorganic Young Investigator Awards
J. M. Bonnaire, Organizer, Presiding
1:30 Introductory Remarks.
1:35 INOR 78. Synthetic micro/nanomachines and their applications: Toward "Fantastic Voyage". W. Gao, J. Wang
2:05 INOR 79. Structure design of silicon anodes for high energy lithium-ion batteries. N. Liu, Y. Cui
2:35 INOR 80. Electronically doped colloidal semiconductor nanocrystals. A.M. Schimpf, D.R. Gamelin
3:05 Intermission,
3:15 INOR 81. Gas separations in metal-organic frameworks with open metal sites. D. Bloch, J.R. Long
4:05 INOR 84. Organometallic palladium complexes as chemoselective bion conjugation reagents. E.V. Vinogradova, C. Zhang, A.M. Spokony, B.L. Pantelute, 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. Burton
4:45 INOR 96. Models of the oxygen-evolving complex of photosystem II. J. Kanadz, T. Agapi
5:15 INOR 97. Efforts toward the next generation of platinum drugs: Monofunctional complexes and nanodendrimeres. 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
2:30 INOR 100. Synthetic chemical approaches to designing and understanding qubits. J. Zadrozny, M. Graham, M. Faharri, S. Costa, 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
Section C
Boston Convention & Exhibition Center Room 162B
Inorganic Catalysts
S. A. Koch, Organizer
K. A. Grice, Presiding
2:50 | INOR 108. Dehydrofluorination of 1,1,1,2,2-pentafluoro propane to produce eco-friendly refrigerant 2,3,3,3-tetrafluoropropane (HFO-1234yf) using Cr-based catalysts. S. Lim, J. Ha, H. Kim
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
3:40 | INOR 112. Hydrocarbon oxidation by bimetallic late transition metal complexes with dual active sites. C. Hes, 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
4:40 | INOR 115. Facile microwave synthesis and catalytic properties of cobalt (II) porphyrinylazin compounds. C.J. McElroy, P. Janu, S. Amoreto, P.O. Vogel

Section E
Boston Convention & Exhibition Center Room 162A
Chemistry of Materials: Metal Organic Frameworks
C. G. Lugnar, Organizer
C. Mottolo, E. Tsivion, Presiding
5:20 | INOR 134. Structural changes in metal-organic frameworks upon light induced disassembly of thin films into catalytically active complexes. A.I. Ivanov, D. Bandyopadhyay, S. Sen
2:30 | INOR 116. Short peptides self-assemble in the presence of metals to produce catalytic metalloamyloids. E.K. Yeh, K. Young
2:30 | INOR 117. Binding of nitrogenase substrates to an iron complex with sulfur and carbon ligands. I. Corp, A.M. Bronsonah, B.O. 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, T. Judd, K. Walsh, B. Levin
4:10 | INOR 121. Water oxidation by photosystem II. G.W. Brudvig
2:10 | INOR 136. Synthesis and characterization of aluminum, gallium, tin, and chromium complexes with a non-innocent bulky dimine ligand. R.A. Zarkesh, M. Anstey
2:30 | INOR 137. Fullerene functionalized phosphorus based dendrons: Building blocks for supramolecular architectures. A. Aghabali, A.L. Balch, M.M. Olmstead
3:10 | INOR 140. Imidacloprid-C coupling reactions in imidium complexes triggered by ligand methyl group deprotonation. R. Arevalo, J.A. Perez, L. Riera
3:30 | INOR 141. Hydroaminoalkylation of olefin catalyzed by silica supported metalazidine. B. Hamzaoui, J.M. Bassett
4:50 | INOR 144. Can polynuclear metal clusters behave as “extended” organometallic complexes? M. Nielsen, T. Breitman

Section F
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 ir(III)bisphosphine complexes of relevance to iron catalyzed cross-coupling. J.L. Kneebone, S.L. Daifuku, V.L. Fleischauer, J.A. Bailey, M.L. Neidig
5:10 | INOR 147. C-H bond amination mediated by high-spin iron complexes. T. Betley, M.J. Wilding, D. Ioan, A. Mikhaline
2:10 | INOR 148. Spectroscopic investigation of in situ formed phenylated iron-bisphosphines and their reactivity in iron-catalyzed cross-coupling. 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
3:10 Intermission.
4:15 | INOR 154. Iridium catalyzed base-free hydrogenation of esters and lactones. T. Brewster, N.M. Rezaeey, Z. Cukalova, M.S. Sanford, K.I. Stepuls

Transition Metal Catalyzed Olefin Polymorphism: Towards Structure Control
Technical Session
Sponsored by PMSE, Cosponsored by INOR‡
INOR

TECHNICAL PROGRAM

SUNDAY EVENING
Section A
Boston Convention & Exhibition Center
Hall C
Biocatalytic Organic Chemistry: DNA, RNA and Inorganic Drugs
S. A. Koch, Organizer
6:00 - 8:00

INOR 159. Withdrawn.

Section B
Boston Convention & Exhibition Center
Hall C
Building Innovative Solid State Materials Through Solution Chemistry
J. R. Nelson, A. J. Norquist, C. M. Oertel, Organizers
6:00 - 8:00

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. Wie, J. Buffet, D. O'Hare
INOR 167. Synthesis of metal-organic frameworks containing organophosphine linkers. R. Stemberg, C.R. Wade
INOR 168. Synthesis of single crystals and nonoligates of lead oxide carboxylates with halogenated benzolate ligands. C. Gang, V.S. Mandalia, M. Zeller, C.M. Oertel
INOR 169. Rational synthesis of dimensionally reduced TiS phases. R.A. Morasse, T. Li, Z. Baum, J.E. Goldberger
INOR 170. Ultrasonic spray synthesis as a route to shape controlled LaTaN nanoparticles. E. Rugen, S.E. Srbatalk
INOR 171. Thermodynamic investigations of actinide and lanthanide complexion: From fundamentals to applications. D. Pau, 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. Electrocatlytic reduction of carbon dioxide to formic acid by manganese carbonyl complexes containing diimines: The need for greater conjugation in the dyopyromethene vs. dipyromethene system. M.R. Wheeler, D. Bhakal, R.J. Hulme, G.A. Felton
INOR 173. Photochemistry and redox non-innocence of electron rich Re(II)-containing 8-diketone and oximinate complexes: A fundamental study toward the application of CO2 reduction. K. Ngo, B. Mananti, N. Lee, J.J. Rochtford
INOR 174. Flow synthesis of magnetic metal-organic frameworks. K. He, C. Tsai, K.L. Young
INOR 177. Recent developments for new Hg2+-fluorescent chemosensors based on 2-[(2)-aminoethyl]sulfanyl/butylsulfanyl)ethanimine. N. Watpathomsub, T. Puangsamie, S. Watpathomsub, S. Kraphoong
INOR 178. Bisimidopyridine nickel complexes as electrocatalysts for the reduction of CO2. R.P. Narayan, J.J. Rochtford
INOR 179. Highly sensitive and selective chemosensor based on cyclic fluorines for Hg2+-detection in aqueous solution. P. Piyanan, S. Watpathomsub, H. Nienamei, N. Watpathomsub
INOR 181. Electrochemistry of cyctohrom c from a cold-adapted microorganism. N. Dilchand, M.C. Buzzo, J.S. Magyar
INOR 182. Synthesis and characterization of a dimanganese Schiff-base complex as an artificial water oxidation catalyst. K. Kat, J.S. Buchwal, P.H. Driessen
INOR 183. 5Co-NMR studies of Co compounds with O-donor ligands for WOC. J. Weber, M. Yumans, L. Doerrer

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. Tabatabaee
INOR 186. Highly fluorinated high-k hybrid dielectric materials for solution-processed electronic devices. Y. Kim, J. Son, J. Lee
INOR 188. Synthesis and processing of core-shell nanoparticles with stitainless surfaces. L. Pathade, T.L. Doane, R.D. Staton, P. Lutz, M.M. Maye
INOR 189. Synthesis and characterization of hollow MnO2 nanoparticles. S. Varaprasam, C. Balasubraman, J.D. Hostetler
INOR 190. Biosorbable 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 192. Unsymmetrical pincer-type palladium complexes containing novel pyrazolyl aminophosphine ligands. C. McConnell
INOR 193. Withdrawn.
INOR 194. Functionalized triazaphospholes: Intriguing phosphorus heterocycles with many perspectives. A. Skorz, C. Mueller

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


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 CMP0 ligands for the sensitization of lanthanide luminescence. E.G. Leach, A.A. Kulesza, S.M. Bisro
INOR 201. Experimental and computational study of lanthanide-CMP0 ligand complexes. A.J. Vanderweide, R.L. Lord, S.M. Bisro
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. Bisro
INOR 203. Synthesis and characterization of dinuclear CMP0 ligands for use in the complexation and extraction of f-elements. A.R. Lear, S.M. Bisro
INOR 204. Withdrawn.

INOR 205. Synthesis, characterization, and the near-infrared luminescence properties of Nd6 and Yb6 complexes containing terpyridine derivative ligand and 3d-f type conjugated terpyridine-alkyne bridging Yb6-Co-carbonyl cluster complex. B. Zhu, Y. Liu, Y. Han
INOR 206. Effect of rotational correlation time and magnetic field strength on the relaxation of Eu(Ill)-containing complexes. C.U. Lenora, M.J. Allen
INOR 208. Carbazole-based coordination polymers of lanthanides and actinides. C.E. Bien, D.P. Manke
INOR 209. Doped hydroxysialpite nanoparticles as scaffolds for solar cells imaging. D. SantaLuzia, A. Washburn, L. Chapman, R. Tan, S. Lapi, A.L. Eckemann
INOR 210. Electronic structure and thermo-dynamic studies of actinide and lantha
dide complexion. 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. Delts Aider cycloaddi
tions catalyzed by aluminum based Lewis acids. D. Vidovic, Z. Liu
INOR 212. Building a Lewis acidic phos
dorus. D. Vidovic, M. Ray, D. Carmichael
INOR 215. Boron based nucleophilic ligands. D. Vidovic, B. Munsempandian
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 diimido-cobanne-supported terminal boron. A. Ledet, T.W. Hudnall
INOR 220. Coordination of N-heterocyclic phosphine (NHP) cations to late transition metals: NHPs as sterically and electronically tunable nitosyl analogues. M. Bezpalco, 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-Tricyanomethylphosphine derivative: Synthesis, reactivity, and coordination chemistry. M. H. Habicht, C. Müller


MONDAY MORNING

Section A
Boston Convention & Exhibition Center Room 162B

Inorganic Chemistry Lectureship
W. B. Tolman, Organizer, Presiding
8:30 Introductory Remarks.
8:35 INOR 223. Semiconductor nanocrystals: Photochemistry and technology. M.G. Bawendi
9:05 INOR 224. In situ phase transformation of colloidal nanocrystals. P. Radvanovec
10:05 Intermission.
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. Rodriguez, Organizers D. E. Freedman, Organizer, Presiding
8:30 INOR 229. New polar and magnetic comonomer - type oxides. A.S. Byer, T.J. White, P. D. Nealey, F. Blum
9:40 INOR 231. Intermission.
10:10 INOR 232. Snapshots of S-adenosylmethionine radical enzymes. C.L. Drennan

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-azoles as blue emitters for OLED solid-state lighting. G.D. Yo
10:05 INOR 239. Synthesis and reactivity of fluorinated NHC carbene complexes. R. Blaski, R.H. Grubbs
10:35 Intermission.
10:50 INOR 240. Industrial water treatment chemistry. C. Mcnins
11:50 INOR 242. Ethylene to 1-hexene: From HTE to continuous unit operations with cyclomethallated pyridyl amine chromium catalysts. S. Brown, J.F. Walzer

Section D
Boston Convention & Exhibition Center Room 160C

Metalloenzyme Mechanisms
G. Ghirlanda, I. V. Korendyych, Organizers, Presiding
9:00 INOR 244. Role of manganese in streptococcal virulence. O. Makhynets, D. Photos, A.K. Boal, J. Khrude, H. Turner, C. E. Waddell
9:30 INOR 245. De novo designed 2(4e)4-5ferroxy mimics: Manipulation of redox and ET properties. G. Ghirlanda, D.J. Sommer
10:00 Intermission.
10:40 INOR 247. Discovery of a novel bacterial nitric oxide sensor. E.M. Boom
11:10 INOR 248. Syntheses 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. Indium(III) bis-pyridil-2-sulfonamidophosphate complexes as efficient and durable catalysts for homogeneous water oxidation. S. Bernhard, M. Li, J.J. Goldsmith, K. Takada
9:00 INOR 251. Capturing 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 mixed hydroxy groups during basic electrolysis. 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-Fiol, 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. Lugnar, Organizer M. M. Maye, P. Radvanovec, Presiding
8:50 INOR 257. Withdrawn.
9:10 INOR 258. Halide passivated colloidal PbS nanocrystals for application in hybrid solar cells. H. Lu, R.L. Brutcher
10:10 INOR 261. Withdrawn.
10:30 Intermission.
11:00 INOR 263. Mechano luminescence and aggregation induced emission of bromine and methoxy substituted naphthyl conjugated 1- diketone compounds. P.T. Butler, W.A. Morris, J. Samonina-Kosicka, C. Fraser
12:00 INOR 266. Morphology-controlled synthesis of WO3 nanostuctures for highly-efficient photocatalysis. Z. Huang, J. Song, W. Zhang, X. Dong, L. Pan, J. Zou

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 microcopy applications of lanthanide centred emission. T.J. Sorensen
9:40 INOR 270. Tuning of the triplet-state energy of new highly luminescent LnIII complexes. A. Duerbeck, A.T. Hor, N.J. Long
10:20 Intermission.
10:30 INOR 272. Synthesis and evaluation of a series of lanthanide chelates that act as T72x MRI contrast agents. I. Daryaee, M. Mompour, M. Pagger
10:50 INOR 273. Multiplex imaging with luminescent lanthanide complexes. E. Borbas
11:10 INOR 274. Molecular recognition of sperm by LnDOTT1: Toward a noninvasive staging of prostate cancer. A. Diahan, L.L. Cheng, P.Z. Sun, P. Caravan

2015 ACS Catalysis Lectureship
Sponsored by CATL, Cosponsored by INOR

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control
Technical Session
Sponsored by PMSE, Cosponsored by INOR

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Monday Afternoon

Section A
Boston Convention & Exhibition Center
Room 103A
Building Innovative Solid State Materials Through Solution Chemistry
A. J. Norquist, Organizer

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. X. Passas
1:50 INOR 277. Atomic-scale derivatives of transition metal chalcogenides. J.E. Goldberger, T. Li, R. Morasse

2:50 INOR 279. Low temperature synthesis of (noncentrosymmetric) oxide-fluoride material. K.R. Poeppelmeier, K. Chang

3:30 INOR 280. Functional nanostructured systems through solution chemistry. M. Aksu, R.D. Robinson
3:50 INOR 281. Towards magnetic or luminescent halide materials synthesized under hydrothermal conditions. R. Gauthier
4:30 INOR 283. New ferrites from hydroxides: From zeolite to hexaferrite related structures. H. Zur Loye

5:00 INOR 284. Hybrid inorganic–organic materials with an aromatic cation and charge transfer: (C₅H₅)₃SnL and C₅H₅PbI₃. A. Maughan, J. Kurzman, J.R. Nellon

Section B
Boston Convention & Exhibition Center
Room 119
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 Tₛ 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-aniions systems. E. McCabe, J.S. Evans, C. Stock

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 157B
Inorganic Nanoscience Award
S. L. Stol, 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 electrical nanoscale controls. P.S. Weiss
10:30 Intermission.
11:15 INOR 344, Electrodepositoped 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
A. Feidman, 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
9:30 INOR 349, Superconducting CuSe, polymorph selection through kinetically-controlled solid-state metallation. A. Martinich, J. Kurzman, J.R. Nelson
10:00 INOR 350, Transition-metal catalyzed reactions that form bonds to phosphorus. R. Waterman
10:20 INOR 354, Small molecule activation by low valent nickel complexes. C.G. Riond
10:40 Intermission.
10:50 INOR 355, Reduction chemistry of rare-earth metal complexes supported by ferrocene diamide ligands. P. Diaconescu
11:30 INOR 357, Tandem catalytic processes for light alkane upgrading and ethylene polymerization. J.E. Boczar, D.C. Latch, A. Satller, J.A. Labinger
12:10 INOR 359, Characterization and reactivity of a series of macrocyclic cobalt-Mabiq compounds. C. Hess
12:30 INOR 360, When there’s a crowd: Reactivity of low-coordinate Ni-NHC polyfluoromacrocycles. R. Baker

Section C
Boston Convention & Exhibition Center
Room 160C
Environmental and Energy-Related Inorganic Chemistry
S. A. Koch, Organizer
M. Emmer, Presiding
8:00 INOR 361, Structural requirements for interfacial proton-coupled electron transfer. M. Jackson, Y. Suresnandan
8:20 INOR 362, Withdrawn.
8:40 INOR 363, Green chemistry design for rare earth recycling. M. Emmer
9:00 INOR 364, Activation of challenging C-O bonds through aldehyde catalysis. C.J. Chang, J.R. Long
10:00 INOR 367, Selective carbon dioxide reduction on rhodium grafted to a glassy carbon surface. D. On, Y. Suresnandan
10:30 INOR 368, Copper(i) bis-perfluorooctylacetate complex for electrochemical reduction of nitrate in water. S.F. Hannigan, L. Doerrer, L. Tahsini
11:10 INOR 370, Effects of solvent on the ionic liquid mediated electrocatalytic conversion of CO, to CO at a Bi-based electrode. T.P. Keane, J.L. DiMeglio, J. Rosenthal

Section D
Boston Convention & Exhibition Center
Room 161
Molecular Water Oxidation Catalysis
M. Albrecht, Organizer
S. Bernhard, Organizer, Presiding
9:50 INOR 374, In situ characterization of molecular water oxidation catalysts. D. Hetterscheid
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 oxidative catalysis of water by indium complexes. A. Macchioni, A. Bucos, I. Cortucci, L. Fagiolan, G. Pastorl, C. Zuccaccia
11:30 INOR 378, Molecular water oxidation catalysis with indium triazolylidene complexes — enhancing catalytic performance. M. Albrecht, A. Patronitho

Section E
Boston Convention & Exhibition Center
Room 160B
Chemistry of Materials: Metal Organic Frameworks
C. G. Lugmar, 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
8:50 INOR 380. Synthesis, structure, magnetic and nonlinear optical (NLO) properties of (Me3C)2, (C4H9) and (NLO) complexes of 3-(2-pyridyl)-5,8-diphenyl-1,2,4-triazine-4, 4'-disulfonate. O.A. Ondulina, O.A. Ibrahim, E.O. Onasimi, M. Hong
9:10 INOR 381. Defect Engineered mixed valence Ru-MOFs: Study on the influence of defect metal sites. W. Zhang, M. Kaur, A. Wuttig, J. Wei
10:30 INOR 383. Improved performance of graphite/LiNi1/2Mn1/2O2 cells cycled to high voltage (4.8 V) with electrolyte additives. Y. Dong, B.L. Lucht, M. Xu, L. Zhou, F. Chen

Section H
Boston Convention & Exhibition Center Room 146A
Chemistry of Materials: Synthesis and Properties
C. G. Lugmair, Organizer
P.J. Cappillino, Presiding
11:40 INOR 387. Effects of alpha substitution and strapped structure on the mechanochromic luminogen and aggregation-induced emission behavior of difluoroboron [B]-diketone dyes. W.A. Morris
9:30 INOR 388. Quantitative direct and indirect mapping of linker distributions in mixed linker MOFs via STEM-EDX. C. Wiktor, M. Melekhina, 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 390. Optimizing the electrocatalytic reduction of CO2 by Re- and Mn-based bipyridine complexes with supramolecular assembly. C.W. Machan, S.A. Achiaba, C.P. Kubiat
8:50 INOR 391. 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
9:30 INOR 393. Graphene as a protective layer for silicon in an aqueous PEC cell. A. Nielsander, N.S. Lewis
9:50 INOR 395. 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 interphase (SEI) formation and gas generation. B. Zhang, B.L. Lucht, M. Metzger, S. Sokolnar, B. Lechler, M. Heinrich
10:30 INOR 395. Improved performance of graphite/LiNi1/2Mn1/2O2 cells cycled to high voltage (4.8 V) with electrolyte additives. Y. Dong, B.L. Lucht, M. Xu, L. Zhou, F. Chen

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. Gadem, R.A. Fischer
8:50 INOR 406. Bis-cyclometalated iridium complexes supported by β-ketiminate (acNac) and β-diketiminate (NacNac) ligands. T.B. Teets, A. Mahy, Y. Radwan
9:50 Intermission.
10:15 INOR 413. Multinuclear osmium carbonyl complexes with dicarbonyl ligands. G.L. Powell
10:35 INOR 414. Understanding electronic structure requirements for iron-catalyzed C-H bond hydroxylation. C. Kleinert, T. Butler

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 metalloccenes (n-C5H5)2M (M = Fe, Ru, Os). I.S. Butler, J. DeArmas-Langais
9:20 INOR 418. Two-photon absorption spectroscopy of inorganic compounds. K. Takematsu, S. Wehlin, J.A. Byers
10:00 Intermission.

2015 ACS Catalysis Lectureship Sponsored by CATAL, Cosponsored by INOR

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace
Sponsored by IAC, Cosponsored by AGFD, AGR, BMTG, CARE, CESS, INOR, MED, ORGN, POLY, PROST, PROF and SBCH
Transition Metal Catalyzed Olefin Polymerization: Towards Structured Control
Technical Session
Sponsored by PMSE, Cosponsored by INOR

TUESDAY AFTERNOON
Section B
Boston Convention & Exhibition Center Room 158
Organometallic Chemistry: Applications to Materials and Polymer Science
N. S. Radu, Organizer
J.A. Byers, Presiding
1:30 INOR 425. On the mechanism of the regio- and stereoselective cyclopolymerization of 1,6-hepta- and 1,7-octadiynes by imido alkyldiene N-heterocyclic carbene catalyst. M. Buchmeiser, K. Herz, J. Haentze, W. Frey
1:50 INOR 424. Withdrawn.
2:10 INOR 428. Mechanistic insights into the stereoselective ring opening polymerization of poly(acrylic acid) catalyzed by achiral iron(II) based complexes. A. Kaur, C.M. Manna, F. Haefter, J.A. Byers
3:10 INOR 428. General mechanism for the synthesis of group II-VI and IV-VI nanocrystals. H. Liu, R. Garcia-Rodriguez

Section C
Boston Convention & Exhibition Center Room 182B
High-Energy Organometallic Complexes: Reactivity Driving New Synthesis and Catalysis
C. G. Cummins, R. Waterman, Organizers
M. R. Smith, Organizer, Presiding
1:30 INOR 429. Self-assembled metallic nanoparticle catalysts for olefin polymerization. R.P. Jordan, J. Wei
2:10 INOR 431. Importance of making molecules in catalysis. M.R. Smith
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
Section E
Boston Convention & Exhibition Center Room 161
Bioinorganic Chemistry: Proteins and Enzymes and Model Systems
S.A. Koch, Organizer
D. Rokhsara, D. K. Wicht, Presiding
1:30 INOR 447. Mimicking [FeFe] hydrogenase by covalent linkage of a synthetic diiron cluster to polymer scaffolds. C.A. Tookey, E.B. Berda, S. Piazzii
1:50 INOR 448. Lewis acid-induced valence tautomerism of a manganese(II) also porphyrinoid complex results in dramatic inhibition of oxygen atom transfer reactivity. J. Zaragoza, R.A. Baglia, M. Siegel, D.P. Goldborg
2:30 INOR 450. Porphyrin-containing polymer nanoparticles for modeling heme proteins iron coordination. K. Rodriguez, S. Piazzii
3:10 Intermission.
3:40 INOR 453. Insights from QM and QM/MM models of carbon monoxide dehydrogenase containing a unique Mo-Cu center. D. Rokhsara, T. Langa, L. Dient, M. Retegan, F. Neese
4:00 INOR 454. Geometrical and electronic structure of the nitrosyl adduct of the non-heme iron active site in anthranilide 1,2-dioxgenase revealed through 1H and 1H ENDOR spectroscopy. V. Hooke, D.M. Kurtz, B.M. Hoffman
4:20 INOR 455. Functional bioorganic peptide assemblies. H.C. Fry, L.A. Solomon
4:40 INOR 456. Spontaneous carbon dioxide activation by bimetallic nickel complexes. M. Mokhtarzadeh, S. Piazzii
5:00 Concluding Remarks.

Section H
Boston Convention & Exhibition Center Room 162A
Organometallic Chemistry: Catalysis
N. S. Radu, Organizer
M. Buchmeiser, Presiding
1:50 INOR 468. New molecular ruthenium and iron electrocatalysts for the reduction of carbon dioxide. C.W. Machan, M.D. Sampson, C.P. Kubik
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. San, R. Schowner, D. Imrich, W. Freytag
3:10 Intermission.
4:00 INOR 474. (NHC)(Pd)(0)-catalyzed cis-bis-silylations of internal alkynes with unactivated disilanes. O. Navarro, J. Spencer, M.B. Arslan, G. Clicke, M. Roe
4:20 INOR 475. Hydroisolation of internal C=C multiple bonds — insights on mechanism and kinetics. T.K. Zimmermann, K. Rener, F.E. Kuehn
4:40 INOR 476. Metal-ligand multiple bonds in iron complexes competent for pnp-loading C-H amiation. M.J. Wilding, T. Betley
5:00 INOR 477. Ring-opening polymerization of lactides and lactones by an iodine alkoxide salen complex. S. Quan, D. Paccones

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5:00  I.NOR  for the 250th ACS National Meeting is available at: www.acs.org/boston2015
Section D
Boston Convention & Exhibition Hall C
Inorganic Spectroscopy
S. A. Koch, Organizer
6:00 - 8:00
_INOR_555. Insight into the active sites and mechanism of alkyl-alkyl cross-coupling with iron. V. Fleischauer, M.L. Neidig
_INOR_556. New iridium pincer complexes for the hydrogenation of carbonyl compounds at room temperature. B. Dori, A. Chalhoub, M.E. Healy, J.A. Krause, H. Guan
_INOR_557. Catalytic dehydroammonolysis of alkanes via an iridium pincer complex: Toward a mechanistic understanding and control of product distribution. A.M. Steffen, A.S. Goldman
_INOR_560. Stoichiometric and catalytic reactivity of hexahydrotris(dimethylglyoxime)obalatane at an (N-heterocyclic carbene)- palladium centre. M.B. Ansell, G. Ciske, J. Spencer, O. Navairo
Section F
Boston Convention & Exhibition Hall C
Solid-State Inorganic Chemistry
C. G. Lugmair, V. Poltavets, Organizers
6:00 - 8:00
_INOR_561. Microporous titanosilicates with band gaps in the visible range for photocatalytic splitting of water. B.C. Hodges, P. Mostafaei, E.E. Rodriguez
_INOR_563. Preparation and characterization of new borophosphates of Pr(BPO_4)_2 and Tb(BPO_4)_2. M.B. Ansell, I.A. Morkan, J.A. Morkan, G.O. Kahveci, E. Gul
_INOR_564. Structural and photoluminescent characterization of anti-perovskite phosphores: Sr_2AlF_6P_2 and Sr_2Na_2AlF_6P_2. D.P. x S. Keil, E.C. Sullivan

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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 tetrahexadecal Au nanoparticles. N. Shukla, D. Yang, A.J. Goldman
9:30 INOR 624. Light or heat? The origin of cargo release from nanomembrane particles containing upconversion nanocrystals under IR irradiation. J. Dong, J.J. Zink, M. Strano
9:15 Intermission.

10:00 INOR 625. Advancements in nanomechanical measurements with scanning probe microscopy based methods. D. Yablon
10:40 INOR 627. Quantum dot luminescent center catalyst 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 measurement of single plasmonic metal oxide nanocrystals reveal considerable peak heterogeneity hidden within ensemble spectra. R.W. Johns, D.J. Milon, H. Bechtel

Section G
Boston Convention & Exhibition Center
Room 162A

Lanthanide and Actinide Chemistry
A. De Bettencourt Dias, Organizer
D. T. de Lili, D. A. Penchoff, Presiding

9:20 INOR 644. Selective and sustainable separation of rare earth elements. K.D. Field, M. Emmer
10:00 INOR 646. Actinide and lanthanide complexes: What is the CSD and structural informatics can tell us about their complexation. K. Miyoe, S. Vyas, P.C. Sanschagrin, J. Brennan
10:20 Intermission.

11:10 INOR 649. Precision design of new multidentate ligands for f-elements. I. Yakovlev, R.J. Agerel

Section H
Boston Convention & Exhibition Center Room 157C

Main Group Chemistry
T. W. Hudnall, Organizer
J. D. Protasiewicz, D. Vidovic, Presiding

8:50 INOR 651. Complexation and activation of silanes with a strongly Lewis acidic alkane: Isolation, structural characterization, and diverse catalysis. J. Chen, E.Y. Chen
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(I) complex with the ambiphilic ligand 3-quinoilindisulfide borane. S.R. Tamang, J.D. Hoefermeyer
10:20 INOR 655. Coordination of N-heterocyclic phosphorane cations to nickel using a chelating ligand framework. M. Bezpaloy, C. Thomas
10:40 INOR 656. Coordination chemistry of Group 1 cations with soft donor nanocarboxylics. M. Champion, M. Everett, A. Jolleys, W. Levason, D. Pugh, G. Reid
11:20 INOR 658. Calcium arylyphosphonates for bone therapy. V. Lopez, M.D. Lijewski, V.N. Bampou, K. Ruhrhardt-Senge

Innovation in Chemical Synthesis
Sponsored by MPFG, Co-sponsored by INOR, MEDI, ORGN

International Symposium on Mesoporous Zeolites
Sponsored by ENFL, Co-sponsored by CATL, IEC and INOR

WEDNESDAY AFTERNOON

Section A
Boston Convention & Exhibition Center Room 160A

Nanoscience: Semiconductors
R. M. Richards, Organizer
M. Znakov, Presiding

2:10 INOR 661. Liquid contacting of PbS quantum dot solids. E. Johansson, V. Denervarik, V. Uzunov
2:30 INOR 662. Hole transfer from photoexcited quantum dots to molecular species: Understanding the relationship between driving force and rate. e.H. Olshansky, T. Ding, Y. Lee, P. Alkidas
MEDI 23:30 Technical program information known at press time. The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015
Enhanced binding affinity by stacking of fluorinated phenyl rings on flat dipeptide fragments. M. Giroud, M. Harder, B. Kuhn, W. Haap, T. Schirmeister, P.N. Diederich

Pharmacophore discovery using extended Hückel Theory. A. Deschenes

Acetylation of lysine residues in Cu,Zn WT and ALS-mutant superoxide dismutase (SOD) with aspin inhibits its aggregation and promotes its amyloid destabilization. A. Abdolvahabi, Y. Shi, B.F. Shaw

Investigating the selectivity of metalloprotein inhibitors (MPI) in the presence of competing metalloproteins. Y. Chen, S. Cohen


Potent small agonists of protease activated receptor 2. M. Yau, J.Y. Sue, S. Wu, J. Lim, L. Liu, M. Adams, Y. He, J. Hooper, R. Reid, D.P. Fairlie

Fate of fluorocarbonones in drinking water treatment plants in China. Y. Xu, S. Liu, Y. Wang, H. Tao, F. Cui

De novo designed metalloprotein captues and stabilizes radicals. G. Ulas, Y. Wu, T. Lemm, W.F. Degrado

Using automated reagent management to dramatically improve efficiency in library synthesis and discovery. D. Miyao

Improved synthesis of trans/cis-4-(boc-amino)-4-methyl cyclohexanol. S. Zhang, L. Chen, Y. Chen, H. Li, X. Wu, M. Yang


Synthesis and SAR of a series of triazine macrocycles for the inhibition of the hepatitis C virus (HCV) series of triazine macrocycles for the ring.


Synthesis of 2'-C-methyl pseudouridines for the inhibition of HCV RNA polymerase. I.K. Sapp, J. Nunari, A.C. Bryant-Friedrich

Identification of active metabolites of lithocholic acid in the presence of competing metalloprotein inhibitors (MPi) in onchocerciasis and drug discovery. A. Abdolvahabi, Y. Shi, B.F. Shaw

Improvement of synthesis of 2,3-dioxygenase.

Enhanced binding affinity by stacking of fluorinated phenyl rings on flat dipeptide fragments. M. Giroud, M. Harder, B. Kuhn, W. Haap, T. Schirmeister, P.N. Diederich

Radiochemistry

Innovation in Health and Medicine

New Strategies and Applications of Aminoglycosides

Cancers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits

Cancer Immunotherapy: The Next Big Thing for Small Molecules

Cancer Immunotherapy: The Next Big Thing for Small Molecules

Antibody drug con-

Radiochemistry

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Cancer Immunotherapy: The Next Big Thing for Small Molecules

Antibody drug con-
MEDI 2:45 MEDI 276. Elution of serum toxicity biomarkers by reduced protein clearance in the absence of organ injury. A. Wolf, Y. Timist, F. Fognan

3:15 MEDI 277. Bromodomain and extraterminal (BET) domain inhibitors induce a loss of intestinal stem cells and villous atrophy. M. Wagner

3:45 MEDI 280. Opportunities for integrated safety assessment — early and ongoing. S. Thoman

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


3:10 MEDI 284. Structure-based design of allosteric inhibitors of hypoxia-inducible factor. U. K. Tambar


4:20 MEDI 286. Multimerization selective inhibitors of HIV-1 inte.

New Strategies and Applications of Aminoglycosides
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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. 78-80, 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. Subsequent listings.

Chemical Innovation and Design (CID) Talks: The Future of Innovation Now
Sponsored by MPRG, Co-sponsored by AFGD, AGR0, BIOT, MED1, PMG and SCHB

8:00 - 10:00
S. Plumlee, W. B. Young, Sci-Mix

MONDAY EVENING
Section A
Boston Convention & Exhibition Center Room 210B
Medicinal Chemistry Toolbox: Understanding the Roles of Inducible Pockets, Water & Small Structural Changes
B. R. Benco, A. Regueiro-Ren, K. Yeung, Organizers

7:30 MEDI 287. Coloring outside the lines: Exploiting induced binding pockets. D. F. Ortwine

10:00 MEDI 288. 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. Than, F. Deflorent

10:30 MEDI 289. Conserved water-mediated hydrogen bond network defines bosutinib’s kinase selectivity. N. M. Levinson

11:00 MEDI 291. Multimodal 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. Lindsey

Section B
Boston Convention & Exhibition Center Room 210A
MEDI Award Symposia
Financially supported by Portola Pharmaceuticals
W. B. Young, Organizer

8:00 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. Portoghese Medicinal Chemistry Lectureship: Curing hepatitis C virus infection with direct-acting antiviral agents: The arc of a medicinal chemistry triumph


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 PLAAG


5:00 MEDI 310. Deuterium-modified drugs: Discovery and development. S. L. Harbison

Section C
Boston Convention & Exhibition Center Room 210C
General Oral
W. B. Young, Organizer
A. S. Ripka, Presiding


Section B
Boston Convention & Exhibition Center Room 210A

General Oral

W.B. Young, Organizer

J. E. Macor, Presiding


Section C
Boston Convention & Exhibition Center Room 210C

Targeted Covalent Inhibitors

S. E. Conner, Z. Pei, Organizers, Presiding

9:00 MEDI 335. Targeted covalent inhibitor- reactivity vs. reactive drug metabolites: A risk-benefit perspective. T.A. Baille

9:30 MEDI 336. Exploring the kinase with selective and promiscuous chemical probes. J.W. Tauntton

10:00 MEDI 337. Discovery of rocile-tinib (CO-1688), a mutant-selective covalent inhibitor of EGFR. D. Niu


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. Koth

Innovation in Chemical Synthesis

Sponsored by MAPP, Cosponsored by INOR, MEDI and ORGN

Computational Toxicology: From QSAR Models to Adverse Outcome Pathways

Sponsored by ACS, Cosponsored by AGRO, ENVR and MEDI

Wednesday Afternoon

Section A
Boston Convention & Exhibition Center Room 210B

First Time Disclosures

L. A. Thompson, Organizer, Presiding


2:05 MEDI 342. Inventing INCB24360 (epacadostat), an indoleamine-2,3-di- oxygenase-1 (IDO1) inhibitor for immuno-oncology. A.P. Combs


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360 MEDI 361. Structured information of potenti and efficacious aminopyrimidines as inhibitors of phosphodiesterase 10 (PDE10). E.M. Jutkiewicz, J.R. Traynor, H.I. Mosberg
370 MEDI 371. Discovery of novel and fibristable SOD1 by small arachynides inhibits fibrillation and destabilizes its amyloid forms. S. Rasouli, A. Abdolvahab, Y. Shi, B.F. Shaw
375 MEDI 376. Novel asymmetric total synthesis of (+)-tetrahydroindole and (+)-3,4-dihydro-2-benzazepine. H. Hsieh, L. Chang, Y. Liu, L. Lin
395 MEDI 396. Fragment-based discovery of the first known inhibitors of PEGHD. N.O. Fuller
405 MEDI 398. Novel class of hsp90 inhibitors that are designed to be solubilizable and chemically accessible. Y. Wu
420 MEDI 401. Second-generation synthetic helix mimetics based on a 2,6,9-tri-substituted purine potently disrupts the McI-1-Bim protein-protein interaction. E.M. Lanning, S. Fischer
430 MEDI 403. Progress towards more potent and cell-active McI-1 inhibitors: Pro-drug and biososicostrogenic optimization of first-generation salicylates. L. Chen, S. Fischer
435 MEDI 404. Structure activity relationships of various β8-substitutions on mixed-modes γ-μ-opioid receptor (DOR) antagonist peptides. A. Harand, A. Bender, W. Grogg, J.P. Anand
440 MEDI 405. Electrolytic modification of quater ammonium salts as prodrugs. T. Zidan, C. Sannae, J.F. Remeran
460 MEDI 409. Identification and optimization of 2,3-dihydrobenzo[b][1,4]dioxine-5-carboxamide derivatives as poly(ADP-ribose)polymerase-1 inhibitors. U. Velagapudi, A. Bhatt, T.T. Talei
475 MEDI 412. Can strong solvents like DMSO and NMP be used as injection solvents in reversed-phase flash chromatography? J.R. Bickler
480 MEDI 413. Organic amine flash purification using a novel stationary phase. J.R. Bickler
490 MEDI 415. Protein and monoclonal antibody functionlization utilizing continuous flow micropore technology. M.M. Siebeika, N.G. Gedeon, S.E. Sadler, G.B. Jones
495 MEDI 416. Facilitating antibody drug conjugation using solid phase purification techniques. J.R. McCombs
505 MEDI 418. Antimycin acid efflux as a surrogate measure of the inhibition of plasmalogen hemoglobin endocytosis by methylamine and related antimarial agents. M. Ghanavi, C. Dapper, S. Dalal, P.M. Krol, M. Katz, P.R. Carpenter

Technical program information at press time. The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015
A.H., C.Y. Zamora, B. Imperiali


MEDI 55. Acrylamide compounds as potent and selective histidine H2 receptor ligands. R. Nirogi, A. Shinde, A. Mohamed, L. Kota, V. Timirin, S. Saraf, R. Subramanian, G. Bhuparne, V. Banade, N. Muddana, P. Jayan


MEDI 57. mGlur3-PAM: A novel approach to neuroprotection in Parkinson’s disease, from HLA to in vivo proof of concept. I. Dorange


MEDI 59. Frequent hitters revisited. E. Schneider


MEDI 61. Discovery of novel selective ER subreceptor ligands by multimodeling approach. A.S. Bayden, J. Jude, D.J. Diller

MEDI 62. Targeting specific interactions to improve binding properties of EGFR-kinase ligands. A. Ajamian

MEDI 63. Distributed drug discovery: Collaborative target repurposing accelerates identification of new leads for neglected tropical diseases. M.P. Pollastri


MEDI 65. Lead optimization studies on PAR-1 antagonist F61168. W. Tan, L. Wang, G. Yao, F. Zhang, C. Hu, J. Shi, Y. Yang, L. Jiang, Y. Xia

MEDI 66. Discovery of the hydantoin based MMP-12 inhibitor drug candidates A2D2324 for treatment of COPD. M. Munck at Rosenchold


MEDI 68. Engineering natural side-chains from leucine and isoleucine using amino acids to inhibit the estrogen receptor/coactivator interaction. T.W. Moore, T. Spetz

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470. RNA-based immune-stimula-
tory liposomal spherical nucleic acids (LNP) for immune antitumor therapy. C. Guan, N. Chernyak, C. A. Mirkin


472. Discovery of isothiazole- and thiourea-containing phenylpro-

473. Identification of novel insulin-
regulated aminopeptidase (IRAP) inhibitors by high throughput screen-

474. High-throughput search for novel PTP1B inhibitors: Targeting both catalytic and allosteric sites via integrated approaches. Z. Xiao, Y. Tang, Y. Yang, T. Tian, F. Ye

475. Novel 1,3,2-triazole analogs as DPP4 inhibitors. H. Park, T. Park


480. Syntheses of spiro-
7-azaindoles. G. Pan, J. Mao, H. Wang, H. Li, X. Wu, M. Yang
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. G. Tyliszczak, 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.
T. L. Sexton, S. Bramley, P. O’Rourke, W. C. Hardy, J. Wilson, M. Jones, M. K. Holland, N. McIntosh
2:40 Intermission.
3:05 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.
3:35 NUCL 6 Development of a dual excitation fiber optic Raman microscope for the identification of mineralogical samples. J. Bello, C. Gasbarr
3:55 NUCL 7 Methods for Pu valence determination in nuclear material processing solutions. R. Lascola, P. O’Rourke, C. Johnson, E. A. Kyser

MONDAY MORNING

Section A
Seaport World Trade Center
Waterfront 2
Analytical Chemistry in Waterfront 2
Division of Nuclear Chemistry
M.D. Powers, Y. Y. Sham, P. S. Portoghese
L. Taylor, D. Giammar, J. G. Catalano
W. R. Heineman, S. B. Clark, S. A. Bryan

TUESDAY AFTERNOON

Section A
Seaport World Trade Center
Waterfront 2
Transformation & Transport of Radionuclides in the Environment Co-sponsored by GECO
M. Boyanova, Organizer
K. M. Kemner, E. J. O’Loughlin, Organizers, Presiding
1:00 NUCL 24 27 Picogram U(VI) and Pu(VI) in marine sediments.
1:20 NUCL 25 Predicting plutonium behavior in the environment: Linking mechanistic behavior to field processes.
A. Kersting
1:40 NUCL 26 Using flow-cell desorption experiments to understand colloid-facilitated Pu transport.
J. Begg, M. Zavarin, S. J. Tumey, A. Kersting
2:00 NUCL 27 Ion-exchange chromatography for the real-time monitoring of Pu and other elements in complex environmental samples.
A. Kersting
2:20 Intermission.
2:40 NUCL 28 Determination of plutonium in spent nuclear fuel.
A. Kersting
3:00 NUCL 29 In-situ analysis of fission products in the Savannah River Site.
J. M. Giaquinto, J. Autschbach
3:20 NUCL 30 Analytical methods in the Savannah River Site.
J. M. Giaquinto, J. Autschbach
3:40 NUCL 31 Determination of the spatial distribution and chemical state of Cs in model environmental samples.
4:00 Intermission.
4:20 NUCL 32 Interactions of uranium and co-occurring elements in abandoned mine wastes.
J. M. Giaquinto, J. Autschbach
4:40 NUCL 33 Determination of the spatial distribution and chemical state of Cs in model environmental samples.
5:00 Intermission.
5:20 NUCL 34 Investigation for source term for the incident in WIPP’S Panel 7 Room 7EHE.
J. Giaquinto, S. Croft, S. Myers, D. K. Vare
5:40 NUCL 35 Determination of the spatial distribution and chemical state of Cs in model environmental samples.
6:00 NUCL 36 Investigation for source term for the incident in WIPP’S Panel 7 Room 7EHE.
J. Giaquinto, S. Croft, S. Myers, D. K. Vare

WEDNESDAY MORNING

Section A
Seaport World Trade Center
Waterfront 2
General Topics in Nuclear & Radiochemistry
J. Braley, T. A. Bredeweg, W. Loveland, Organizers
W. Loveland, Organizer, Presiding
1:00 NUCL 37 Nuclear structure and dynamics of mixtures of molten salts for pyroprocessing of nuclear waste.
D. Corradini, M. Levesque, P. Maddin, M. Salanne
1:20 NUCL 38 Development of block copolymer microphase-separated micelles for f-element separations.
L. Mitchell, T. T. Nguyen, B. J. Holiday
1:40 Intermission.
2:00 NUCL 39 Spectroscopic identification of Ti and in situ nuclear reactions and isotope production.
A. Roman, R. S. Rundberg
2:20 NUCL 40 Update on the observation of gamma rays from the nuclear isomer of 229Th.
R. S. Rundberg

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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 01. Bioactive peptide nanofibers for bone regeneration. G. Tansik, E. Ergul, A. Tekinay, M.O. Guler
8:20 | ORGN 02. Targeting anti-apoptotic Bcl-2 proteins with synthetic biologics. J.M. Holub, Z. Coon, M. Harris, B. Swords
8:40 | ORGN 03. Synthesis and conformational studies of pseudopeptidic macrocycles [a-w-Hydrazin]-catalyzed carbon-carbon bond formation of adjacent acyclic quaternary-tertiary amines. A. Adhikari, D. Beckers, M. Gattis
9:00 | ORGN 04. Regeneration of cartilage tissue and chondrogenesis in 3D microenvironment by supramolecular glycopeptide nanofibers. E. Arslan, M. Sardan, A. Tekinay, M.O. Guler
11:20 | ORGN 22. Self-assembled supramolecular chiral peptoid nanofibers and catalytic structures. M. Hatip, M. Khalify, M. Guler

Section C
Boston Convention & Exhibition Center Room 204B

New Reactions and Methodology
M. C. McIntosh, Organizer
T. Kah, Presiding
8:00 | ORGN 24. Synthesis of di-, tri-, and tetrasubstituted pyridines from (phenyl)acrylcarboxylic acids and 2-(aryl)tosylaminomethylac- rylates. 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. Calaza-Friede, P. P. V. Domingo, B. Hafemeyer, M. Gaunt
10:00 | ORGN 30. Nickel in the high speed ball mill: A new concept for metal mediated cyclodaddion reactions. R. Haly, A. Zelnir, J. Mack, H. Guan
10:40 | ORGN 32. First pinacol coupling under micellar conditions: Key role of surfactant and impact of alternative activation tech- nologies. C. Len, M. Blamboz
11:00 | ORGN 33. Development of regioselective allene functionalization methodology. Y. Xing
11:20 | ORGN 34. Mechanosynthesis as a powerful tool for reaction discover- y: New mechanochemic copper catalyzed C-N coupling reactions for the synthesis of pharmaceutically attractive compounds. D. Tan, T. Friscic
11:40 | ORGN 35. Aromatic H-D exchange using CF3COOD and an NH2-amine/palladium catalyst. K. LaCroix, R. Naran, R.A. Giles

Section D
Boston Convention & Exhibition Center Room 206A

Asymmetric Reactions and Syntheses
M. C. McIntosh, Organizer
T. Benkovics, Presiding
8:00 | ORGN 36. Stereoselective synthesis of a C2-symmetry reverse transition inhibitor via organocatalytic dynamic kinetic resolution. T. Benkovics
8:40 | ORGN 38. Enantioselective redox olefin azidiradion via Cu(0)-based metallo- catalytic cycle. X. Cai, Y. Zhan, K. Bai
9:00 | ORGN 39. Bridged D-symmetric chiral amorphophidones for Cu(0)-based metallo- radical catalysis: Highly enantio-switch- able, intramolecular Csp3-H radical amination controlled by bridge-regul- ated cavities. K. Lang, P.X. Zhang
10:00 | ORGN 42. Metal-free metathesis reaction of C-aryl alkylic sulfiliums with any isocyanates: Construction of chiral nonracemic allici- cyanates. R. Grange, P. Evans
10:20 | ORGN 43. Palladium-catalyzed asymmetric alkylic alkylation of imines nucleophiles with cycloalkene carbonates. N.K. Zaware, D. Kastinsky, G. Narla, M. Ohtme
11:00 | ORGN 45. Development of a catalytic enantioselective Mannich reaction. J. Shikora, S.R. Chem
11:20 | ORGN 46. Cu-catalyzed asym- metric allylic amination with aryl lithium reagents. S. Gudungula
11:40 | ORGN 47. Stereocatalytic synthesis of adjacent acyclic quaternary-tertiary motifs and its application to a concise total synthesis of (–)-Filorfin. 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 units to manipulate binding strength in linear H-bond arrays. D.K. Smith, L.A. Cane, R. He
8:20 | ORGN 49. Bowl-shaped molec- ular probe for xenon-129 magnetic resonance imaging. B.L. DeBoef
8:40 | ORGN 50. Multistate regula- tion of anion binding affinity by light and heat. S. Wezenberg, M. Vaktov,J. Kistemaker, B. Feringa
9:00 | ORGN 51. Construction of chiral materials using supramo- lecular atropisomers. Q.R. Chu
SUNDAY EVENING

Section A
Boston Convention & Exhibition Center Hall C

Asymmetric Reactions and Synthesis: Chemistry of Fullerenes, Carbon Nanotubes, and Graphene; Materials, Devices and Switches; Nanomaterials; Physical Organic Chemistry
R. D. Brown, Organizer

0:00 - 10:00
100. Structure activity studies on a 4-component assembly for HTS of chiral alcohol ee values. C. Lin, E. Anslyn
101. Supramolecular polymers as high performance binders for silicon anodes in lithium ion batteries. A. Coskun
102. Self-assembly of cat ion dicationic peptide hydrogels: Supramolecular nanostructure and rheological property dictating antimitochondrial activity. L. Jiang, D. Xu, H. Dong
104. Revealing self-assembly processes that underlie fibration of β-lactoglobulin through dynamic light scattering, Raman spectroscopy, and optical microscopy. S. Blake, S. Ann, N. Lewis, W. Qi, M. Majumdar
105. Copper-catalyzed enantioselective addition of silane nucleophiles to aldimines using new planar chiral [2.2] paracyclophane-based triazolic copper carbene precursors. Y. Ma, Z. Chen, C. Song
106. Enantioselective iodination of vinyl iodides using organic iodine reagents. A. Chen, C. Song
107. Enantioselective iodination of vinyl iodides using organic iodine reagents. A. Chen, C. Song
108. Conjugate addition of hydroxyl and aryl trifluoroborates: A synthetic strategy for discovery. R. S. Hughes
110. Novel convergent total synthesis of biologically active small molecules containing cyanovinyl aziridine derivatives from the fungus Penicillium sumatrense MA-92. L. Eliopoulos
111. Formation of acyclic quaternary N-nitroso compounds by diazo substitution. O. Schwarz, R. J. Appleby
112. Assembly of amphiphilic borylnitro compounds into discrete cavities. S. Chen, Y. Ruan, M. Yamazaki, J. D. Badjo
113. Click-fluors: Synthesis of fluorescent saccharide sensors via a copper-catalysed azide-alkyne cycloaddition reaction. W. Zhai, L. Mao, J. S. Bossey

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

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Section C
Boston Convention & Exhibition Center Room 203
Young Investigator Symposium
S. Dreher, Organizer, Presiding
8:30 Introductory Remarks.
9:00 ORG 232. Development and imple- mentation 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 ORG 233. Organic acid applica- tions within the cosmeceutical industry “chemical peels”. P.M. Brevia
10:40 ORG 236. Continuous process- ing: Chemical route development and GMP implementation. K.P. Cole
11:05 ORG 237. DNA-programmed chemistry toward macrocycle libraries for drug discovery. T.F. Briggs

Section D
Boston Convention & Exhibition Center Room 304A
Magnetically Recyclable Nanocatalysts
A. M. Pericas, O. Reiser, Organizers, Presiding
8:00 Introductory Remarks.
8:05 ORG 239. Development of magnetic-core @ catalytic - shell nanostructures. D. Ma
8:30 ORG 240. Magnetically recover- able fibrous nanosilica (mKCC-1), V. Polshettidwar, A. Raghavan, B. Singh

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Section B
Boston Convention & Exhibition Center Room 205B/C

Young Academic Organizer 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 bipyridyl organophospho- nate catalysts. A.T. Radosovec
8:30 ORGN 349. No strain, no gain: Advances in the synthesis and use of cyclobutanes. M.K. Brown
9:00 ORGN 350. Structure and reactivity of gold (I) complexes relevant to catalysis. A.C. Jones
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 sarcopine alkaloids. T. Giai, S. Kriger

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. Ayitou, 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. Micra, J.B. Rainzabek, T.M. Swager
8:40 ORGN 358. Molecular design and synthesis of heliconical twist-bend nematic liquid crystals. Y. Wang, H. BisoY, Q. Li
9:00 ORGN 359. Stimuli directing self-organized 3D liquid crystal nanostructures. Q. Li
10:00 ORGN 362. Photoswitchable phosphine ligands for Pd-catalyzed asymmetric reactions. D. Zhao, B. Feringa

Section D
Boston Convention & Exhibition Center Room 206A

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species
M. C. McIntosh, Organizer
M. S. Oderinde, Presiding
8:00 ORGN 343. Surprising impact of the 2,2,6,6-tetramethylpiperidinyl group on the chemical shift and conformation of singly-masked 1,2-diolos. S. Chatterjee, E. Fought, J.S. Chen, T.L. Winds
8:40 ORGN 345. Understanding solvent-induced red-shifts for the protons stretch vibrational frequency in a hydrogen-bonded complex. P.M. Kief, D. Pinos, E. Pinos, J.T. Hynes
9:00 ORGN 346. 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. Choudhry, A. Greer
9:20 ORGN 347. New photooxygene-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
10:00 ORGN 439. Design, synthesis, and computational studies of novel rhodamine dyes for imaging applications. A.K. Muthusamy, J. GrIm, L.D. Lavis
10:40 ORGN 441. Measurement of substitut-ent interactions. J. Huang, K.D. Shum
11:20 ORGN 443. Synthesis of tetracene derivatives, study of their stability, and photooxidation with singlet oxygen. R.N. Baral, S.W. Thomas

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. Leizman, D.E. Bergbreter
9:00 ORGN 380. Studies towards ligand-enabled (Sp3)-H activation using Pd(II) and Pd(II) catalysts. J. He, J. Yu
9:20 ORGN 381. Polyelectrol oligomers as solvents and tools for Ru(II)-catalyzed metathesis reactions. J. Surbooth, W. Guzman, D.E. Bergbreter
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. Tokor
10:40 ORGN 385. Withdrawn.
11:00 ORGN 386. Transition metal and phosphorous mediated transforms for C-C and C-N bond formations. A. Lepore, B.L. Ashfield

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 phenoins. J. Lumb, Z. Huang, K. Esquana
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 functiona- lization reaction. D. Mait
9:00 ORGN 470. Stereocontrolled radical C-H alkylation via Cofibr-based metalorganic catalysis. X. Cui, X. Xu, J. Lin, L. Wojas, P.X. Zhang
9:20 ORGN 471. Directing group strategies for the beta-functionalization of ketones via C-H activation. M. Young, G. Dong
10:20 ORGN 474. Control of reaction selectivity in palladium-catalyzed transformations through tuning of ligand structures. K.H. Shaughnessy

Biological Inspiration for Environmental Sustainability: Biospired 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 CEF, ENFL, ORGN and PHYS

Glycolipid Immunostimulants
Sponsored by CARB, Cosponsored by MEB 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
Section C
Boston Convention & Exhibition Center Room 203

Materials, Devices and Switches
M.C. McIntosh, Organizer

D. Chidron, Presiding
1:20 ORGN 425. Pyrene-based compounds in organic optoelectronic applications. B.R. Kaarfarani
1:40 ORGN 426. Noncovalent aromatic interactions that control the geometry and piezoelectricity of conjugated oligomers. S.W. Thomas
2:00 ORGN 427. Withdrawn.
2:20 ORGN 428. Benzothiadiazine and benzothiadiazolene donor-acceptor (D-A) small molecules for solution-processed small molecule organic solar cells. M. Chong
3:00 ORGN 430. Electrochemical molecular switching using thiathreene-containing cavitand. W. Ong, F. Bartani, T.M. Swager
3:20 ORGN 431. Design and prototyping of biodegradable polymeric drug delivery system for inner ear disease treatment. J. Wang, A.M. Ayoub, J.T. Borenstein

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 Δ11,12,13-triazolines to form aziridines. T. Chung, M.A. García-Garbay
2:00 ORGN 368. Exploring excited-state catalyzed 1,3 dipolar cycloaddition reactions. J. Ortiz Sanchez, T.J. Heavey, M. Lakewicz, 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
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
3:40 ORGN 373. Solution and solid state photochemistry of spiroynans. V.M. Breslin, M.A. García-Garbay
4:00 ORGN 374. Quinoline based α,ω,ω,ω-tetrahalogenation: Synthesis and gas phase reactivity by using a linear quadrupole ion trap (QIT) mass spectrometer. R.R. Kotha, H.I. Kantamma

Section E
Boston Convention & Exhibition Center Room 204B

New Reactions and Methodology
M. C. McIntosh, Organizer
P.S. Hanley, Presiding
1:20 ORGN 446. NHC-Cu-catalyzed nucleophilic fluorination of propargyl electrophiles. L. Cheng, C. Gorder
1:40 ORGN 447. Withdrawn.
2:00 ORGN 448. Hypervalent activation as a key step in accessing the ortho-CH position of iodoarenes. Y. Wu, I. Arenas, L. Broomfield, A. Shaffir
3:00 ORGN 451. Inter- and intramolecular decarbonylation of bis-alicylic esters lacking anion-stabilizing groups. I.D. Hyatt, M.P. Gramt
3:20 ORGN 452. Selective functionalizations of tetracoordinated sulfur derivatives. R.A. Bohmann, C. Bröm
4:00 ORGN 454. Metal free C-H coupling of aromatic compounds by graphene oxide activated by acidic additives. Y. Nishina, N. Morimoto, K. Morikawa
4:20 ORGN 455. Modified Friedel-Crafts quinoline synthesis in water. F. Li

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TECHNICAL PROGRAM

Section G
Boston Convention & Exhibition Center Room 208B

Metals-Mediated Reactions and Syntheses
M. G. McIntosh, Organizer
J. S. Fossey, Presiding
1:00 ORGN 401, Organotransition metal catalysis 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. Mousselli
1:40 ORGN 403. Direct, efficient, and general gold-catalyzed synthesis of fused-imidazo heterocycles. M. Garzon Sanz, P.W. Davies
2:20 ORGN 405. Rapid Cu(II)-mediated formation of 5,5′-bis[1,2,3-triazole] from organic azides and terminal alkynes. C.J. Brassard, X. Zhang, R.J. Clark, L. Zhu
4:00 ORGN 410, Iron (II)-catalyzed stereoselective intramolecular olefin amination and aminochlorination. C. Zhu, D. Lu, T. Jian, H. Xue

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Bioinspired Desigms: From Molecules to Functional Materials

Glycolipid Immunostimulators
Sponsored by CARB, Cosponsored by MED and ORGN

Green Chemistry Makes a Difference: Pharmaceutical Industry/Academic Collaborations

Sponsored by iMEC, Cosponsored by 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
Section B
Boston Convention & Exhibition Center
Room 205B/C
Technical Achievements in Organic Chemistry
K. L. Lee, Organizer, Presiding
T. D. White, Presiding

9:00 Introductory Remarks.

9:10 ORGN 574. Grignon reagent formation in continuous stirred tank reactors with sequestered magnesium. T. Braden, M.D. Johnson, S.A. May, M.E. Harman


10:40 ORGN 577. Flow chemistry: A technology for control freaks. M.W. Bundesen, J.E. Davon, M.S. Lall, C.I. Li, J. Yan, Q. Yan

11:10 ORGN 578. New streamlined methods of sulfone and sulfonamide synthesis from aromatic halides and their hybrids for engineering of free-standing 2D carbon materials and C–N bonds via oxidative functionalization of unactivated sp3 C–H activation and sequestered magnesium. C.A. Parish, M. Reibarkh, E. Streckfuss, T.F. Pahutski

Section C
Boston Convention & Exhibition Center
Room 203
Frontiers of Functional Interfaces
A. Cattani-Scholtz, 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


9:30 Internessment.


Section D
Boston Convention & Exhibition Center
Room 204A
Heterocycles and Aromatics
M. C. McIntosh, Organizer

8:00 ORGN 582. Green synthesis of divergent heterocyclic scaffolds. W. Zhang

8:20 ORGN 583. Progress towards the synthesis of a bowl-shaped fragment of C31N. D. Dodge, A. Whaley, D.P. Sumy

WEDNESDAY MORNING

Section A
Boston Convention & Exhibition Center
Ballroom East

On the Importance of Synthetic Organic Chemistry in Drug Discovery
J. A. Elman, 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


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


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.G. Khazhnya, E. Rodriguez, A.B. Charrette


9:40 ORGN 589. Thiohydrazidic acids as versatile reagents for heterocycle synthesis. B.C. Lemerier, J.G. Piena

10:00 ORGN 590. Catalytic functionalization of unactivated sp3 C–H bonds through intramolecular oxygen nucleophiles affording cyclic ethers. S. Thompson, G. Dong


11:00 ORGN 592. Mechanistic studies to enable a scalable Friedel-Crafts reaction. J. Albrecht, G. Beutner, B. Cohen, A. Dorr, J. Fan, D. Fanter, M. Lawler


Section E
Boston Convention & Exhibition Center
Room 204B
New Reactions and Methodology
M. G. McIntosh, Organizer

8:00 ORGN 595. Reactivity of photoclonally derived tri cyclic vinyl aziridines. E.E. Blackham, K. Booker-Milburn, J. Knowles


8:40 ORGN 597. New rearrangement and substitution reactions of ethenylbenzylamines. X. Shi, A.C. Ono, A. Hsu, W.F. Kekeman

9:00 ORGN 598. Unexpected retroaldol-aldehyde reaction during O-alkylation of hydroxylated Vincet lactam derivatives. J. Braën

9:20 ORGN 599. Withdrawn.
Biologically-Related Molecules and Processes
M. C. McIntosh, Organizer
D. H. Appella, Presiding
8:00  ORGN 657, Disubstrate analogs and inhibitors of farnesyl dipiphosphate synthase: Synthesis and enzymatic studies. G. Ramamoorthy
8:40  ORGN 659, Synthesis and chemical biology of the morpholine fragment of the monocyclins. Y. Shi, J.G. Pence
9:00  ORGN 660, Natural products with the 6-7-5 ring scaffold. A.S. Bayden
9:40  ORGN 662, Diastereoselective design of privileged structures: Forward chemical genetics for phenotypic screening of chemical probes. T.H. Atell
10:00 ORGN 663, Copper-catalyzed synthesis of 2-arpyrrolidines. C. Um, S.R. Chemler
10:20 ORGN 664, Multivariant display using a synthetic, PNA-based scaffold to characterize ligand-receptor interactions of alphaVbeta3 integrin, adenovirus A2A, and dopamine D2. D.H. Appella

Technical program known at press time.
The official technical program for the 250th ACS National Meeting is available at: www.acs.org/boston2015
Synthesis of some aryl amides — potential double-acting inhibitors under microbial conditions.
S.A. Santo, L.S. Longo Jr, A.C. Reis

Flexible synthetic entry into the dienophile class of natural products. Bar, C. Schirmeister

Refinement of a biaxial coupling reaction. S. Corning

Design of small molecule libraries. T. Flagstaff, T.E. Nelson, M. Mausen

Cinchona alkaloid-catalyzed synthesis of chiral trifluoromethylidene diphosphoranes. K. Kasten, A.D. Smith

Isotiochore-mediated one-pot synthesis of functionalized pyridines. D.G. Stark, L.C. Monti, A.D. Smith


Scope of strainselective active monosubstitution of aldehyde. L. Tian, H. Lin, L.J. Krauss

Unsymmetrical 1-haloallynes — synthesis, isomerization, and reactivity. B.Z. Puglisi, N. Gula, S. Szafert

Nickel-catalyzed decarboxylative C--H arylation of azoles with perfluoro- and nitrobenzeno-ethanol. J. Crawford, K. Sheltton, B. Sadarananda, E. Reeves, D. Kalyani

Nickel-catalyzed decarboxylative cross-coupling of perfluorozenobenzoates with anhydrides and sulfonates. L.W. Sardzinski, W.C. Welter, A.M. Schnaith, D. Kalyani

Efficient method for the preparation of styrene derivatives via Rh(II)-catalyzed direct C-H vinylation. K. Ottey, J.A. Elman

Transition metal catalyzed functionalization of anilines. B. Catano, Y. Yang, C.C. Kim, J. Lee


Novel annionic cascade for synthesis of chiral 3-pyrrolines. I. Chogi

Palladium catalyzed oxidative arylation of nitrobenzenes. A.M. Schnaith, S.B. David, D. Kalyani

Selective access to heterocyclic sulfonil halides in a parallel medicinal chemistry platform. J. Tucker, L. Chander, J.M. Young


Catalytic turnover in Friedel-Crafts catalysis of tertiary aliphatic fluoroiodides. M. Dryzhakov, J. Moran

Wild and metal-free N-arylation of secondary acyclic amides at room temperature. G. Tenis, E. Stefab, H. Lundberg, H. Adolfsson, B. Olfsen

Redox neutral alkylation of electron rich heterocycles using photoredox catalysts. T.M. Williams, E. Swift, C. Stephenson

Withdrawn.

Development of a biomimetic biaryl coupling reaction to access strained cyclophanes. R. Watson, C. Schirmeister

Mild and direct lactamization protocol for the synthesis of pyridyl-3-glyoxylate-2-one. C.M. Stift, C. am Ende, J.M. Humphrey

Catalytic asymmetric synthesis of α-amino acid derivatives through [2+2]-rearrangement. T. West, A.D. Smith, D.S. Daniels


Palladium-catalyzed α-arylation of aryl nitromethanes. K. Van Gelder, M. Kozowski

Effective nitrogen radical reactions via Co(I)-based metalloradical catalysis. L. Jin, J. Tao, H. Lu, X. Cui, P.X. Zhang

Improved general synthetic route to dialkylphosphono-alkanes: Featuring the first synthesis of Me-DIOR. A.J. Kendall, D.T. Schneider, D. Tyser

Development of predictive models to elucidate the roles of ligand and substrate in tunable sulforhodium(I)-containing transmetallation catalysis. R.J. Scap, R.C. Johnston, S. Hare, P. Cheng, D.J. Tantillo, J.M. Schomaker

Development of a novel Bronsted acid composite material and study of its catalytic performance using cloud computing. W. Wang

Metalloaryl radical-mediated stereoselective radical reactions via Co(I)-catalyzed metalloradical catalysis. X. Cui, X. Xu, L. Jin, P.X. Zhang

Route to polysubstituted β-naphthol from coumarins by the directed remote metalation reaction. J. Patel, J. Board, M. Hossain, V. Sinetsky

Taming carbon dioxide: Access to 1,2-azodicarbonitriles from alkenes. R.A. Vailin, S.K. Mammudaly, M.G. Finn

Ruthenium-catalyzed cross coupling reaction of 1-phenylthiophenes with internal alkynes. K. Sugita, Y. Toroko, S. Fukuzawa

Regioselective acetylation of TMS ethers: Application to cycloalkanes, carbohydrates, glycolipids, and their conjugates. S.S. Park, J. Gervay-Hague

Conversion of aldehydes to β-hydroxyboronates. C.J. Ferber, C.M. Moore, C.P. Medina, P. Csanad, T. Clark

N-Alkylation of anilines and sulfonylamides with trichloroacetimidates. D. Wallach, P. Stege, J.D. Chisholm


Triazabutadiene chemistry in organic synthesis and chemical biology. F.W. Kim, J.C. James

Development of directed photochemical arylation of tertiary aliphatic carbon. A.K. Contreras, I.M. Chapa, I. Bálderes-Renteria, G. Rivera, B.K. Bank

Biocatalysts for hydroxamic acid. K. Albritton, A.C. Smith

Investigation of ureas and thioureas as H-bonding chiral hosts. A. Shrestha, N. Camasso, M. Shin, E.C. McLaughlin


Cinchona alkaloid-catalyzed oxidative arylation of nitroarenes. A.K. Contreras, I.M. Chapa, I. Bálderes-Renteria, G. Rivera, B.K. Bank


Development of directed photochemical arylation of tertiary aliphatic carbon. A.K. Contreras, I.M. Chapa, I. Bálderes-Renteria, G. Rivera, B.K. Bank


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 dihalo-carbenes to a n-bowl. C. Dubocac, A.S. Flatoz, A. Zubala, M.A. Petrukhina
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 acetylides. S. Hein, H. Arslan, I. Kesnitz, W. Ditten
9:40 ORGN 804. Ambient-processed transition metal oxide free-Peroxysilite solar cells enabled by a new organic charge transport layer. G. Han, S. Chang, S. Gradiocak, 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 (Csp3)-H arylation. J.A. Bull, D.P. Atton
9:20 ORGN 809. Directed ortho-meta-ligation (DOM) and directed metatlation group (DMG) — dance strategies for the synthesis of C7-G (C7)-substituted benzimidazoles. S. Singh, A. Friedman, S. Gomes, K. Mitchel, V. Samudra
9:40 ORGN 810. Iron trichloride-catalyzed biaaryl synthesis via ring-opening Friedel-Crafts arylation of 1,4-epoxy-1,4-di-hydroxynaphthalenes. S. Asai, T. Kawasaki, Y. Monguchi, H. Saiki, Y. Sawama
10:00 ORGN 811. Expedient synthesis of gem-dialkylbenzyl heterocycles through olefinic hydroarylation. Y. Lian, K. Burford, A.T. Lendrium

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 diatratror diazo reagents: In-flow generation and purification. E. Levesque, S.T. Laporte, S. Varier, A.B. Charette
9:00 ORGN 816. Continuous flow halogenation: Challenges and opportunities. R.V. Jones, L. Kocsis, T. Sipocz, F. Darvas

Section D
Boston Convention & Exhibition Center
Room 206A
Biologically-Related Molecules and Processes
M. C. McIntosh, Organizer
M. D. Distefano, Presiding
8:20 ORGN 819. Discovery and optimization of peptide-based ligands for the CuAAC reaction. A. Googhan, L.C. Dahora, M.G. Finn
8:40 ORGN 820. Probes to perturb the protein-protein interface in e-anti-thrombin. D. Xin, K. Burgess
9:00 ORGN 821. Application of 1,3-dipolar cycloaddition reaction for protein labeling. Z. Wang, A. Laverette, A. Daughta
9:40 ORGN 823. Marine very-long-chain methylated Δ5,9 fatty acids are effective inhibitors of lipopolysaccharides β. N.M. Barballeira, N. Montano, A. Rodriguez, L.A. Amador, R. Balana-Fouce, R. Regueira
10:00 ORGN 824. Drug discovery: From computational screening to synthesis of lead compounds. J. Brown, J. Stiles, B.L. Delboel
10:20 ORGN 825. Maltose containing a thioacetel linkage is resistant to hydrolysis and efficiently targets bacteria in vivo. X. Wang, N. Murthy
10:40 ORGN 826. Theoretical modeling of α-lipoic 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, K. Zhou, J. Guo

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials
Biodesigned: From Molecules to Functional Materials
Sponsored by ENVR, Cosponsored by CEI, ENFL, ORGN and PHYS

OTHER SYMPOSIUM OF INTEREST:
Accelerated Discovery of Chemical Compounds: Design New Polymers & Inorganic Materials from Integration of Polymer Science, Materials Science, & Informatics
Calculating pKa’s & Redox Potentials
Molecular Dynamics Simulations in Drug Discovery
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 252A
Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds
Cosponsored by ENVR
D. A. Knopf, S. Lee, Organizers, Presiding
8:30 PHYS 14. Chemical imaging of atmospheric particles. A. Laskin


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 complex molecular environments. W. Deering
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. Epitanovksy, A. Krylov
10:00 PHYS 12. Withdrawn.

Section C
Boston Convention & Exhibition Center
Room 252B
Environmental Sustainability: Bioinspired Designs: From Molecules to Architectures
Cosponsored by ENVR, ORGN/PHYS
H. Arslan, I. Kesnitz, W. Ditten
8:00 PHYS 1. 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

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Section B
Boston Convention & Exhibition Center Room 252A

Electronic Structure Methods for Large Systems

Fragment-Based Approaches
Co-sponsored by COMP
M. P. Head-Gordon, J. Herbert, Organizers

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. Pau

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-Davidy exciton model. A. Morrison, J. Herbert


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
Co-sponsored by ENVY

D. A. Knopf, S. Lee, Organizers

N. Ng, J. A. Thornton, Presiding


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


10:00 PHYS 123. Withdrawn.

10:30 PHYS 124. Molecular dynamics of clusters formed by ammonia, sulfuric acid, and water. N. Chen, A.W. Duster, H. Lin

11:00 PHYS 125. Growth mechanisms of ambient nanoparticles. M.V. Johnston


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
Co-sponsored 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 Internmission.


11:00 PHYS 131. Tracking viral membrane mannol melanocyte dynamics through temporally-resolved plasmon coupling microscopy. A. Feazour, H. Aiyama, S. Gummuluru, B.M. Reinhard
Section I
Boston Convention & Exhibition Center
Room 257B
From Diradicals & Polyradicals to Functionalized Materials: Theory Meets Experiment
Co-sponsored 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 diradicals. J. Musfeldt, A. Clune, J. Fasso-Tande, R. Harrison, P. Lathi
2:10 PHYS 213. Revisiting the chemistry of the phenalenyls. T. Kudo, K. Uchida
2:30 Intermission.
4:00 PHYS 215. Theoretical molecular design for singlet fission based on the diradical character: Tetrathiafulvalene and bisimidazol diradicals. S. Ho, N. Itô, M. Nakano
4:50 PHYS 217. Ab initio wave function studies of organic photovoltaic systems. I. Borges, E. Uhi, 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, 177-179, 184, 190, 192, 211. See previous 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
Co-sponsored by COLL
A. E. Bragg, A. T. Kummel, Organizers
P. B. Petersen, Organizer, Presiding
8:00 PHYS 219. When complicated things happen to simple liquids: Nitriles at silica interfaces. J.T. Fourkas
8:55 PHYS 221. Nonlinear coherent vibrational spectroscopy of electri
tified interfaces. N. Garcia-Rey, B.G. Nicolau, B. Dryzkov, D.D. Drott
9:30 PHYS 222. Effect of energy level alignment on heterogeneous electron transfer: Injection from porphyrinoids into TIO, 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

Section B
Boston Convention & Exhibition Center
Room 252A
Electronic Structure Methods for Large Systems
Excited States and Strongly Correlated Electrons
Co-sponsored by COMP
M. P. Head-Gordon, J. Herbert, Organizers
R. A. DiStasio, Presiding
8:00 PHYS 226. Bioluminescence chal-
lege: Simulating and exploring thermal nonadiabatic chemistry. R. Lindh
8:40 PHYS 227. On the nature of a large Stokes shift in midinfrared fluores-
cent protein. S. Faraji, A. Knylov
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 improv-
able multiscale methods for cor-
rrelated electron systems. D. Zgid
10:20 PHYS 230. Multireference excited state method applied to acenes and phenental 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 correlation interaction singles (ALMÖ-CIS). K.D. Closser, O. Ge, M.P. Head-Gordon
11:00 PHYS 232. Modeling middle-size to large-size multireference molecular systems. R. Carlson, C. Hoyer, A. Sonnenger, D.G. Truhlar, L. Gagliardi

Section C
Boston Convention & Exhibition Center
Room 252B
Chemical Processes Involving Atmospherically Relevant Trace Gases Aerosols & Clouds
Co-sponsored by ENV
D. A. Kropf, S. Lee, Organizers
F. Geiger, F. Veres, Presiding
8:00 PHYS 233. Tracking aerosol chemical age through stable carbon isotopes. A. Krider-Schar, I. Gensch, X. Sang, A. Khan, W. Laumer, P. Schlag, S. Schmitt
8:30 PHYS 234. Using single parti-cle mass spectrometry (SPMS) to characterize chemical composition of atmospherically-relevant aerosol particles. M.A. Zawadowski, J.T. Jeng, P. Croteau, D.R. Worsnop, D. Cziczo
8:45 PHYS 235. Polytopic aromatic hydrocarbon photocytolysis kinetics in aqueous, organic, and aqueous-or-ganic environments. J. Grossman, A. Stern, M. Kirch, T.F. Kahn
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 mech-
anism of sunlight irradiated aqueous pyruvic acid. A.J. Eugene, M. Guzman
9:45 PHYS 239. Computational screening of possible brown carbon compounds in the atmospheric aerosol. M. Caricato
10:00 PHYS 240. Dynamics of sec-
ondary organic aerosol: 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
Co-sponsored 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
9:20 Intermission.
9:40 PHYS 244. Mimicking photosynthetic electron, energy, and proton trans-
s. J.D. Gust, T.A. Moore, A.L. Moore
10:20 PHYS 245. Proton transfer in cyto-
ochrome c oxidase. E. Knapp, A. Woolke
11:00 PHYS 246. Channelrhodopsin: Molecular dynamics studies of hydration and cation transport. M.R. VanGorden, S.W. Rick, S.L. Rampe
Section E
Boston Convention & Exhibition Center
Room 254B
Hydrophobicity, Ion Solvation, & Interfaces: Theory, Simulations, & Experiments
Nanoflowers
D. Ben-Amarz, S. Garde, Organizers
S. L. Rempel, Presiding
8:00 PHYS 247, Reversible control of nanoflower 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. Wysolovsl, H. Pathak, A. Obidat, G. Wiersma
9:20 PHYS 250, Understanding freezing point deviations and the Gibbs-Thomson equation for fluids confined to nanopores, S. Simizu, L. Drahushuk, N. Manohar, M. Strano
9:40 PHYS 251, Experimental measurement of extreme phase transition temperatures for water confined inside carbon nanotubes, K. Agrawal, S. Simizu, M. Strano
10:00 PHYS 252, Understanding surfactant structure on the SWCNT sidewall via single molecule photoluminescence spectroscopy, R. Pramanik, S.K. Ioom, 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
Organizer
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(ERSRS), H. Moehwald
8:30 PHYS 255, Analytical superrefractiﬁcation as a tool for characterization of protein nanoparticle 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. Welsh, S. McManus, C. Hia, S. Yin
10:00 PHYS 258, Multiplexing nanoparticle-based SET and FRET to measure correlated distances on DNA, R.A. Risikowski, R. Armstrong, G.F. Strouse
10:20 PHYS 259, Spectroscopic properties of semiconductor quantum dots embedded in biological medium, B. Ellis, W. Jang, J. Elward, F. Iudayananth, S. Narga, 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
Organizer
G. E. Johnson, Organizer, Presiding
J. A. Dionne, Presiding
8:00 PHYS 261, Controlling protein conformation on surfaces by soft-lathing electrospore 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 Au$_{12}$, (SR)$_{12}$ nanoparticle revealed by X-ray crystallography, C. Zeng, R. Jin
9:10 PHYS 264, Core-shell metalloccations: Property alteration and charge-control of substrates, F.Y. Naumkin, R. Chhital, B. Irving
9:30 Intermmission
9:50 PHYS 265, Gold nanoclusters with the protection involving alkyln 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
Organizer
M. S. El-Shall, R.C. Forbenerry, Organizers, Presiding
E. Fayolle, Presiding
8:00 PHYS 269, Spectral features and nanostructural properties of soot as analog of the carbonaceous cosmic dust, T. Pino, T. Le, L. Gavilan, I. Alata, D. Deidique, J. Pouzaud, E. Darmon
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. Rovers, A. Ricca Bauschlicher
9:45 Intermmission
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, F. Gerakines, M. Leofter

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. Piechuch, Presiding
8:00 PHYS 274, Plasmon resonances in acenes and silicones, C.M. Aikens, E. Guizel, 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 Intermmission
9:50 PHYS 276, Structure-Property relationships of curved aromatic materials from first principles, K.K. Baldrige
10:30 PHYS 277, Radical and polycyclic characters of polycyclic aromatic hydrocarbons: A theoretical study, A. Das, H. Lischka
10:55 PHYS 278, Oxygenated quinoid 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 analog of the carbonaceous cosmic analog, S.A. Sandford, C.K. Materese, G.W. Cooper
11:45 PHYS 280, Conduction and efficient rectiﬁcation in unmolecul- lar hemi benzoquinone 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 ANW1, BOLI, BIOT, BMGT1, COMP, DAZC, ENFL1, 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, OMGN 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
13:35 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, G.P. Jaroniec
3:05 PHYS 284, New approaches to simulating biological and molecular catalysts, T.F. Miller
3:35 Intermmission
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. Flaha, O. Holtsz, M. Thomas, J. Sancho Sans
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. Rojas, S. Sukhatev, 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
4:10 PHYS 293, Enabling large-scale hybrid density functional theory calculations in condensed-phase systems, R.A. DiStasio
Section C
Boston Convention & Exhibition Center Room 252B
Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds
Co-sponsored 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. R.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
2:45 PHYS 298. Atmospheric hetro-reaction kinetics related to organic aerosols. H. Aikimoto
3:15 PHYS 299. Single particle time of flight mass spectrometry utilizing a femtosecond desorption and ioniza-tion laser. D. Cziczo, M.A. Wozniakiewicz, A. AbdiEmonen, C. Mohr, H. Saathoff, D. Murphy, K.D. Floyd, T. Lissner
3:30 PHYS 300. OrganoSulfate formation in the secondary organic aerosol produced from photooxidation of various VOCs in the presence of NOx and sulfuric acid aerosol using natural sunlight. M. Jang, H. Jiang, J. Park, R. Beardsky
4:00 PHYS 301. Chemical speciation of organic aerosol driven by phase partitioning. M.J. Walker, B.W. James, W. 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. P. Ault, R.L. Craig, A. Boddy

Academic Innovations for Tomorrow's Industries: GSSPC Symposium
Sponsored by CHEED, Cosponsored by ANI/l, BOTT, BMGT, CORP, D3C/2, ENFL, PHYS2 and POLY*

Innovation in Materials for Emerging Uses
Sponsored by NPPG, Cosponsored by PHYS, PMSE and POLY

Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials

Biologicalinspired Designs: From Molecules to Functional Materials
Sponsored by ENVR, Cosponsored by CE, 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. Kunnmel, 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. Verna
8:35 PHYS 305. Structural dynamics and heterogeneities of localized excited states in conjugated polymers. A.E. Bragg
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. Ho, Y. Taga, K. Hristova, S. Takai, D. Kitagawa, S. Kobatake, H. Miyasaka

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. Herbst, 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 wave-function theory to perturbative-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
11:00 PHYS 317. Energy decomposition analysis for second-order Möller-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 molecules with heavy atoms. T. Shiosaki

Section C
Boston Convention & Exhibition Center Room 252B
Chemical Processes Involving Atmospherically Relevant Trace Gases, Aerosols & Clouds

Section D
Boston Convention & Exhibition Center Room 254A
MolecularBiophysics: 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. Gounet, Presiding
8:00 PHYS 327. Dynamics and conformational changes coupled to changes in pronation states: Should we always blame the histidines? A.E. Roeilberg
8:40 PHYS 328. Mechanism of pH-Triggered self-assembly of polysaccharide. J. Shen
9:20 Intermission.
10:20 PHYS 330. Molecular multipole models for water and biological macromolecules. T. Ichiy
11:00 PHYS 331. Electrostatic effects and spatially extended enzyme active sites. M.J. Ondruch, P.J. Bunting, R. Parasuram, T. Couflli, 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. Bélhuis
8:30 PHYS 333. Efficient and accurate characterization of protein hydration and interactions. E. Xi, R. Rensing, 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
10:50 PHYS 338. Solvation structure and ion-pairing for biological relevant ions using density functional theory. M.D. Baer, C.J. Mundy
11:10 PHYS 368. Reactions in complex biomimetic media. C.D. Keating
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

S. Vajda, D. Kozakov, P. Vakil, I.C. Paschalis

2:10 PHYS 390. Predicting molecular interactions by using protein-protein and protein-RNA docking.
Z. Zou

2:50 Intermission.

P. Carey, H. Haridas Torkabadi

3:50 PHYS 392. Structural modeling of interactome.
I. Arshinchenko, P. Kundratova, I. Vakeva

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. Sarde, 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. Sampat, C. Kingsley, C. Halfen

2:30 PHYS 396. Structure and dynamics of the quasi-liquid-layer on ice I.
T. King, M. Suplu, D. Donadio

WEDNESDAY EVENING

Section A
Boston Convention & Exhibition Center Hall C
Poster Session
E. L. Sibert, Organizer

6:00 - 8:00

4:15 PHYS 386. Using mass spectrometry to determine residual chemical composition in coagulated aerosol experiment.
K. Ardon-Dryer, Y. Huang, D. Cziczo

4:30 PHYS 387. Equilibrium structure of liquid-liquid phase separated aero-

4:45 PHYS 388. Quantitative comparison of mineral-rich aerosol mass spectra and ice nucleating efficiency.
S. Garimella, M. Zawadowicz, Y. Qiu, V. Molinero

Section H
Boston Convention & Exhibition Center Room 257A
Bringing Astrochemicals Back to Earth: Formation Mechanisms, Stability, & Spectroscopic Signatures

S. E. El-Shall, R. C. Fortenberry, Organizers
W. K. Peters, Presiding

S. Ioppolo, B. McGuire, X. de Vleeshouwer, B. Cardell, M.A. Alkob, G.A. Brake

2:05 PHYS 416. Structural studies of reactive molecules by rotational spectroscopy: HOON, HOCOH, and CH2O.
K.N. Crabtree, C. Womack, O. Martinez, J. Stanton, M. Moddel

N. Shuman, S.G. Arai, 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. Hallen, L.M. Zurbur

4:20 PHYS 419. Large amplitude motions and feasible proton per-

4:50 PHYS 420. Multipolar Raman on chiral plasmonic nanoribbons.
M. Banik, H. Rodriguez, E. Huikko, V.A. Aptakhan spectroscopy.
Y. Zhang, E. Anit-Dano, A.N. Dinesh

5:00 PHYS 421. Synthesis and char-

5:40 PHYS 422. Configuration interac-

3D discrete variable calculations of X-ray absorption in isolated AuBr nanoclusters.

PHYS 320. Detailed quantum studies on the m-benzyne and o-benzyne diradicals. B. Zhang, C.A. Parish, C. Annas

PHYS 321. Synthesis and characterization of highly purified bimetallic Au-Nanoclusters. M. Kim, K. Kwak, D. Lee

PHYS 355. Computational study of intermolecular interactions in L-cysteine and 2-mercaptoethylamine compounds using DFT, QAIM, and NBO methods. I.A. Morkan, A.U. Morkan, H.C. Yazed


PHYS 357. X-ray absorption in insulators with non-Hermitian real-time dependent functional theory. R.G. Fernande, M.C. Bahhoff, K. Lopata

PHYS 358. Valence bond theory study of charge-shift binding resonance energy. C. Laconsay, A. James, J.M. Galbraith


PHYS 360. SERS studies of chemo-therapeutic agents. M. Duplanty, C. Marsid, N. Mirsaleh-Kohan

PHYS 361. Energetics of methanol decomposition of graphene-supporte nanoparticles. R.J. Gasper, A. Ramasubramaniyan


PHYS 364. Electrochemical and photophysical studies of Au/bi, for microscopio-photochromic-tether-adsorbed on surface. C.N. Latratta, C. Wheeler, E. Reed, P. Lawrence, G. Anway

PHYS 365. Spectroscopic characterization of electron-lattice coupling in the cooperative proton-electron transfer photocatalytic reaction. A. Fury, S. Sorensen, E. Driscoll, J.M. Davitt

PHYS 366. Modeling nonadiabatic energy transfer dynamics in photosynthetic complexes. M. Lee, D. Cokelaer

PHYS 367. Energetic 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 368. Electrocatalytic efficiency of functionalized multivalved carbon nanotubes toward the oxygen reduction reaction and antiinflammatory drug ibuprofen from aqueous solutions. A. Bakr, M. Rahman

PHYS 369. Determining conformational dynamics of specific regions of a model peptide by 13C isotope-edited ATR-FTIR in H2O. J.D. Combs, V. Wang

PHYS 377. Timescale and energetics of hydrogen level change in an internal cavity of cytochrome c oxidase. C. Son, A. Yehyia, O. Cui

PHYS 378. Photocatalysis of green fluorescent protein: A computational investigation. P. Gunanathan, L.V. Cherkis

PHYS 379. Atomic vibration of FUS N-terminal domain liquid-liquid phase separated states. K.A. Burke, A. Janke, N. Fawzi


PHYS 542. Electrochemical and photophysical studies of Au/bi, for microscopio-photochromic-tether-adsorbed on surface. C.N. Latratta, C. Wheeler, E. Reed, P. Lawrence, G. Anway

PHYS 543. Spectroscopic characterization of electron-lattice coupling in the cooperative proton-electron transfer photocatalytic reaction. A. Fury, S. Sorensen, E. Driscoll, J.M. Davitt

PHYS 544. Modeling nonadiabatic energy transfer dynamics in photosynthetic complexes. M. Lee, D. Cokelaer

PHYS 545. Energetic 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 546. Electrocatalytic efficiency of functionalized multivalved carbon nanotubes toward the oxygen reduction reaction and antiinflammatory drug ibuprofen from aqueous solutions. A. Bakr, M. Rahman

PHYS 547. Determining conformational dynamics of specific regions of a model peptide by 13C isotope-edited ATR-FTIR in H2O. J.D. Combs, V. Wang

THURSDAY MORNING Section A

Structure and Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

Structure, Dynamics, and Behaviors of Material Systems

Cosponsored by CCL, ENFL, CRGN and PHYS

Section A

Boston Convention & Exhibition Center Room 251

Structure and Dynamics in Complex Chemical Systems: Gaining New Insights through Recent Advances in Time-Resolved Spectroscopies

Structure, Dynamics, and Behaviors of Material Systems

Cosponsored by CCL, ENFL, CRGN and PHYS

A. E. Bragg, P. B. Petersen, Organizers

A. T. Krummel, Organizer, Presiding

8:00 PHYS 597. Investigating the influence of composition on excitation dynamics in organic thin films.

P. Goët, B. Cappy, D.A. Blank

8:35 PHYS 598. Origins of recombin-...
Section B
Boston Convention & Exhibition Center Room 252A
Electronic Structure Methods for Large Systems
SCF Functionalons and Algorithms
Cosponsored by COMP
M. P. Head-Gordon, J. Herbert, Organizers
R. Steele, Presiding
8:00 PHYS 605. Multipletetopos 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. Schör, 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 EBRV
D. A. Knopf, S. Lee, Organizers
J. H. Kroll, J. B. Nowak, Presiding
8:00 PHYS 610. Immersion ice nucleation properties of fieldspar mineral. S. A. Kanji, A. Wettl, U. Lohmann
8:15 PHYS 611. Why does acid treatment inhibit ice nucleation on alumino-silicate 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. Shvovon, K. Murphy, G. Schill, M. Tolsberg, K. L. Mueller, M. Freedman
9:00 PHYS 613. How important are glassy SOA ice-nucleus 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.

Section D
Boston Convention & Exhibition Center Room 25A
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. Minor, 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 mechanisms. P. Blevacs, 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. Tolok, A. Drozdtski, N.A. Bakar, L. Pollack, A.V. Othonov

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. Stienemann, 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 hydrophobic 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. Patten ande

Section F
Boston Convention & Exhibition Center Room 255
Protein-Nanomaterial Interfaces & Protein Coronas: Physical Properties, Biocompatibility, & Biological Impact
Fundamentals and Applications
Cosponsored by COLB
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. MacDermid, Z. Qian, C.J. Lenci, 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. Meinser, G.H. Findenegg
8:40 PHYS 629. Shape matters for protein-nanoparticle interactions in biosensing. D. Jin, J. He, E. Lehnhoff, C. Math, L. Sagie
9:00 PHYS 630. Engineered repeat-protein enabled synthesis of gold nanoparticles with tunable morphology. T. Zarkovic Grove, X. Gong, M. Freyman
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. Lewis
8:30 PHYS 635. Raspberry-like metallocules exhibiting strong magnetic resonances. Z. Qian, S. Park, Z. Fakhraii
8:50 PHYS 636. State-resolved electronic relaxation dynamics of structurally precise metal nanoclusters studied using femtosecond and magneto-optical spectroscopy. K. Knappner
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. Hinchluff

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.
9:10 PHYS 642. Photodestruction and reactive processes of interstellar carbon chain anions. R. Weter
9:45 Intermission.
10:15 PHYS 643. Computational study of possible ion-molecule reactions leading to precursors of biocatalysts 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.P. Anantharaman

Section I
Westin Boston Waterfront Grand Ballroom C
Protein-Like Structure & Activity in Synthetic Systems
J. Foster, Y. C. Simon, Organizers
E. B. Berda, Organizer, Presiding
A. Prashe, Presiding
8:00 Introductory Remarks.
8:05 POLY 1. Modular approach to single chain nanoparticles using alternating radical copolymerization. C. Lyon, E.B. Berda
9:35 Intermission.
10:20 POLY 5. Radical polymerization ketenes. Y. Xiang, R. Drout, T. Denmore, E. Pentzer
10:50 POLY 6. Rational design of macro-molecular superstructures. K. Zhang
11:20 Concluding Remarks.
Section D
Westin Boston Waterfront
Commonwealth B
Silicones
S. J. Clarson, J. M. Mabry, Organizers, Presiding
1:00  POLY 73, Silicone-based hyperbranched polymers. P.R. Dvornic
1:30  POLY 74, Silicone polymers in Australia. S.R. Clarke, E. Markovic, K. Nguyen, T. Atchison, N.A. Trout, C.A. Williams
2:00  POLY 75, Water soluble polysiloxanes and their use in Intercalating Polymer Networks (IPN). D. Graiver, K.W. Farriner, S. Dewhasteh, R. Narayan
2:30, Intermission.
2:45  POLY 76, Manufacture and characterization of multifunctional siliconic 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. Hvidt, A. Skov
4:00  POLY 79, Silsesquioxane-based thermosetting oligomers: Chemistry and delivered properties. T.S. Haddad, G.R. Yanotk, 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. Ketyer, 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

Tuesday, January 10

Section A
Westin Boston Waterfront
Grand Ballroom 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
9:05  POLY 89, Response and function in peptide-based block copolymers. G. Strange, I. Smith, C. Machado, D.A. Savin
9:30, Intermission.
9:50  POLY 90, Toward polymer-based artificial metalloenzymes: Modeling second-sphere interactions in synthetic systems. S. Piazzini, 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 antibodies with double selectivity. H. Liang, Y. Jiang, W. Zheng, H. Ma
11:40, Concluding Remarks.

Section B
Westin Boston Waterfront
Grand Ballroom B

Surface Modification of Polymeric Materials
K. J. Wynne, Organizer
C. Wohi, Organizer, Presiding
8:00  POLY 106, Surface-attached polymer layers via C,H insertion reactions. O. Prucker, J. Rushe
8:20  POLY 107, Bioactive and anti-fouling poly(vinylamine) nanoﬁber meshes. J.S. Hersey, M.W. Grinstaff
8:40  POLY 108, Self-organization of ε-caprolactone/poly(caprolactone) pseudopolyoxotannates for nonfouling surfaces with enhanced surface reactivity. M. Oster, A. Hébraud, A. Lapp, E. Polet, L. Ausvais, G. Schlatter
9:00  POLY 109, Non-protein fouling polyisobutylene-based biomaterials via modular surface functionalization. A. Alvaraz Albarran, E.O. Rosenthal-Kim, L. Liu, Z. Nikolou, J.E. Puntes
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. Kizombi
10:40  POLY 113, Dual cyclodextrin polyelectrolytes multilayer coatings on tissue-controlled drug delivery. J. Junthip, N. Tabaey, B. Martel
11:00  POLY 114, Temperature controlled fluorescence resonance energy transfer on poly(propargyl acrylate) nanoparticles modified with oxadiazole and naphthalimide derivatives. Ö. Klep, S.H. Fowler
11:40, Intermission.
11:50  POLY 116,Clickable nanoparticles designed for reagent-free functionalization. O.I. KalogaUi Altan, 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 PE-Si-silane amphiphiles: Impact of structure and concentration. M. Grunlan
8:30  POLY 118, Introducing mixed polyol in polysiloxane and polysiloxane-based structures: Hydrophobic or oleophilic behavior? B. Arkles, Y. Pan, F. Gonzalez
9:00  POLY 119, Designing durable icerophobic surfaces. K. Golovin, A. Tuteja
9:30, Intermission.
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) nanoparticle (Silgard® 184). C. Wang, J.K. Wynne, S. Nar, V. Sharon, T. Shresta
11:00  POLY 123, Wetting properties of polysiloxane networks networked in situ with fluoroalkyl-substituted linear and POSS cage structures. R. Campos, S.M. Ramirez, J.M. Mabry

Section E
Westin Boston Waterfront
Commonwealth E
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. Nos, K.L. Wooley
9:00  POLY 126, Rapid synthesis of a liposomal polymer delivery library via ring-opening polymerization of amine and alkyl functionalized valencianolocenes as potent form for PEG-PAH delivery nanoparticles. D.J. Siegwart, J. Hao, P. Kos, K. Zhou, J.B. Miller
Section A
Westin Boston Waterfront

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, M. Mehmert, M.T. Buchill, G.E. Moelter
2:30 POLY 137. Inter-polymer complex hydrogels formed by thermal and/or pH triggered gellation. P. Sullivan, J. Goddy, B. Bustay
3:00 POLY 138. Innovation in medical adhesives. K. Tsia
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
1:15 POLY 141. Size and shape changes of polymer aggregates and monomer droplets during air-immune polymerization under an optical microscope. J.K. Szymbanski, J. Perez-Mercader
1:40 POLY 142. Synthesis and characterization of phosphonium-containing polyelectrolytes and investigation of their antibacterial activity. T. Eren, C. Suer, C. Demir, T. Kocagöz, A. Yetinlik Unutul
2:00 POLY 143. Green(er) routes toward the synthesis, functionalization, and use of polymers. C.E. Hobbs
2:40 POLY 145. Stereo- and regioregular ring opening metathesis polymerization and cyclopolymerization of cyclic olefins and dinyes containing porc functional groups by functional group-tolerant olefin metathesis catalysts. M. Buchmeiser, R. Schovner, S. Sim
3:00 POLY 146. Hyperbranched-polydendrons: A new branched linear-dendrimer hybrid polymer architecture. F. Hatton, H. Rogers, A. dever, P. Chambon, S. Rannard
3:20 POLY 147. Functional polymer particle 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. Shuman, 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. Arlington, A.R. Whittington, A. Goldstein, D.J. Irvine
4:20 POLY 150. Living anionic polymerization of dihydropyrophosphine styrne for high temperature thermoplastic elastomers. A. Schultz, M. Chen, C. Jiang, T.E. Long

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. Hanken, B. Tuten, Presiding
1:00 Introductory Remarks,
1:05 POLY 175. Tuning volumetric display of peptide antigens on nanoparticles in vaccine design. T. Moyer, C. Ke, D.J. Irvine
1:45 POLY 177. From synthetic mimics of antimicrobial peptides to new delivery reagents inspired by cell penetrating peptides. G.N. Twe
2:35 Intermission.
2:50 POLY 179. OPG-functionalized phenylalanine-based poly(ester ureas) for enhancing osteoinductive potential of human mesenchymal stem cells. G.M. Policasto, 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
3:50 POLY 182. Green routes to peptides that enable its use in a broader range of applications. A. R. Gross
4:10 Concluding Remarks.
TUESDAY MORNING

Section A
Westin Boston Waterfront
Grand Blrm D

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, Glycoproteins for stabilization of therapeutic proteins. H. D. Maynard, E. Palagi-D’Oyay, Y. Liu, J. K. Jo, 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, Thermoelastic elastomers with semicrystalline, glassy, and rubbery blocks. A. Burns, W. Muhran, R. A. Register
10:05 Intermission.
10:20 POLY 156, Synthesis, morphology, and ion transport properties of block copolymer electrolytes. M. Park
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 additives. J. Liu
8:35 POLY 184, Existed and advanced rheological measurements of polymers and rubber compounds. M. Namani
9:05 POLY 185, Free volume and water vapor transport properties of non-chromatized prime films. W. Zhang, M. Jaworowski, G.S. Zafris
9:35 POLY 186, Enhance resource efficiency through innovative polymer design. J. Wang
10:05 POLY 187, Beyond polyhexa-hydrotriazines: From high strength materials to self-healing polymerizable organogels and the development of new polymer-forming reactions. J. M. Garcia

Section C
Westin Boston Waterfront
Grand Blrm D

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 poly-peptide copolymers. P.T. Hammond
8:30 POLY 190, Self-assembly and properties of glycolipidylpolymer bihybrid materials. S. Lecommandoux
9:00 POLY 191, Engineering energy dissipation in protein gels. L. Dong, D.A. Tirrell
9:30 Intermission.
9:45 POLY 192, Hypersialylation via Glycoxalyx Engineering Confers Resistance to Immune Surveillance. C.R. Bertozzi
10:15 POLY 193, Functional poly-peptides and thermoresponsive responsive hydrogels. T.J. Deming
10:45 Award Presentation.
10:50 POLY 194, Synthetic glycopoly-peptides for biomedical applications. J. Kramer, T.J. Deming, C.R. Bertozzi

Section D
Westin Boston Waterfront
Commonwealth B

Silicones
S. J. Clarsom, J. M. Mabry, Organizers, Presiding
8:00 POLY 195, Making alternating siloxane copolymers. J.G. Matison
8:30 POLY 196, Functional siloxane copolymers and elastomers with high dielectric permittivity. F.B. Madsen, A. Daugza, S. Holsted, A. Sun
9:00 POLY 197, High elongation silicon elastomers derived from dual functional siloxane macromonomers. J.D. Goff, S. Salzman, A. Akkas
9:30 Intermission.
10:10 Intermission.
10:20 POLY 199, Stabilization to UV of polysiloxane resins in geostationary environment. M. Planes, S. Cartotti, S. Leonowicz, S. Remaudi
10:35 POLY 200, Conformal polysiloxane- thin film electrolytes for lithium ion batteries. N. Chen, B. Reja-Jayan, J. Lau, P. Mon, 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 HST, PMSE, FNES and PROF
G. N. Tew, Organizer
M. Jeffress-El, L. Korkey, Organizers, Presiding
8:00 Introductory Remarks.
8:05 POLY 202, Advanced materials for regenerative engineering. R. James, C. Laurenici
8:35 POLY 203, Soft multifaced colloids by constrained volume self-assembly. R.D. Priestley
9:05 POLY 204, Printed electronic resolution: 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. Desmone

Academic Innovations for Tomorrow’s Industries: GSSPC Symposium
Sponsored by CHED, Co-sponsored by ANLY, ROLK, BIOTI, BMGT1, CORP1, DAC1, ENFL1, PHR2 and POLY

International Entrepreneurship: How To Start a Business and Thrive in the Global Marketplace
Sponsored by IAC, Co-sponsored by AGFD, AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY: PNSQ, 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. McCreary, J. Wie, V. Tondiglia
1:55 POLY 210, Dual networks incorporating both reversible and irreversible polymers. G. Berg, T. Gong, C. Fernol, A.D. Baranek, C. Bowman
2:20 POLY 211, Biinspired mucin-mimetic brush polymers with selective antiviral properties to influenza A. S. Tang, B. Seltfried, X. Dong, W. Putyear, J. Runstader, 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.
3:50 POLY 214, Poly(propargyl L-glutamate)-based block copolymers for smart drug delivery applications. M. Quadir, S. Morton, L.B. Mensah, K. Shoposzcz, P.T. Hammond
4:40 POLY 216, RAFT polymerization of hydroxy-functional methacrylic monomers under heterogeneous conditions: Effects of varying the core-depolymerizing block. B.A. Blanazs, S.A. Eastman, R. S. Moore, R.M. Laine

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. Body
2:05 POLY 219, Bioinspiried technology: Basic research catalyzes new materials discovery. A. 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.
1:45 POLY 224, New materials from polymeric ionic liquids. J. Texter
2:10 POLY 225, Reactive polyionic liquid s (PILs) and precision synthesis of PIL-based nanostructures. D. Taton, P. Coupillaud, J. Vignolle, M. Weiss-Maurin, D. Dercyere, C. Detremo"
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 Convention & Exhibition Center Ballroom West

Polymeric Materials

T. S. Haddad, R. Campos, J. M. Mabry, Organizers
6:00 - 8:00

345. Applications of anthracene and pyrene as fluorescent probes in targeted cancer therapy.
J. H. T. S. Haddad, S. S. Campos, J. M. Mabry, Organizers
6:00 - 8:00

346. Study of Fenton catalysis in the elimination of binding agent interaction, within polymer bonded explosives.
C. A. Williams, S. Walker, I. Lochert, S. Clarke

347. Improved curing of sodium silicate solutions for soil stabilization.
S. R. Clarke, N. A. Trout, A. K. A. Tufa, T. S. Haddad, R. Campos, J. M. Mabry

348. Polydimethylsiloxane-based materials formed by nanoscale ordering of monodisperse supramolecular building blocks.
H. Zha, B. F. de Groot, J. W. Meijer

349. Study of the polymer - solvent interactions for polyisoxazoles with different functional groups using dissipative particle dynamics.
J. Valeo, A. Gama, G. A. G. Gracia, J. A. C. Carvalho, S. C. Malve, A. V. Villegas Gasca

B. Wenning, J. Frayn, N. Aldred, A. Clare, C. K. Oser

351. Silsesquioxane-based amine-functionalized monomers as building blocks in thiol-ene polymerization: Chemistry and delivered properties.
J. Lamb

Section F
Boston Convention & Exhibition Center Ballroom West

Surface Modification of Polymeric Materials

C. Wohi, K. J. Wynne, Organizers
6:00 - 8:00

352. Effect of cross-linking agent on the grafting modification from sodium rubber.
J. Wang, P. Du, S. Tu, X. Ren

353. Xanthate mediated sequential thiol-acrylate Michael addition polymerization.
R. M. Chiguru, A. A. M. S. Amini, T. J. M. Mabry, Organizers
6:00 - 8:00

354. Grafting of poly(N-isopropylacrylamide) brushes on the surface of cupric mesoporous organosilica via atom transfer radical polymerization.
A. S. Manchanda, M. Krug

355. Tailoring of PVA cryogel porosity using ionic liquids.
A. S. Papanea

356. Hybrid hydrogels for cell therapy.
A. C. Kumar, T. Srithuition, A. A. M. S. Amini, T. J. M. Mabry, Organizers
6:00 - 8:00

357. Functionalization of nanopartic- les with pH sensitive co-polymers for smart self-assembling.
J. Tinklepaugh, O. Sheppard, M. M. M. Mabry, Organizers
6:00 - 8:00


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POLY 360. Surface and interfacial modification of polyethersulfone films via POSS modified chain ends. K.M. Krauer, L. Moore, S.E. Morgan

POLY 361. Lipid clustered nanoparticles to target Er8B3 in high grade serous ovarian cancer. L. Gu, C. Kolt, K. Rangii, L. Mensah, B. Imperati, L. Gittin, P.T. Hammond


POLY 363. Surface attached hydrogel films via novel diazo-ester cross-linkers. P. Kotade, O. Pruckler, J. Rushe


Joint PMSE/POLY Poster Session

Sponsored by PMSE, Cosponsored by POLY

**WEDNESDAY MORNING**

**Section A**

Westin Boston Waterfront
Grand Ball C

Multi-component & Sequential Reactions in Polymer Science: Efficient Synthesis of Structural Diverse Polymers

M. Meier, P. Theato, Organizers, Presiding

8:00 POLY 386. Polyimidazolium salts – novel versatile cat-ionic polymers. J. Lindner


8:50 POLY 388. Synthesis and characterization of polycrylates with different pendant groups for thermoplastic elastomers. W. Lu, N. Kang, K. Hong, J.W. Mays


9:40 Intermittion.


10:45 POLY 372. Withdrawn.

11:10 POLY 373. Synthesis of alkyne macro-molecules with structural diversity through multi-component polymerization. B. Tang

11:35 POLY 374. Sequence-defined polymers via multicomponent reactions. S.C. Solloder, M. Meier

**Section B**

Westin Boston Waterfront
Grand Ball D

Charles Overberger Award Symposium in Honor of Krzysztof Matyjaszewski

R. M. Lane, Organizer, Presiding

8:00 Introductory Remarks.

8:05 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


9:35 Intermittion.

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, D. Montana

10:10 POLY 384. Ionic liquid microemulsions for directing the assembly and morphology of cellularuc nanoparticles. J.R. Alston, A. Guenterth, J.N. Mabry


**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 poly-peptides for exploring the role of shape and sequence on polymer self-assembly. R.A. Segalman, R.N. Zuckermann, H. Buss, A. Patterson, G. Nits


9:35 Intermittion.


10:20 POLY 390. Polymer-peptide hybrids: Tuning mechanics via nature’s building blocks. L. Korley, J. Johnson, M. Targe

**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-phenylendiamine and terephthaloyl chloride. J. Williams, M. Meador, L. McCrindle

8:20 POLY 392. Synthesis and characterization of poly(malic anhydride) 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. Lille, W.C. Searsruse, T.M. Reinke, W.B. Tolman

9:40 POLY 396. Vulcanization of silicone conformal coatings for anti-corrosion applications. J. Wertz, B.M. Koblica, J. Kuczynski, J. Zhang, D. Boslav

10:00 POLY 397. Sulfer-rich polymer nanoparticles through interfacial polymerization: Synthesis, size control, and sulfur content varia- tion. J. Lim, U. Jung, J. Pyun, K. Char


10:40 POLY 399. Degradation of thermostox shape memory polyurethanes and foams. A.C. Weems, D.J. Martin

11:00 POLY 400. Studying of supercritical carbon dioxide effect on physicochemical properties of cassava-based cellulose. P. Nanta, W. Blokamp, K. Kasemwong


12:05 POLY 403. Cu-catalyzed multi-component polymerization. T. Choi


13:00 POLY 405. Passerini multi-component polymerization for new polymers with a range of diversity in both structure and function. Z. Li


2:40 POLY 407. Multicomponent coupling approaches to conjugated poly(3,4-diphenyl) and polyhetero- cycles. L.Y.Kayser, B. Arntzen

3:05 Intermittion.

3:20 POLY 408. Functionalyzed ABC triblock copolymers: Multicompartiment micelles as a scaffold for advanced nanoreactors. A. Cohen, M. Week


4:35 POLY 411. Tandum living radical polymerization with transterification as modular synthetic approaches to gradient, telechotic, and pinpoint-functionalized polymers. T. Tarashima, Y. Ogura, M. Sawamoto


**Section B**

Westin Boston Waterfront
Grand Ball D

Charles Overberger Award Symposium in Honor of Krzysztof Matyjaszewski

R. M. Lane, 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 materials and tissue. E. Kumacheva

2:30 Intermittion.

3:00 POLY 416. Polymer-protein conjugates for the treatment of disease. O.S. Tucker, C.A. Figg, B.S. Sumerlin


4:00 POLY 418. From new catalytic and initiating systems for ATRP to new materials. K. Matyjaszewski
**Section C**

Weston Boston Waterfront
Grand Ballroom 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. Makakui, C. Appiah, P. Zare, A. Stojanovic-Marino, F. Kremer, W.H. Binder

2:40 | **POLY 421.** Conductivity scaling relationships in nanostuctured membranes based on proton polymerized ionic liquids. - R.A. Segalman, G. Sanjana, C.M. Evans, B. Beckingham, Y. Schneider

3:30 | Intermission.

2:45 | **POLY 422.** Dynamics of polymerized ionic liquids and their monomers. - U. Choi, A. Mittra, T. Price, H.W. Gibson, J.P. Runt, R.H. Colby

3:10 | **POLY 423.** Multirole responsive polymer actuators: A matter of speed and sensitivity. - H. Lin, O. Zhao, J. Yuan


**Section D**

Weston 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 graphenes. - E.L. Thomas, J. Lee

2:05 | **POLY 427.** Self-assembly and ion transport in sequence-defined block copolyelectrets. - N.P. Balsa, 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 microphase separation in globular protein polymer diblock copolymers. - B.D. Olsen, C. Lani, A. Huang, M. Kim

**Wednesday Evening**

Joint PMSE/POLY Awards Reception and Plenary Lecture

Sponsored by PMSE, Cosponsored by POLY

**Thursday Morning**

Section A

Weston Boston Waterfront
Grand Ballroom 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

9:25 | **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. Fere, 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. Epeel

10:20 | **POLY 447.** Sequential post-polymerization modifications. - P. Theato, F. Friesinger

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. Jaeckle

12:00 | Concluding Remarks.

**Section B**

Weston Boston Waterfront
Grand Ballroom D

**Ring Opening Polymerization**

B. Bodas, M. Jeffries-El, Organizers, Presiding

8:00 | **POLY 451.** Fabrication of semi-conductor block copolymers via ring-opening metathesis polymerization. - F. Elicata, M. Wick

8:25 | **POLY 452.** Ring-opening metathesis polymerization as a strategy to prepare organic electronic materials via backbone-driven molecular self-assembly. - S. Muench, M. Nguyen, J.D. Bledsoe, B.J. Holiday

8:50 | **POLY 453.** Renewable furan-based epoxy systems for self-healing applications. - F. Cu, G. Palmese

9:15 | **POLY 454.** Controlling NCA ring opening polymerisation to achieve well-defined hydrogels. - C.D. Vacone, H. Schlaad

9:40 | **POLY 455.** Linear and branched polyesters with a high affinity to polyolefins: Synthesis, characterization, and their application. - L. Jansska-Walc, M. Bouyayhi, R. Duchateau

10:05 | **POLY 456.** Tailoring hyperbranched polyether polyls with adjustable degree of branching and hydrophilicity by random anionic copolymerization of alkyne oxides and glycidol. - J. Seiwert, M. Schoemer, M. Bauer, H. Frey

10:30 | **POLY 457.** Poly(caprolactone-ran-methacrylic acid) block copolymer with light-actuated shape memory properties. - X. Xu, B.M. Budhia

10:55 | **POLY 458.** Grignon-based anionic ring-opening polymerization of propylene oxide activated by trisobutylalumini um. - K. Roos, S. Carlotto


9:05 | **POLY 462.** 1,2,3-Trimiazolium-based polyionic liquids: A new class of functional ion conducting materials. - E. Dekkenmuller

9:30 | Intermission.


10:10 | **POLY 464.** Polymeric ion networks: Synthesis and application in catalysis. - P. Zhang, X. Jiang, S. Dai


**Section E**

Weston Boston Waterfront
Commonwealth C

**General Topics: New Synthesis & Characterization of Polymers**

B. Barkakaty, D. Garcia, Organizers

M. von Czapiewski, Z. Zhang, Presiding

8:00 | **POLY 466.** Dodecagonal quasicyrstalline morphology in a poly(propylene-b-isoprene-b-styrene-ethylene oxide) tetrablock terpolymer. - J. Zhang, F.S. Bates

9:20 | **POLY 467.** Cyclodextrin strategies to polyhologenated carbon-rich architectures: Ortho-arylene foldamers, polyyclic aromatics, and graphene nanoborbons. - D. Lahmert, M.J. Aztala, W. Dichtel

8:40 | **POLY 468.** Fragmentable oligoionic liquids assembled through anhimeric-assisted nucleophilic substitution of thiabicyclo[3.3.1]nonane derivatives and their application in transsections. - Z. Geng, M.G. Finn

9:00 | **POLY 469.** Accessing block copolymers containing conductive and insulating segments through multilinking catalysts. - K. Souther, E. Palermo, A.J. McNiel


9:40 | **POLY 471.** Living anionic polymerization of 4-vinybenzyl piperidine ABC triblock copolymer thermoplastic elastomers. - M. Chen, A. Schultz, C. Jiang, 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. Budhia

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**Division of Polymeric Materials Science and Engineering**

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

**SUNDAY MORNING**

**Section A**

Westin Boston Waterfront

**Harbor Bldm III**

**Eastman Chemical Student Award in Applied Polymer Science**

Financially supported by Eastman Chemical Company

J. W. Gilmer, Organizer

**C. J. Jenkins, Presiding**

8:30 **PMSE 1.** Probing percolation pathways in binary polymer nanoparticulate films. L. Renna, M. Bag, T. Gehan, X. Han, P.M. Lahd, D. Marx, H. Y. Kim and S. Agrawal

9:00 **PMSE 2.** Ternary blend polymer solar cells with enhanced power conversion efficiency. L. Lu


10:00 **PMSE 4.** Bicomponent nano-fibers produced by GPG process. S. Rajgarhia, S.C. Jana

**PMSE**

**OTHER SYMPOSIA OF INTEREST:**

Innovation from Discovery to Application Plenary Session (see PMPP, 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

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**THURSDAY AFTERNOON**

**Section B**

Westin Boston Waterfront

**Grand Bldm D**

**Ring Opening Polymerization**

D. Bodat, M. Jeffries-El, Organizers, Presiding

1:00 **PMSE 476.** 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. Hom, G.O. Jones, J.E. Rice, V. Purova


1:50 **PMSE 480.** Controlled ROMP of cyclotetubenes by tuning the steric bulk of the monomer pendant chains: An efficient route towards well-defined cyclotetubene-based diblock copolymers. J. Vio, S. Granados Focil

2:15 **PMSE 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 **PMSE 482.** Thermoresponsiveness and mechanical properties of highly concentrated aqueous poly(L-proline) solutions. M. Gikas, R.K. Avery, B.D. Olsen


3:30 **PMSE 484.** Enzymatic ring-opening polymerization of α-pendentacalcetone by reductive extraction. S. Spinella, G.L. Re, J. Raquez, P. Dubois, M. Ganesh, R.A. Gross

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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**
Section D
Westin Boston Waterfront
Alcott
Advanced Materials for High Performance Formulations
Financially supported by The Dow Chemical Company.
C. 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
9:30 PMSE 22. Passive cooling with UV-resistant siloxane coatings in direct sunlight. J.J. Benkoski, C.M. Hoffman, K.S. Caruso
10:10 Intermission.
10:55 PMSE 25. Controlling crystallization and polymorphism to enhance charge mobilities in conjugated polymers. E. Gomez
11:45 PMSE 27. High power factor, completely organic, thermoelectric polymer nanocomposite thin film multilayer assemblies. J.C. Gunlani, C. Yu, C. Cho

Section E
Westin Boston Waterfront
Fanueil
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 polymethyl methacrylate/poly(styrene) triblock copolymers. M. Mahanappra
9:30 Intermission.
10:05 PMSE 31. Influence of polycrylic acid content on phase separation and water uptake in polysobutylene based micromark star polymers. K.M. Knauer, Y. Zhu, R.F. Storey, S.E. Morgan
10:45 PMSE 33. Effects of high speed extrusion on catalyzed interchange reaction in biobased polyester/polyamide blends. J. Gu, M.J. Sobkowicz, A. Farahanchi, M. Palacios, J. Banntting
SUNDAY AFTERNOON
Section A
Westin Boston Waterfront
Harbor Bld 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. Werring, J. Jiang, C.K. Ober
1:30 PMSE 35. Radical polymers in solid-state organic electronic devices. B.W. Boudours
2:00 PMSE 36. Directed self-assembly of block copolymers for high resolution lithographic applications: From materials design to pattern transfer. G. Hadzioannou
2:30 PMSE 37. Close look at the surface orientation of semiconducting molecules with X-rays. M.L. Chabinyc
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. Incoccia
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 peptide polymers. R.N. Zuckermann
4:30 PMSE 41. Consequences of identity 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 ACSR
G. A. Vaughan, Organizer
R. F. Jordan, Organizer, Presiding
L. R. Sita, Presiding
1:00 PMSE 43. Linear low density polyethylene 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. Golberg
2:00 PMSE 45. Advances in alkene polymerization. G.W. Coates
2:30 PMSE 46. Development of fourth generation metallocene catalysts for high temperature Ethylene-o-olefin copolymerization reactions. J. Klosin, P. Fontane, R. Figuera
3:00 Intermission.

Section C
Westin Boston Waterfront
Douglas
Patternning Materials for Bio-Interface
Financially supported by Nature Chemistry.
J. Hedrick, A. Nelson, Organizers, Presiding
1:00 PMSE 47. Nano- and microfabricated hydrogels for regenerative engineering. A. Khademhosseini
1:30 PMSE 48. Tunable micro and nanostuctures for the modulation of fibrosis and wound healing. T. Desai
2:00 PMSE 49. Printing living tissues. J. Lewis
2:30 PMSE 50. Advanced technologies in biomimetic and biofabrication for on-chip tissue models. U. Demirci
3:00 Intermission.
3:10 PMSE 51. Free-form microfabrication of bioimplants into structures capable of guiding cell morpholgy and alignment. J. Jaworski
3:30 PMSE 52. Surface-attached polymer layers for the control of surface-cell interactions. O. Prucker, M. Eschhorn, K. Anselm, J. Ruehe
3:50 PMSE 53. Decreased bacterial activity on nanopatterned PDMS replica for catheter-associated infection prevention. L. Liu, B. Luan, L. Sun, T. Webster
4:30 PMSE 55. Surface patterning of ionically cross-linked alginate hydrogels. M. Bruchet, A. Mülman

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 56. Advantages of precision in functional copolymers: Mechanical properties and chain dynamics. K.I. Winey
2:00 PMSE 57. High performance water-based coatings with improved eco-footprint through the use of self-assembled polymer pigment composites. J. Bohling
3:10 Intermission.
3:25 PMSE 60. Direct integration of polymers and colloidal nanocrystals for electrochemical memories. D.J. Milliron, E.L. Runerstrom, J. Kim, G.K. Ong, B. Halms
3:55 PMSE 61. Experimental approach to direct characterization of the Z-mer in gradual addition emulsion polymerization. R. Ewen, V. Gao, D.A. Kline, T. Zhang

Section E
Westin Boston Waterfront
Fanueil
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, B. Zhang, Presiding
1:30 PMSE 63. Self-assembly of block copolymers with bottlebrush architecture. J. Rayez
2:50 PMSE 65. Chemical and morphological changes of sulfonated poly(styrene-2-phenoxymethyl methacrylate): Effect of block composition. M. Perez Perez, D. Sukliman Rosado
3:50 Intermission.
4:05 PMSE 66. Double-stage phase separation in dynamically asymmetric ternary polymer blends. C. Kuang, S. Gai, R. Foudazi
3:45 PMSE 68. Shape memory polymer blends. K.A. Cavicchi, H. Fairbairn, J. Lee, M. Pantoja

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**MONDAY MORNING**

**Section A**
Westin Boston Waterfront
Burroughs

New Advances in Nanostructured Polymeric Membranes for Filtration

**Section B**
Westin Boston Waterfront

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

**Section C**
Westin Boston Waterfront

Olefin Metathesis for Functional Polymer Materials

**Section D**
Westin Boston Waterfront

Advanced Materials for High Performance Formulations

**Section E**
Westin Boston Waterfront

Fanueil

Phase Separation and Morphology Development in Polymers

**MONDAY AFTERNOON**

Section A
Westin Boston Waterfront

Burroughs

New Advances in Nanostructured Polymeric Membranes for Filtration

**Section B**
Westin Boston Waterfront

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

**Section C**
Westin Boston Waterfront

Materials for Printed Electronics

**Section D**
Westin Boston Waterfront

Advanced Materials for High Performance Formulations

**Section E**
Westin Boston Waterfront

Fanueil

Phase Separation and Morphology Development in Polymers

**Section A**
Westin Boston Waterfront

Burroughs

New Advances in Nanostructured Polymeric Membranes for Filtration

**Section B**
Westin Boston Waterfront

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

**Section C**
Westin Boston Waterfront

Materials for Printed Electronics

**Section D**
Westin Boston Waterfront

Advanced Materials for High Performance Formulations

**Section E**
Westin Boston Waterfront

Fanueil

Phase Separation and Morphology Development in Polymers
Section A
Westin Boston Waterfront

Section B
Westin Boston Waterfront


10:00 Intermission.


10:40 PMSE 156. Metalocene-catalyzed olefin polymerization studied by solution dynamic nuclear polarization (DPN) NMR. C. Chen, W. Shi, C.B. Htily

Monday Evening

TUESDAY MORNING

Section A
Westin Boston Waterfront

New Advances in Nanostructured Polymeric Membranes for Filtration

Nanostructured Membranes for Water Purification

B.T. Chu, B.S. Hsiao, Organizers

V. Fregel, A. Taniski, Presiding

8:00 PMSE 145. Highly permeable nonfibrous membranes for water purification. B.S. Hsiao, B.T. Chu

8:30 PMSE 146. Reusable bacteria immobolized electropun nonfibrous web 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.


10:15 PMSE 149. Ultrafiltration membranes by reversible assembly of polymer brush nanoparticles. I. Zhavor

10:45 PMSE 150. Bottom up self-assembly strategies for the fabrication of nanostructured polymeric membranes. M. Mahanthappa, G. Sorensen, J. Jennings

11:15 PMSE 151. Adsorption of bacteria into electropun cellulose nanomats: Effect of surface functional- ality. J.D. Schafman, K. Fieger

Section B
Westin Boston Waterfront

Adams

Transition Metal Catalyzed Olefin Polymerization: Towards Structure Control

Technical Session

Corrsoned 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-Bu,P-igated methylpalladium complex. D. Kim, A. Bell, R.A. Register

9:00 PMSE 153. Organometalllic chromium catalysts in olefin polymerization. G.E. Alliger

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Section D
Westin Boston Waterfront
Alcott
Roy W. Tess Award: Symposium in Honor of Jamil Bagdachi
K. Matyjaszewski, G. K. Ober, Organizers
B. D. Freeman, D. C. Webster, Organizers, Presiding
9:00 PMSE 163. Synthesis and characterization of oligoconjugated compounds and their applications as polymer coatings. R. Zarras
10:00 PMSE 165. Concepts for the deposition and structure of films—graphene nanocomposites and enzyme triggered deposition of cassein 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 carbbid functional resins: Polyurethanes through epoxy chemistry. D.C. Webster

Section E
Westin Boston Waterfront
Fanueil
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
8:30 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. Trelil

Henry A. Hill Centennial Symposium: Innovation in Polymer Science
Sponsored by POLY, Cosponsored by HIST, PMSE, FRES and PRF2

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
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 176. Molecular mechanisms of membrane desalination. V. Freger
2:00 PMSE 177. Icon:supporting understanding fundamental structure-transport relationships for RO membranes. A. Roy, S. Rosenberg, R.C. Gleskowi, M. Paul, I. Tomlinson, M. Perey, S. Jons
2:30 Intermission.
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. Elmelech

Section B
Westin Boston Waterfront
Adams
Adhesion Science and Adhesive Materials
Mechanism of Adhesion
Financially supported by IM Company, ExxonMobil Chemical Company
R. Topali, Organizer
A. Crosby, A. R. Forrof, Organizers, Presiding
1:00 Interim Remarks.
1:10 PMSE 180. Adhesion aspects of polymeric materials. J. Bagdachi
2:00 PMSE 181. Surface tension and its effect on the mechanics of contact and fracture of soft matter. 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
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
G. Gilmore, J. J. Watkins, Organizers, Presiding
1:00 PMSE 185. Advanced micro- and nanomanufacturing of large-area functional surfaces. B. Stadiolob, D. Nees, U. Pafliger, S. Ruttilo, M. Belegats
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 nanomanufacturing 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. Kovacik, K. Glasbon
3:40 PMSE 190. Highly conductive PEDOT/PSS nanofilbs induced by solution-processed crystalline formation and its application as flexible and transparent parent electretes. S. Lee, N. Kin, K. Lee

Section D
Westin Boston Waterfront
Alcott
Roy W. Tess Award: Symposium in Honor of Jamil Bagdachi
B. D. Freeman, D. C. Webster, Organizers
K. Matyjaszewski, C. K. Ober, Organizers, Presiding
1:00 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.
4:00 PMSE 196. Smart and functional materials. J. Bagdachi

Section E
Westin Boston Waterfront
Fanueil
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. Razev
1:30 PMSE 198. Polymer chemistry’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.

TUESDAY EVENING
Section A
Boston Convention & Exhibition Center
Ballroom West
Joint PMSE/POLY Poster Session
Sponsored by POLY
C. L. Soles, Organizer
6:00 - 8:00 PMSE 203. Carbazole-assisted electrodeposition of graphene oxide: Synthesis, characterization, and directed deposition. R. Advincula, J.O. Madrigal, R.C. Advincula
PMSE 204. Polymer grafted graphene oxide (GO) nanoparticle dispersions. A. Advincula, J. Madrigal, R.C. Advincula
PMSE 205. Post-synthetic modification of a bis(mino)pyridine-linked porous polymer with inorganic fluorinated ions for highly selective CO2 capture. P. Arab, H.M. El-Kadi
PMSE 206. New polyurethane-like material based on proteins. A. Araujo, A. Machado, B.D. Olsen
PMSE 210. Removal of heavy metal ions by a polymer matrix containing dithiocarbamate as a chelating group. F. Darmaki, B. Boke Sankahya, H. Sarkahya, V. Nt, A. Alewada
PMSE 212. Hydrogel based protein microarray for SIRS detection. A. Buderer, T. Brandtbaeter, O. Pruckler, J. Ruhe
PMSE 213. Emission tuning of boron nitride-coordinated β-diketone poly(lactic-acid) materials through methoxy substitution. T.P. Butler, C.A. DePissa, C. Fraser
PMSE 214. Hydrophilic yet non-water soluble electrospin nanofibers for specific contamination detection using microfluidics. L. Buttar, O. Druva, M.W. Frey
PMSE
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. Arinzeh
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. Cazzell, 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. Chyasnavichyus,

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 dinaphthoylmethane polylactide. C.A. DeRosa, J. SamoninaKosicka, 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 Janustype 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. Filikci, 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. Ostanen

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. Chyasnavichyus, 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 Miscarthus x.
Giganteus. M. Hunsen, A. Way,

Z. Xue, E. Cudjoe, S.J. Rowan
PMSE 251.

Controllable wettablity of layerby-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 of 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. Woltornist, 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 Sejoubsari,
T. Xu, S.J. Woltornist, D.H. Adamson

PMSE 281.

New technique for preparation of uniform brush polymers
using surface-initiated atom transfer
radical polymerization. R. Mohammadi
Sejoubsari, 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. Matsuura,
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. Adibhatla


TECHNICAL PROGRAM

WEDNESDAY MORNING

Section A
Westin Boston Waterfront

General Papers/New Concepts in Polymeric Materials

Biological and Biomedical Materials

C. L. Soles, Organizer, Presiding
8:00 347. Complete biobased polymer derived from polyactic acid and starch nanocrytal: The preparation process for practical model of green disposable plastic. K. Laohasurayut, P. Songkhum, K. Kasamwong, W. Pinkrit


8:40 349. Polyethylene glycol (PEG) polymer brushes protect nuclear acid from DNase degradation by steric hindrance. X. Lu, P. Xu, J. Tan, K. Zhang

9:00 350. Efficient synthesis of multiblock copolymer microfibers via interfacial bioorthogonal polymerisation. S. Liu, H. Zhang, J.M. Fox, J. Xu


9:40. Intermission.

10:00 352. Characteristics of polycaprolactone grafted propargyl dehydroabiatic ester (PCL-g-DAPE) by on-line differential pressure viscometer and light scattering detectors. N. Hamidi, F. Clemens


Section B
Westin Boston Waterfront

Adhesion Science and Adhesive Materials

Interfacial Wettting

Applications Supported by IM Company, ExxonMobil Chemical Company

A. R. Formak, Organizer
A. Crosby, T. Tripathy, Organizers, Presiding

8:30 Introductory Remarks.

8:40 357. Contact mechan- ics of soft solids. E. Dufresne


10:00 Intermission.

10:15 359. Withdrawn.


11:15. Modulating wet adhesion properties of polyelectrolyte multilayers. C. Li, Y. Gu, N. Zacharias

11:15. Conclusion 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

10:30 PMSE 360, Materials for epi-

dermal and water-soluble forms of

flexible electronics. J.A. Rogers

9:00 PMSE 363, Thin and flexible organic
devices for wearable or implantable
electronics. P. Zalar, T. Sotome

9:30 PMSE 364, 3D printing of flexible
electronics and sensors. J. Lewis

10:00 Intermission.

10:30 PMSE 365, Field-effect transis-
tors 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 biosen-

sors. H.E. Katz, K. Besar, X. Guo, Wu Huang

11:10 PMSE 367, Parasitic capacitance
effect on dynamic performance of

printed sub-2 volt electrolyte-gated

poly(3-hexylthiophene) transis-
tors. F. Zare Bidoky, C.D. Friddle

11:30 PMSE 368, Flexible microop-

cular parylene cages as spacer/spring

elements for REWOD energy harvesting
devices. A. Menner, Q. Jang, A. Bimarck

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. Adakam, A. Luthi,
C. LaGuzyder, M. Hahn, N.C. Gianneschi

8:20 PMSE 370, SNAPSHOT Gram-negative

bacteria with star-shaped polypep-

dides. S. Lam, N. O’Brien-Simpson,
N. Pantarat, A. Sulitio, 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 medi-

cine. G. Ginar, M. Goktas, I. Orijapoff,
J. Ade, T. Ikhay, M.O. Ouler

9:00 PMSE 372, Thin-film catalysts from

enzymatically active polymer biocon-

jugates. A. Huang, G. Qin, B.D. Olsen

9:20 PMSE 373, Nanoparticle delivery of

Vibrio cholerae communication signals.

H. Lu, N. Weissmüller, A. Speigel, A. Hurley,
D. Perez, K. Maset, L. Ensign, J. Hanes,
B. Basfier, M.S. Sammonhak, R.K. Prudhomme

9:40 PMSE 374, Supramolecular

gel polymer as an enteric elastomer

for safe gastric devices. S. Zhang,
J. Zhu, R.S. Lange, G. Traverso

10:00 Intermission.

10:20 PMSE 376, Hybrid liposomal

polymeric nanoparticle delivery of

combination chemo-, immuno-, and RNA

therapy for triple negative breast cancer.
C. Scandone, R. Jaska, C. Tanos, P. Pae, F. Ekez

10:40 PMSE 376, Development of

multifunctional DNA-based nano-

molecules for biomedicine applica-
tions. 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. Valucic, S. Kuss, G. Bisker, A. Landry,
S. Islam, R. Jan, 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. Bencewicz

11:40 PMSE 379, Phospholipid polymer

interfaces reveal activation dynamics of

C-reactive protein. T. Goda, Y. Miyahara

Section E
Westin Boston Waterfront
Fanueil

Celebrating 50 Years of Polymer
Science and Engineering

K. Carter, E.B. Coughlin, G. N. Tew,
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, TissuGlue: 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 morphol-

ogy and performance of organic

photovoltaics. T.P. Russell

10:30 PMSE 384, Nanostructure and mate-
ial construction through peptide or block
copolymer solution assembly. D.J. Pochan

11:00 PMSE 385, Illumination alters the

assembly and conformation of conju-
gated 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

scanning model for characterization of

water channel in diblock copo-

lymer 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 sulfon-

ated polyether 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 morphol-

ogy-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

impregnated conjugated polymer films.
A. Serreman, S. Krishnan, S.J. DeLuca,
M.C. Turk, D. Roy, E. Honavar, P. Goulou

2:40 PMSE 391, Physical and trans-

port properties of functionalized

poly(phenylene)s, and their applica-
tion in vanadium redox flow bat-

teries. T. Largier, C.J. Cornelius

3:00 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

3:30 Concluding Remarks.

PMSE

Westin Boston Waterfront

Advances in Polymer
Synthesis and Processing

C. L. Soles, Organizer, Presiding

1:00 PMSE 403, Synthesis and char-

acterization of a supramolecular

thermostatic elastomer. L. Voooraar,
M. Diaz, F. Lenou, A. Abakumov, G. Van
Assche, B. Van Mele, R. Hoffmann

1:20 PMSE 404, Preparation and char-

acterization of copolymer containing

cadmium. Y. Jiang, L. Shu, Q. Liu, H. Zhang

1:40 PMSE 405, Preparation and charac-

terization 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. Ertas, T. Uyar

2:20 PMSE 407, Introducing met-

al-containing monomers in emulsion

polymerization for the preparation of smart

stimuli-responsive polymeric

capabilities. D. Scheid, M. Galbi

2:40 PMSE 408, Continuous process-

ing of polyanilides with superfried

water. G.C. Evans, A.J. Lesse

3:00 Intermission.

3:20 PMSE 409, Chemical vapor

deposition of 2D polymeric carbon

nitride. J. Thieren, D.F. Schmidt, Y. Li

3:40 PMSE 410, Utilizing electron

transfer mechanism of chlorophyll A under

visible light for living polymeriza-

tion. C. Boyer, S. Shannugam, J. Xu

4:00 PMSE 411, Investigation of dose

rate effects in electron-beam initi-

ated polymerization. S.M. Schissel,
S.C. Lapin, J.L. Jessop

4:20 PMSE 412, Synthesis and pho-

tophysical properties of triblock
copolymer-carbon nanotube hybrid materials functionalized with ruthe-

nium complex photoinitiators.

4:40 PMSE 413, Photopolymerized

thiol-ene networks made from natural

products. J.R. Davidson, R. Reit,
B.R. Lund, W. Volt, R. Smaldea

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 respon-

sive elastomer based hybrids with
tunable multifunctionality. S. Zeng,
W. Huang, H. Nguyen, A.T. Smith,
L. Sun

1:20 PMSE 415, Multiresponsive surface

via wrinkling. S. Zeng, W. Huang,
H. Nguyen, A.T. Smith, L. Sun

1:40 PMSE 416, Withdrawn.

2:00 PMSE 417, Facile fabrication of

hyperbranched polymer nanoparti-

cles via nonemulsion polymerization.
C. Hyon, H. Jeong, Y. Jang, B. An

2:20 PMSE 418, Designing of poly-

meric microstructures using a dynamic reaction-diffusion

process. T. Shim, S. Yang, S. Kim
PMSE TECHNICAL PROGRAM

WEDNESDAY EVENING

Section A
Westin Boston Waterfront

Adams

Wednesday Science and Adhesive Materials

Bio-Inspired Adhesion

Financially supported by 3M Company, ExxonMobil Chemical Company

A. Crosby, Organizer

A. R. Forrom, 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. Dhinowala

10:00 Intermission.

10:15 PMSE 447. Developing new adhesive designs and capabilities from the biomimicry of pollinators. J.C. Meredith, H. Lin, D. Shin


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


8:20 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-ProDOT cross-linked PEDOT films. B. Wei, J. Lu, L. Ouyang, N.S. Bhagwat, D.C. Martin

9:00 PMSE 454. Hydrogen assisted growth of conducting polymer microstructures for supercapacitors. K.P. Diaz Orejana, 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. Her, N.J. Long


10:00 Intermission.

10:20 PMSE 457. Hybrid TEOS-TiPenta block copolymer composite membranes: Morphology, physical properties, and liquid transport. F. Huang, C.J. Cornelius


11:00 PMSE 459. Design of assemblies based on polymer-coated quantum dots and organic dye. A. Machado, I. Mousa, A.S. Abu


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. Multicomponent 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. Colart, B.D. Olsen

8:40 PMSE 464. Self-assembly of nanostructured materials through irreversible covalent bond formation and their application. G. Yun, K. Kim


9:40 Intermission.

10:00 PMSE 467. Direct mapping of local director field of nematic liquid crystals at the nanoscale. Y. Xia, F. Sama, 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


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
Westin Boston Waterfront
Faneuil

General Papers/New Concepts in Polymeric Materials
C. L. Soles, Organizer, Presiding

8:00 PM  PMSE 473. Preparation, cyclization, and pyrolysis of poly(methyl vinyl ketone) as a carbon fiber precursor polymer. J.W. Knumpfer, M. Krapper, A. Müller, M. Buchmeiser, K. Muelen
8:20 PM  PMSE 474. Modulator synthesis of functional polymer nanoparticles from poly(2entafluoropropyl methacrylate). Y. Lee, J. Lim, P. Thaot, J. Fuyu, K. Char
8:40 PM  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 PM  PMSE 476. Stimulus-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 PM  PMSE 477. Withdrawn.
10:00 PM  Intermission.
10:40 PM  PMSE 480. Exfoliated boron nitride polymer composites by a solvent trapping technique. C. Chapman, Z. Cui, A.V. Dobryn, D.H. Adamson
11:00 PM  PMSE 481. Cellulose nanocrystal-polyamide 6 nanocomposites with improved creep resistance prepared via in-situ polymerization. S. Kashani Rahimi, J. Otaigbe
11:20 PM  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 PM  PMSE 483. Mechanical, morphological, and rheological properties of PBS/silica nanocomposites manufactured using a high-speed twin-screw compounder. X. Chen, M.J. Sobkowiak

SUNDAY AFTERNOON
Section A
Westin Boston Waterfront

Adams

Adhesion Science and Adhesive Materials

Anti-Adhesion
Financially supported by 3M Company, ExxonMobil Chemical Company
A. Crosby, Organizer
A. R. Fororn, R. Tripathy, Organizers, Presiding
1:30 Introductory Remarks.
1:40 PM  PMSE 495. Everything SLIPS: Anti-adhesive properties of liquid-infused surfaces. J. Atzenberg, P. Kim, T. Wong
2:25 PM  PMSE 496. Stimulus-responsive superoleophobic polymer brushes showing excellent oil drop motion and low adhesion properties underwater. G. Dandertle, M. K. C. Ura, A. Hozumi
2:45 Intermission.
3:00 PM  PMSE 497. Mechanism-based approach to reduce biological adhesion. C. Del Grosso, T. McCarthy, C. Clark, J. Cloud, J.J. Wilkin
3:20 PM  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 PM  PMSE 499. Shedding light on new benefits. B. Tylkowski, M. Giambonni, S. Fernandez Perez, J. Smeltz, J. Otaigbe
1:20 PM  PMSE 500. Characterization of MgO-PA-PLLA nanocomposites as antibacterial scaffolds for orthopedic tissue engineering applications. D.J. Hickey, T. Webster
2:00 PM  PMSE 502. Light-responsive nucleic acid-drug nanostructures. X. Tan, B. Li, X. Lu, F. Ja, C. Santor, P. Menon, B. Zhang, H. Li, J. Zhao, K. Zhang
2:20 PM  PMSE 503. DNA polymer amphi\philes as mRNA regulation agents: Properties and applications. S. Barnhill
2:40 PM  PMSE 504. Turning bacteria’s defense mechanism against them: Towards beta-lactamase-triggered release of antibiotics. Z. M. Hudson, A. McGrath, C.J. Hawker, D. Kinger

1:00 PM  PMSE 505. Nonsmall-cell-lung-cancer treatment using Hsp90 inhibitor carrying magnetic nanotheranostics. J. Kallu, B. Heckert, S. Sultiana, S. Santra
2:00 PM  PMSE 502. Light-responsive nucleic acid-drug nanostructures. X. Tan, B. Li, X. Lu, F. Ja, C. Santor, P. Menon, B. Zhang, H. Li, J. Zhao, K. Zhang
2:20 PM  PMSE 503. DNA polymer amphiphiles as mRNA regulation agents: Properties and applications. S. Barnhill
2:40 PM  PMSE 504. Turning bacteria’s defense mechanism against them: Towards beta-lactamase-triggered release of antibiotics. Z. M. Hudson, A. McGrath, C.J. Hawker, D. Kinger

SUNDAY AFTERNOON
Section A
Boston Convention & Exhibition Center Room 210C

Professional Legacy of Henry Hill
Professionally supported by GEPA, CMA, ETHI, HIST, ORGN, PMSE, POLY, PRES and SCHB
E. A. Nailey, 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. Nailey
2:00 PROF 2. Henry Hill, on of the founding fathers of professionalism. A. E. Pavlah
2:50 Intermission.
3:00 PROF 4. Facets of professionalism: Writing and editing. M. Ora
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
Professionally supported by AGRO, CARB, CHAS, CHED, ONF, COLLE, ENFL, PROF and SCHB

National Science Foundation’s Centers for Chemical Innovation
Professionally supported by PMSE, Cosponsored by AGRO, CARB, COLL, ENFL, PROF and SCHB

True Stories from Entrepreneurs: BizTalk
Professionally supported by SCHB, Cosponsored by CARB, COLL, I&EC, JAC, PRES and PROF

MONDAY MORNINg
Section A
Boston Convention & Exhibition Center Room 51
Getting Your First Industrial Job
Professionally supported by YCC‡
N. A. LaFranco, Organizer
A. C. Myers, Organizer, Presiding
8:30 Introductory Remarks.
8:35 PROF 7. Finding the trampline, avoid the black holes. K.C. Glasgow
8:55 PROF 8. Finding the career that fits: My life away from the bench. N.A. LaFranco
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 next graduate and a recruit’s perspective. K.M. Allen
11:05 Prof:Discussions.
11:25 Concluding Remarks.

21st Century Chemistry Education: Formal and Informal
Professionally supported by AGRO, CARB, CHAS, CHED, ONF, COLLE, ENFL, PROF and SCHB

ACS Scholars: Rising Stars in Academe
Professionally supported by AGRO, CARB, CMA, ENFL, PROF, SCHE and YCC

Careers for Young Professionals in Green Chemistry: Breaking Bad Chemistry Habits
Professionally supported by CHED, Cosponsored by BMGT, CEI, ENVIR, IECC, MEDF, SCHB and YCC

The Chemistry Enterprise in 2015
Professionally supported by BMGT, Cosponsored by PMSE and PROF

Managing Transitions
Professionally supported by WCC, Cosponsored by PROF

Memories of Henry Hill: His Legacy in Science and in Professional Service
Professionally supported by HIST, Cosponsored by AGRO, CARB, COLL, ENFL, POLY, PRES, PROF and SCHB
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.
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, Co-sponsored by AGRO, CARB, CMA, COLL, HIST, I&EC, POLY, PRESS, and PROF

The Legacy of Henry Hill: Commercial Enterprises in the Polymer Sector
Sponsored by SCHB, Co-sponsored by CMA, COLL, HIST, I&EC, POLY, PRESS, and PROF

Leadership Skills as a Strategic Advantage: the Chemist's Competitive Edge
Sponsored by BMGT, Co-sponsored by CEPA, PRESS, and YCC

Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais
Sponsored by YCC, Co-sponsored by CHED, I&EC, 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. Par, Organizer
D. Chamot, Presiding
8:30 Introductory Remarks.
8:40 PROF 15. Career tune-up.
L. M. Bailey, L.B. Robinson
9:35 PROF 17. Maximizing your volunteer experience. D.B. Hauser
9:55 Intermission.
10:10 PROF 18. Smart money moves in your 20's and 30's. S. Toscano

SCHB
Division of Small Chemical Businesses
J. Sabol, Program Chair

SUNDAY 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.
9:05 SCHB 14. Chemical management for safe, secure, and environmentally sound chemical facilities. N.B. Jackson
9:35 SCHB 15. Chemosynthetic livers: Generating effective and harnessing amphotericin B. M. Burke

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.
9:05 SCHB 14. Chemical management for safe, secure, and environmentally sound chemical facilities. N.B. Jackson
9:35 SCHB 15. Chemosynthetic livers: Generating effective and harnessing amphotericin B. M. Burke
10:55 SCHB 17. Olefin metathesis chemistry as a catalyst for building businesses. BRIC by BRIC. R.H. Grubbs


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, ENWR, I&EC, MED, PROF, SCHB and YCC

MONDAY AFTERNOON

Section A
Westin Boston Waterfront

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 Renagen and WeChem. 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

Chemical Innovation and Design (CID) Talks: The Future of Innovation Now
Sponsored by APPPC, Cosponsored by AGRO, AGRO, BMGT, MED, 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

8:00 Networking.
8:30 Introductory Remarks.
8:35 SCHB 25. Delivery to biotech: Alkermes’ and TransForm’s stories. J.F. Remenar


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. Tobe

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 AGRO, AGRO, BMGT, CARB, COLL, INOR, MEDI, ORGN, POLY, PRES†, PROF and SCHB

Transforming University-Industry Partnerships for an Innovative Future
Sponsored by Pres, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MED, PROF, SCHB and YCC

Women in Innovation: Business and Commerce
Sponsored by PROF, Cosponsored by BMGT, SCHB, WCC and YCC

Transforming University-Industry Partnerships for an Innovative Future
Sponsored by Pres, Cosponsored by AGRO, CARB, CHAS, COLL, ENFL, ENVR, MED, PROF and SCHB

TUESDAY AFTERNOON

Section A
Westin Boston Waterfront

Big Chemistry from Small Businesses
Sponsored by IAC, Cosponsored by AGRO, BMGT, CARB, CELL, INOR, MEDI, ORGN, POLY, PRES and SCHB

Biological Techniques
Sponsored by CHAS, Cosponsored by AGFD, AGRO, BMGT, CARB, CHAS, COLL, ENFL, ENVR, MED, PROF, SCHB and YCC

WEDNESDAY MORNING

Section A
Westin Boston Waterfront

 compliment from ACS.

Lab Safety 25 Years After Promulgation of the OSHA Laboratory Standard
Sponsored by CHAS, Cosponsored by CCS

MONDAYafternoon
Lab Safety 25 Years After Promulgation of the OSHA Laboratory Standard
Sponsored by CHAS, Cosponsored by CCS

MONDAY AFTERNOON

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‡

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or to stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from ACS.
MONDAY AFTERNOON
Leadership Skills as a Strategic Advantage: the Chemist’s Competitive Edge
Sponsored by BMGT, Cosponsored by CEPA, PMSE, PROF and YCC

TUESDAY MORNING
Academic Innovations for Tomorrow’s Industries: GSSPC Symposium
Sponsored by CHED, Cosponsored by ANVL, BIOT, BMGT, CHED1, CORP1, DAC1, ENFL1, PHYS1 and POLY1

TUESDAY AFTERNOON
Academic Innovations for Tomorrow’s Industries: GSSPC Symposium
Sponsored by CHED, Cosponsored by ANVL, BIOT, BMGT, CHED1, CORP1, DAC1, ENFL1, PHYS1 and POLY1

GENERAL SESSIONS

CEI
Committee on Environmental Improvement
C. Middlecamp, Program Chair

MONDAY AFTERNOON
Citizens First: Using Real-World Contexts for Engaging Students in Learning Chemistry
Sponsored by CHED, Cosponsored by CEI

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
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

DAC
Committee on Divisional Activities
M. J. Morello, Program Chair

TUESDAY MORNING
Academic Innovations for Tomorrow’s Industries: GSSPC Symposium
Sponsored by CHED, Cosponsored by ANVL, BIOT, BMGT, CHED1, CORP1, DAC1, ENFL1, PHYS1 and POLY1

TUESDAY AFTERNOON
Academic Innovations for Tomorrow’s Industries: GSSPC Symposium
Sponsored by CHED, Cosponsored by ANVL, BIOT, BMGT, CHED1, CORP1, DAC1, ENFL1, PHYS1 and POLY1

CEPA
Committee on Economic and Professional Affairs
D. Kneeland, Program Chair

SUNDAY AFTERNOON
Professional Legacy of Henry Hill
Sponsored by PROF, Cosponsored by CEPA, CORP, ETHC, HIST, ORGN, PMSE, POLY, PRES and SCHB

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

TOXICITY AND ENVIRONMENTAL IMPACT IN THE CHEMISTRY CURRICULUM: SCIENCE AND STRATEGIES FOR EDUCATORS - STATE OF THE ART SYMPOSIUM

citizens first: using real-world contexts for engaging students in learning chemistry

sponsored by ched, cosponsored by cei

The Debate: How Do We Respond to Climate Change
Sponsored by ENVR, Cosponsored by CEI

Professional Legacy of Henry Hill
Sponsored by PROF, Cosponsored by CEPA, CORP, ETHC, HIST, ORGN, PMSE, POLY, PRES and SCHB

WEDNESDAY MORNING
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
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
Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials
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
Sponsored by ENVR, Cosponsored by CEI

THURSDAY MORNING
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

ETHC
Committee on Ethics
K. Vitenese, Program Chair

SUNDAY AFTERNOON
Professional Legacy of Henry Hill
Sponsored by PROF, Cosponsored by CEPA, CORP, ETHC, HIST, ORGN, PMSE, POLY, PRES and SCHB

TECHNICAL PROGRAM
TECHNICAL PROGRAM

MONDAY MORNING

Section A
Boston Convention & Exhibition Center
Room 52A
What's in Your Chemical Toolbox?
Co-sponsored by ENFL and ENVR
G. Muller, Organizer, Presiding
12:00 SOCED 1, Eminent Scientist Lecture: What's in your chemical toolbox? J.C. Warner

SUNDAY MORNING

High School Program
Sponsored by CHED, Co-sponsored by SOCED
Undergraduate Research Papers
Sponsored by CHED, Co-sponsored by SOCED

SUNDAY AFTERNOON

21st Century Chemistry Education: Formal and Informal
Sponsored by PRES, Co-sponsored by AGRO, CARB, CHAS, CHED, CINF, COLL, ENFL, PROF and SOCED
Undergraduate Research Papers
Sponsored by CHED, Co-sponsored by SOCED

MONDAY MORNING

Section A
Seaport Hotel and World Trade Center
Hampton A/B
Managing Transitions Co-sponsored by PROF
M. J. Shultz, Organizer, Presiding
N. Bridges, Presiding
8:15 Introductory Remarks.
9:20 WCC 1. After school: Diverse paths in the chemical enterprise. K.L. Lee
9:30 WCC 2. Diverse paths in the chemical enterprise: A career in publishing. H.L. Tierney
9:40 WCC 3. Still love science, but don’t want to DO science? H. Eracher
10:00 Discussion.
10:45 Intermission.
11:30 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.

MONDAY AFTERNOON

Incorporating Green Chemistry Innovations and Applications into the Classroom and Outreach
Sponsored by CHED, Co-sponsored by CEI, I&EC and YCC
Undergraduate Research Posters
Sponsored by CHED, Co-sponsored by AGRO and SOCED

MIDNIGHT EVENING

Successful Student Chapters
Sponsored by CHED, Co-sponsored by SOCED

WCC

Women Chemists Committee
K. Wozniak and A. Deballie, Program Chairs

SOCIAL EVENTS:
WCC Breakfast, 7:30 AM: Monday
WCC/Eli Lilly Travel Award Poster Session, 11:15 AM: Tuesday
WCC Luncheon, 12:00 PM: Tuesday
Just Cocktails, 4:00 PM: Tuesday
BUSINESS MEETINGS:
WCC Division Executive Session, 7:30 PM: Saturday

YCC

Younger Chemists Committee
A. Gavrilenko and T. Matos, Program Chairs

SOCIAL EVENTS:

MONDAY AFTERNOON

Women in Innovation: Business and Commerce
Sponsored by PROF, Co-sponsored by BMGT, SCHB, WCC and YCC

WEDNESDAY EVENING

Green Chemistry and the Environment
Sponsored by ENVR, Co-sponsored by YCC

MONDAY AFTERNOON

Section A
Seaport Hotel and World Trade Center
Seaport Blm B
Younger Chemists Exchanging More than Currency: First—Euros and Dollars; Next—Rupees, Rands, and Reais
Co-sponsored 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 expansion of cultural representation among ACS student chapters. N. Di Fabio
2:00 YCC 8. Expanding beyond the Boston area for young chemists. K.R. Lucci
2:40 Intermission.
2:50 YCC 10. Where chemistry meets wanderlust: A continuing journey. C. Dunne
3:10 YCC 11. Chemistry without borders: International activities at ACS. H. Cheng, B. Miller
3:50 Discussion.
4:00 Concluding Remarks.

ACS Scholars: Rising Stars in Industry
Sponsored by PRES, Co-sponsored by AGRO, CARB, CHAS, COLL, ENFL, ENV, PROF, SCHB and YCC
Green Chemistry and the Environment
Sponsored by ENVR, Co-sponsored by YCC
Leadership Skills as a Strategic Advantage: the Chemist’s Competitive Edge
Sponsored by BMGT, Co-sponsored by CEI, PRES, PROF and YCC

TUESDAY MORNING

Checklist for Turning Thirty
Sponsored by PROF, Co-sponsored by YCC
Green Chemistry and the Environment
Sponsored by ENVR, Co-sponsored by YCC
Starting-Up & Spinning-Out: Commercializing Innovative Chemistry
Sponsored by SCHB, Co-sponsored by AGRO, COLL, I&EC, PRES, PROF and YCC

TUESDAY AFTERNOON

Starting-Up & Spinning-Out: Commercializing Innovative Chemistry
Sponsored by SCHB, Co-sponsored by AGRO, COLL, I&EC, PRES, PROF and YCC
Women in Innovation: Business and Commerce
Sponsored by PROF, Co-sponsored by BMGT, SCHB, WCC and YCC

WEDNESDAY EVENING

Green Chemistry and the Environment
Sponsored by ENVR, Co-sponsored 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. Ulrich
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. Gütter
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.
ACS Publications, CAS and so much more from American Chemical Society will be in one convenient location. Visit the ACS Booth and experience more than chemistry.

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- Experience SciFinder® from CAS, the world’s authority for chemical information
- Learn about your personal and professional benefits from ACS membership
- Contests and giveaways including gift cards and more!

**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

**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.

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915

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Humio, Inc. 743
Implen, Inc. 43
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Camag, Scientific, Inc. 410
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Cedarlane 1207
CEDM Corp. 617
CCEP 210
Edinburgh Instruments 318
EMD Millipore 438
Enlab, Inc. 325
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NIST 543
Organix Inc. 942
OriginLab Corp. 538
Park Systems, Inc. 427
Parr Instrument Co. 1100
Particle Sizing Systems 310
PerkinElmer, Inc. 211
PharmAgra Labs, Inc. 1126
Pine Research Instrumentation 844
Piramal Healthcare 343
Polymer Source Inc. 450
PSS USA, Inc. 750
Pure Chemistry Scientific Inc. 1315
Robertson Microlit Laboratories, Inc. 1037
Royal Society of Chemistry 801
SciAlps, Inc. 100
Semichem 1014
Simulations Plus, Inc. 654
Specac, Ltd. 1032
Spectradyne LLC 448
Thermo Scientific 1114, 1115
SuperCritical Fluid Technologies 912
TSI, Inc. 126
Vacuum Technology Inc. 431
VWR International LLC 1316
Wilmad-LabGlass 1300
Wiley 700
Wyatt Technology Corp. 510
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Affs Aesar-A Johnson Matthey Co. 300
Ark Pharm, Inc. 1112
Astatech, Inc. 1205
BASF - The Chemical Company 517
Bellen Chemistry, Ltd. 648
Berry & Associates 1324
Biochromato (Amuza Inc.) 1245
Biolin Scientific 851
C/D/N isotopes 429
Carbosynth LLC 641
Cedarlane 1207
Chembird Corp. 919
CombBioPhos Catalysts, Inc. 1027
DEEP PhARM-CHEm PVT. LTD. 1243
EMD Millipore 438
Enamine LLC 443
Frontier Scientific, Inc. 1218
Flinn Scientific Inc. 110
Guizhou Wylton Jinglin Electronic Material Co., Ltd. 744
HeChem 316
Heidolph North America 1224
Hielscher Ultrasonics 434
Hitgen Ltd. 1149
Industrial Test Systems 312
Interchim Inc. 1109
JoVe 1133
Kishida Chemical Co., Ltd. 339
LabNetwork 442
Life Chemicals, Inc. 236
Materia, Inc. 1211
Metrohm USA, Inc. 424
MDP Chemicals 1244
Nanalyses Corp. 500
Neo-Advent Technologies, LLC 1240
Oakwood Products Inc. 1101
Organix Inc. 942
Oxenham Corporation 1216
Pharmablock USA, Inc. 1418
PharmAgra Labs, Inc. 1126
PolyDesign LLC 1046
Riek Metals, LLC 943
Sapala Organics PVT. LTD. 1002
SciAlps, Inc. 100
Semichem 1014
Sigma-Aldrich 901
Small Molecules, Inc. 1229
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Sorbent Technologies 606
Spectrum from Chemical Mfg Corp. 843
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Strem Chemicals 1011
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Booth # 1324
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L-Histidine-1-13C
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Booth # 537
SP-50/150
QFM-400
SFM-400
Accessories
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Booth # 642
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<tr>
<th>Company</th>
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</tr>
</thead>
<tbody>
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</tr>
<tr>
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<td><strong>Boston Park Plaza Hotel and Towers</strong></td>
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<td><strong>Courtyard Boston Downtown</strong></td>
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<tr>
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<td>10</td>
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<tr>
<td>11</td>
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<td>marriott.com</td>
<td>15</td>
</tr>
<tr>
<td>12</td>
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<td>16</td>
</tr>
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<td>1 Seaport Lane</td>
<td>16</td>
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<td>16</td>
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<td></td>
<td>seaportboston.com</td>
<td>16</td>
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<tr>
<td>13</td>
<td><strong>Sheraton Boston Hotel</strong></td>
<td>17</td>
</tr>
<tr>
<td></td>
<td>39 Dalton Street</td>
<td>17</td>
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<td>14</td>
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<td>18</td>
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<tr>
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<td>100 Stuart Street</td>
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<td>18</td>
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<td>18</td>
</tr>
</tbody>
</table>

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### Shuttle Schedule

**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 26**
- 7:00 AM – 6:00 PM .......................... 60 minute intervals

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ROUTE 2
ROUTE 3
ROUTE 4
ROUTE 5
WALKING
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

**HOTEL ROUTE INFORMATION**

**Map#** | **Hotels** | **Route**
--- | --- | ---
1 | Boston Marriott Copley Place | 1
   | Boarding: Walk to Westin Copley Place | 
2 | Boston Park Plaza Hotel and Towers | 2
   | Boarding: Valet Entrance on Columbus Avenue | 
3 | Courtyard Boston Downtown | 2
   | Boarding: Curbside on Tremont Street | 
4 | Doubletree by Hilton Hotel Boston- Downtown | 2
   | Boarding: Walk to Courtyard Boston Downtown | 
5 | Fairmont Copley Plaza | 1
   | Boarding: Walk to Westin Copley Place | 
6 | Hilton Boston Back Bay | 3
   | Boarding: Cross Dalton Street to Sheraton | 
7 | Hilton Boston Downtown / Faneuil Hall | 4
   | Boarding: Curbside on Broad Street | 
8 | Hyatt Regency Boston | 5
   | Boarding: Curbside on Avenue DeLafayette | 
9 | InterContinental Boston | 4
   | Boarding: Curbside on Atlantic Avenue | 
10 | Omni Park House Hotel | 5
   | Boarding: Corner of Beacon St. - at the Citizen Bank | 
11 | Renaissance Boston Waterfront | W
   | Walk to Boston Convention & Exhibition Center | 
12 | Seaport Hotel | W
   | Walk to Boston Convention & Exhibition Center | 
13 | Sheraton Boston Hotel | 3
   | Boarding: Curbside on Dalton Street | 
14 | W Boston | 2
   | Boarding: Walk to Courtyard Boston Downtown | 
15 | Westin Boston Waterfront | W
   | Walk to Boston Convention & Exhibition Center | 
16 | Westin Copley Place | 1
   | Boarding: Curbside on Huntington Avenue |
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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), Environmental Protection Agency (EPA), and the Air Force Office of Scientific Research (AFOSR).

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

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Check with your division for your deadline. Presenters — Abstract submission varies by division.
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