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Letter from the Co-Chairs

Chemistry continues to be an exciting field, with the ingenuity of chemists continuing to create great new opportunities. The Chemical Sciences Roundtable looks at trends in chemistry and attempts to illuminate them for the broader community. Being anticipatory is always challenging, especially in a field as diverse as chemistry.

This Second Edition of the Chemical Sciences Roundtable (CSR) Newsletter comes at a time of great change in the Roundtable. Roundtable members and staff have accomplished a lot in the past six months, and we are excited to share the highlights of our work with you.

CSR members held a two day meeting in December 2016 in Washington, D.C. where we welcomed new members, explored potential topics for future activities, and held strategic planning sessions. In addition, CSR convened a session on Artificial Molecular Machines. Invited speakers included David Leigh, The University of Manchester, Josef Michl, University of Colorado, and Miguel Garcia-Garibay, University of California, Los Angeles. Shortly after the CSR meeting, Prof. Leigh’s group reported the fourth ever synthesized molecular braid. The selection of topic coincided with the award of the Nobel Prize in Chemistry to Fraser Stoddart, Jean-Pierre Sauvage, and Ben Feringa for the “design and synthesis of molecular machines”. The second topic, covered at the CSR meeting, was Toxic Substances Control Act Reform.

More details on the new CSR members, and sessions on Artificial Molecular Machines and Toxic Substances Control Act Reform can be found in the Meeting Minutes section of this newsletter.

Recently, a series of four Microbiome Seminars, examining what is currently known about earth, marine, and human microbiomes, as well as the opportunities for additional research, were held in Washington, DC. The seminars reached a broad audience with ~100 in-person participants and about 700 virtual participants for the combined seminars. Virtual attendees were able to actively participate by submitting their questions on-line. If you have missed any of the seminar series you can find them here, look for the upcoming report which is anticipated in May 2017. Let us know what you thought about Microbiome Seminars by writing to CSR@nas.edu.

CSR members are constantly exploring the most relevant and important topics for future activities. Currently, the topics under consideration are Astrochemistry, Big Data Analytics and Machine Learning, and Molecular Machines. Let us know what topic is the most interesting to you by sending us a comment to CSR@nas.edu, and don’t forget to follow us on Twitter @NASEM_Cham.

Thank you and best regards,
CSR Co-Chairs
Jennifer Sinclair Curtis (jscurtis@ucdavis.edu)
Mark Jones (markjones@dow.com)
On December 6-7, 2016, the Chemical Sciences Roundtable (CSR) held their business meeting at the National Academies Building in Washington, DC. During the meeting, CSR members explored potential topics for their next and future workshops. In addition, the recently-formed internal committees of CSR met to discuss their ongoing activities and provide a report to the remainder of the CSR membership.

This was the first meeting for a number of new CSR members, as CSR membership has recently expanded to include a broader representation across many sectors. Eight new members joined the roundtable, including a new CSR Co-Chair Dr. Mark Jones who has replaced Dr. Bill Carroll as CSR Co-Chair. We are very grateful to Bill for his insight and wonderful service to CSR for the past 6 years. Our new Co-Chair Mark Jones is the Executive External Strategy and Communications Fellow with the Office of the CTO of Dow Chemical in Midland, Michigan. Other new CSR members include Michelle Chang (UC Berkeley), Michael Fuller (Chevron Energy Technology Company), Malika Jeffries-El (Boston University), Mary Kirchhoff (American Chemical Society), David Myers (GCP Applied Technologies), Ashutosh Rao (Food and Drug Administration), and Laurie Locascio (National Institute of Standards and Technology). The Roundtable seeks more industry representatives, so we welcome your suggestions for potential new members. As a way of orientation for these new CSR members, Dr. Teresa Fryberger (Director, Board on Chemical Sciences and Technology (BCST), NAS) gave a short background on CSR and BCST, as well as a summary of their ongoing activities.

During the business meeting, two potential topics for the next CSR workshop were explored. The first was ‘Artificial Molecular Machines (MM)’. A number of specific focus areas for such a workshop were considered - characterization techniques for MM, biomolecular MM, smart polymers/smart materials, multiscale autonomous machines, improvements in force fields, MM in space, control of MM, and safety and toxicology of MM, to name a few. Speakers included Miguel Garcia-Garibay (UCLA), David Leigh (University of Manchester) and Josef Michl (University of Colorado). Discussion on this topic concluded that while this topic certainly has basic research implications, industry interest is low and if the workshop took place that it needed to focus on applications.
The CSR members also delved into a second topic for a potential CSR workshop that is related to the Toxic Substances Control Act (TSCA) Reform. The themes for such a workshop would center on the challenges and opportunities for innovation that could complement this new bill. Jim Jones (EPA) spoke on this topic as well as panelists Sarah Vogel (Environmental Defense Fund), Mike Walls (American Chemistry Council) and James Aidala (Bergeson & Campbell, PC). After the talks, CSR members felt that a possible workshop focusing on alternative testing approaches would be the best theme, as well as possible coordination with ACS’s Division on Toxicology.

Other topics that were discussed more briefly amongst the CSR membership, without the benefit of talks from invited guests, were possible workshops on the ChemRxiv, desalination, biodegradation of plastics, concerted electrochemical reactions making a single product, and multiphotonic events associated with better lasers and microscopes.

There was also time during the business meeting for the CSR committees to meet in person to supplement their ongoing monthly teleconference meetings. Committee chairs then presented brief reports. A report from the Program Committee was presented by Michael Fuller. Michael emphasized leveraging the relationship with ACS in idea generation, capturing perspectives from graduate and undergraduate students in the chemical sciences, reaching out to CSR alumni, and strategizing on ways to get public input for topics. The Marketing/Outreach Committee report was presented by Malika Jeffries-El and she highlighted numerous activities to expand the impact of CSR. In addition, she discussed how to more effectively expand CSR’s social media presence and followers on Twitter. Finally, Miles Fabian reported on the activities of the Communications Committee that included continued development of content for the CSR website and ways to leverage other topics and things that have already been written for inclusion on the CSR website.

For comments and feedback, write to the Chemical Sciences Roundtable at CSR@nas.edu.

Meeting Minutes were prepared by
Jennifer Sinclair Curtis
University Of California, Davis
Chemistry in Upstream Oil and Gas: A World of Possibilities

“In 2004, I finished my graduate degree at Northwestern University and entered a career in an unknown technical realm: the world of oil and gas development. Where many peers went onto successful careers in academia or chemical manufacturing, the upstream oil and gas segment presented an alternative career path with opportunities to solve chemical challenges around the world.

Common upstream tasks within oil and gas development include drilling, completion, and cementing of a well, as well as stimulation of the hydrocarbon productivity (such as hydraulic fracturing). And while career paths in oil and gas development are historically associated with petroleum engineering programs, the upstream oil and gas industry employs technical experts across dozens of technical fields. Chemistry is one subject matter expertise critical to the development of hydrocarbon resources.

Many scientists enter careers in upstream research and development expecting a simple laboratory environment to develop and qualify new chemical products and fluids. But many are surprised to find that in their first 10 years, they may also be expected to:

- Develop additional skills in geology, biomacromolecules, metallurgy, and environmental sciences
- Travel to dozens of countries worldwide to teach about and consult on various technical topics
- Solve chemical challenges across six continents at well sites ranging from deserts to offshore platforms
- Volunteer in the local community with hundreds of peers, on projects ranging from supporting local STEM programs (such as volunteering at the local Science and Engineering Fair) to working at the local Children’s Hospital

There is a literal world of opportunity for scientists and engineers to share their expertise in the upstream oil and gas sector. “Never a dull moment” doesn’t begin to describe the experience…

Michael J. Fuller, Completion Fluids and Stimulation Advisor Chevron Energy Technology Company
New Technologies for an Old, Familiar Material

“...chemistry and engineering of portland cement is quite complex, and there are still important technical problems to solve and opportunities for improved performance”

People are often surprised to learn that my research work, now and for much of the last 30 years, is focused on cement and concrete. Seemingly, everything should be known by now about such a common material, in use in its current form for well over a century.

It turns out that that the chemistry and engineering of portland cement is quite complex, and there are still important technical problems to solve and opportunities for improved performance.

Approximately 4.3 billion tons of cement are produced in the world each year, mainly for use as the primary binder in 7.5 billion m³ of concrete, that the world requires annually for the construction of buildings, dams, roads, and bridges. The cement hydration reactions, which cause concrete to be transformed from a liquid slurry to a solid mass with high compressive strength, are perhaps the most widely practiced chemical reactions used industrially in the world. And there have been major technical advances over the last 25 years. New catalysts for cement hydration chemistry have been discovered that provide up to 20% more strength compared to the same cement without these catalysts. A new generation of water-soluble polymer dispersants has been developed to reduce the amount of water required to make concrete flowable, greatly reducing the porosity and increasing the durability of concrete. To compensate for concrete’s brittleness, Polymer fibers have been engineered to replace steel used in concrete, reducing the problem of steel corrosion due to the use of deicing salts on roads or exposure to marine environments.

Despite this good progress, there is still much that can be done to make concrete more durable, less prone to cracking, and more attractive. Recent work aims to reduce the CO₂ footprint of concrete (cement production accounts for about 5% of global CO₂ emissions) and to deploy sensors, wireless communications, and databases to improve delivered concrete quality. Since concrete is unlikely to be displaced as the primary construction material used globally, these opportunities for improved performance and lower environmental impact will continue to make R&D on cement and concrete an important area of focus for years to come.

David F. Myers, Vice President
Product Development and Technical Support
GCP Applied Technologies, Inc.
Preprint publication, long a staple of other scientific disciplines, is coming to chemistry. The American Chemical Society (ACS) will soon launch a preprint server ChemRxiv.

The Chemical Sciences Roundtable will host a joint session with the American Chemical Society at the August 2017 ACS National meeting in Washington, D.C. The symposium will explore the advantages and challenges associated with adoption of ChemRxiv. The participants will include representatives from various sectors of the chemical community: funding agencies, scientific journals, and academia; as well as representatives from other scientific disciplines, such as physics, engineering, and biology. The half-day session will include individual talks, panel discussions, live Twitter chats, and a townhall style Q&A session.
MEET THE ROUNDTABLE MEMBERS

Co-Chairs:

Jennifer S. Curtis, University Of California, Davis
Mark Jones, Dow Chemical

Members:

Tina Bahadori, U.S. Environmental Protection Agency
Michael R. Berman, Air Force Office of Scientific Research
Donna G. Blackmond, Scripps Research Institute
Emilio Bunel, Argonne National Laboratory
Allison Campbell, Pacific Northwest National Laboratory
Richard R. Cavanagh, National Institute of Standards and Technology
Michelle Chang, University Of California, Berkeley
Miles Fabian, National Institutes of Health
Michael J. Fuller, Chevron Energy Technology Company
Miguel Garcia-Garibay, University Of California, Los Angeles
Bruce Garrett, Department Of Energy
Malika Jeffries-El, Boston University
Jack Kaye, National Aeronautics And Space Administration
Mary M. Kirchhoff, American Chemical Society
Joann Slama Lighty, National Science Foundation
Laurie E. Locascio, National Institute Of Standards And Technology
David F. Myers, GCP Applied Technologies
Ashutosh Rao, Food And Drug Administration
Angela Wilson, National Science Foundation