CALL FOR PAPERS

The Division of Physical Chemistry has organized the following topical oral symposia, consisting of both invited and contributed papers, as well as topical and general poster sessions.

The abstract submission deadline is 6 April 2017. For those interested in an oral presentation, please submit abstracts to the appropriate symposium. For each symposium, the organizers (listed below) will select some contributed papers for oral presentations; contributions not selected for oral presentations will be assigned to the poster session.

SPECTROSCOPIC AND COMPUTATIONAL INSIGHTS INTO SOLID/LIQUID INTERFACES FOR ENERGY CONVERSION

This symposium will feature recent, complementary and synergistic research efforts devoted to understanding the fundamental physical chemistry of solid/liquid interfaces relevant for energy conversion. Session will include both invited talks and participation of presentations of 1 recent spectroscopic and computational investigations on battery and catalysis technologies, 2 recent advances in understanding atomic and nanoscale phenomena at interfaces between liquids and metals, oxides, and carbon materials, and 3 novel solar and energy technologies and future applications. Our aim is to bring together different communities of basic scientists and engineers to share knowledge and improve the rational design of technologies that efficiently convert, store, and utilize energy.

A. A. Keith, University of Pittsburgh, jashe@pitt.edu

LIQUID THEORY: IN HONOR OF BEN WIDOM'S 60TH BIRTHDAY

This symposium will highlight talks by liquid theory and numerical modeling pioneers whose work builds on fundamental foundations to describe increasingly complex fluid systems. The central role of liquids in chemistry and biology has ensured that the theoretical description of liquid structural, thermodynamic, and dynamic properties is a grand challenge that must be met. Given the daunting complexity of liquids, it is necessary that numerical modeling must take over where pure theory leaves off, in order to link molecular and macroscopic properties of fluids spanning a wide range of length and time scales.

Dor Ben-Amotz, Purdue University, bendor@purdue.edu
Kenichiro Koga, Okayama University, koga@cc.okayama-u.ac.jp
Roger F. Loring, Cornell University, roger.loring@cornell.edu

GASEOUS ION CHEMISTRY AND SURFACE REACTIONS

This symposium will focus on emerging trends in experimental approaches to studying gaseous ion reactivity, which lies at the border of physical, analytical, biological and environmental chemistry. Therefore, the proposal aims to assemble speakers from diverse backgrounds, each making physical measurements with different instrumentation and focus. Chemical systems of interest include cold ions, micro-solvated ions, ionsurface and ion-solid interactions, and gaseous biopolymers. Such a forum is expected to expand our scientific vocabularies and provide new opportunities to think in different ways about the scientific challenges we face.

Abraham Badu-Tawiah, The Ohio State University, badu-tawiah.1@osu.edu
Hao Chen, Ohio University, chenh2@ohio.edu

EXPERIMENTAL AND COMPUTATIONAL ADVANCES IN UNDERSTANDING ENZYME SPECIFICITY AND PROMISCUITY

Recent years have produced ever-increasing evidence that many, if not even most, enzymes are highly non-specific, catalyzing diverse reactions (‘‘catalytic promiscuity’’). This behavior has been argued to be crucial to the evolution of life, as providing a perfect training ground for artificial enzyme design. Our symposium will showcase recent advances in our understanding of enzyme multifunctionality, covering both methodological developments as well as applied insights. The invited speakers are all current or emerging leaders in their respective sub-fields, and bring together the interface between chemistry, biology, and computer science. The combination of these speakers in one symposium has been ensured that the theoretical approaches and bring normally scientifically disparate communities together to engage in active discussion, while maintaining a strong link to both academic and industrial applications. The program is organized into 6 sessions, each of which can accommodate 2-3 contributed talks. Due to the interdisciplinary nature of the topic, we welcome high-quality abstracts from any area related to the topic of the symposium, from microbiology, evolutionary biology and biochemistry, through to synthetic organic chemistry and biomolecular simulations.

Caroline Lynn Kamerlin, University of California, Berkeley, kamerlin@icm.uu.se
Qu Cong, University of Wisconsin, cui@chem.wisc.edu
Gerrit Poelemonds, University of Groningen, g.poelemonds@rug.nl
 Nobuhiko Torukai, The University of British Columbia, btorukai@ubc.ca

PHYSICAL CHEMISTRY SYMPOSIUM WORKSHOP

The Workshop for Undergraduate Career Majors is targeted for current junior chemistry majors who will be seniors at the time of the Washington DC meeting. Up to 25 outstanding undergraduate chemistry students will be selected for a series of undergraduate-focused talks and social events during the DC meeting. In addition, they will be expected to present posters on their research as part of the PHYS poster session. More information and application materials can be found at http://www.acs.org/ypgrd_workshop/2017.html. The application deadline is 26 February 2017. Cayce Londergan, Haverford College, clondergan@haverford.edu

PHYSICAL CHEMISTRY PAPER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday evening, 30 August 2017. See announcement below for information about the Physical Chemistry Student Poster Awards.

Joan-Emma Shea, University of California Santa Barbara, shea@chem.ucsb.edu

On-Line Abstract Submission Deadline: 06 APRIL 2017

POSTDOCTORAL RESEARCH AWARDS

PHYS Division Postdoctoral Research Awards and invited talks will be presented at the relevant PHYS Symposia.

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

Six awards with monetary prizes will be awarded for posters presented by students at the Physical Chemistry Poster Session on Wednesday evening of the meeting.

To be eligible for the award, the presenting author must be a graduate or undergraduate student at the time of the poster presentation and must present during the session.

JOAN-EMMA SHEA, PROGRAM CHAIR

University of California, Santa Barbara, Department of Chemistry and Biochemistry (805) 893-5604 shea@chem.ucsb.edu

FOR INFORMATION ABOUT THE PHYSICAL CHEMISTRY DIVISION, VISIT OUR WEB SITE: http://phys.acs.org/

ELECTRONIC STRUCTURE METHODS FOR COMPLEX CHEMICAL SYSTEMS

Electronic structure methods are providing insight into complex chemical systems with a scope and realism unimaginable just a few years ago. For example, transition states involving large and complex subsystems with a multitude of interacting sites can now be modeled without truncation, including effects of light with materials, reactions at interfaces, and heterogeneous catalysis can be studied using predictive many-body methods; and weak interactions of nanosystems and soft matter can increasingly be investigated with correlated wannier function methods. This workshop will highlight the latest developments in electronic structure method and examine their impact on modeling of complex chemical systems. Topics will include emerging directions, correlated electronic structure methods, noncovariant interactions, nanosystems, and solvation of the electron in new and future applications. Our aim is to bring together different communities of basic scientists and engineers to share knowledge and improve the rational design of technologies that efficiently convert, store, and utilize energy.

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