



ACS DIVISION OF PHYSICAL CHEMISTRY  
254<sup>TH</sup> NATIONAL ACS MEETING  
Washington DC 20-24 August 2017  
Meeting Theme: "Chemistry's Impact on the Global Economy"



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.

**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 substrates with a multitude of interactions can now be modeled without truncation; interaction 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 wavefunction methods. This symposium will highlight the latest developments in electronic structure theory and examine their impact on modeling of complex chemical systems. Topics will include emerging directions, correlated electronic structure methods, noncovalent interactions, nanosystems, and solvation, ultra-efficient electronic structure methods and molecular dynamics, many-body perturbation theory, random phase approximation methods, and electronic structure of extended systems. We aim to bring together scientists with diverse backgrounds and foster discussion and exchange of ideas beyond the traditional boundaries of the physics, chemistry, materials and computational science communities.

James J. Shepherd, Massachusetts Institute of Technology, [jshep@mit.edu](mailto:jshep@mit.edu)

Sahar Sharifzadeh, Boston University, [ssharifz@bu.edu](mailto:ssharifz@bu.edu)

Filipp Furche, University of California, Irvine, [filipp.furche@uci.edu](mailto:filipp.furche@uci.edu)

**PHYSICAL CHEMISTRY RESEARCH AT UNDERGRADUATE INSTITUTIONS**

One rewarding aspect of teaching at a primarily undergraduate institution (PUI) is collaborating with undergraduate students on research. This symposium will showcase the quality and breadth of physical chemistry research occurring at PUIs. This symposium will provide an opportunity for PUI faculty to gather and present physical chemistry research conducted with undergraduate students, including research in a variety of areas such as astrochemistry, biophysical, energy, materials, and atmospheric chemistry. This symposium will include experimental, computational, and theoretical studies. Speakers will include both established and young faculty with productive research programs.

Todd Hopkins, Butler University, [tahopkin@butler.edu](mailto:tahopkin@butler.edu)

**MOLECULES IN SPACE:**

**LINKING THE INTERSTELLAR MEDIUM TO (EXO)PLANETS**

Molecules from simple to as complex as fullerenes have been identified in various astrophysical environments such as the interstellar media, dark clouds, hot cores, outflows of carbon stars, protoplanetary disks, and in the atmospheres of (exo)planets. We are only beginning to understand by sustained laboratory experimental, spectroscopic, computational, modeling, and observational efforts how these molecules are synthesized in the gas phase and on grain surfaces, evolve in those exotic conditions, and become incorporated in to planetary bodies. With the advent of new and upcoming capabilities such as the Atacama Large Millimeter Array (ALMA) and the James Webb Space Telescope (JWST), the scope of molecular exploration will increase many folds over the next decade. The symposium will cover a wide breadth of subjects that will include organic inventory of the gas phase, the chemistry of the dark clouds, interplay of gas and dust, hot-cores and corinos, organic inventory of protoplanetary disks, high-resolution spectroscopy, the diffuse interstellar bands, the chemistry of atmospheres of stars and planets, and present and future opportunities such as ALMA, SOFIA, and JWST. Each session will begin with an overview talk by an eminent scholar in the field, followed by talks on astronomical observation, laboratory experiment, quantum chemistry calculations, and modeling. In addition, there will be a poster session.

Alexander Tielens, Leiden University, [tielens@strw.leidenuniv.nl](mailto:tielens@strw.leidenuniv.nl)

Partha P. Bera, NASA Ames Research Center, [partha.bera@nasa.gov](mailto:partha.bera@nasa.gov)

**MEMBRANE PROTEINS: STRUCTURE, ACTIVITY AND DRUG DEVELOPMENT**

Membrane proteins play essential roles in human health and are major targets for drug development. Understanding their structures and functions is key for harnessing their therapeutic potential. Recent studies based on NMR spectroscopy and computational methods have shed light on key aspects of membrane protein structure and function, and pave the way for their development as drug targets or therapeutic agents. This symposium will focus on holistic approaches where the protein and lipid components are treated as one, rather than separate parts. Advances in the areas of membrane protein sample preparation, structure determination, molecular dynamics and structure-based drug development will be discussed. The symposium will feature invited and contributed talks on experimental and computational work, covering the areas of solution NMR, solid-state NMR, molecular dynamics calculations, and NMR-based drug development. Abstract submissions covering these key areas are invited. The goal is to provide a forum for discussion of interdisciplinary ideas in this rapidly evolving area of chemistry.

Francesca Marassi, Sanford Burnham Prebys Medical Discovery Institute, [fmarassi@sbp.edu](mailto:fmarassi@sbp.edu)

Melanie Cocco, University of California, Irvine, [mcocco@uci.edu](mailto:mcocco@uci.edu)

**CHEMICAL BONDING AND REACTIVITY SPANNING THE PERIODIC TABLE:  
A SYMPOSIUM IN HONOR OF ROALD HOFFMANN**

This symposium, honoring distinguished American chemist and Nobel Prize winner, Prof. Roald Hoffmann, offers a broad perspective on recent developments in the field of theoretical chemistry applied to study a wide variety of compounds and chemical reactions. Recent advances in theoretical approaches to organic, organometallic, inorganic, and biological chemistry, as well as to materials subject to conditions of high external pressure will be discussed. Thus, this symposium will cover virtually all key branches of modern chemistry. The choice of topics reflects the enormously broad research interests of Prof. Hoffmann, who began his scientific career by looking at mechanisms of a certain class of organic reactions (culminating in the development of the "Woodward-Hoffmann" rules) and later moved on to study the electronic structure and magnetism of inorganic compounds, including matter at high pressures, while always trying to build bridges between the fields of organic and inorganic chemistry, as well as chemistry and physics.

Eva Zurek, University at Buffalo, SUNY, [ezurek@buffalo.edu](mailto:ezurek@buffalo.edu)

Wojciech Grochala, University of Warsaw, [w.grochala@cent.uw.edu.pl](mailto:w.grochala@cent.uw.edu.pl)

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

This symposium will feature recent, complementary and synergetic research efforts devoted to understanding the fundamental physical chemistry of solid/liquid interfaces relevant for energy conversion. Sessions are tentatively planned to include 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 tools and methods for 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.

John A. Keith, University of Pittsburgh, [jakeith@pitt.edu](mailto:jakeith@pitt.edu)

Katherine Jungjohann, Sandia National Labs, [kjungj@sandia.gov](mailto:kjungj@sandia.gov)

**LIQUID THEORY: IN HONOR OF BEN WIDOM'S 90<sup>TH</sup> 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 assured that the theoretical prediction 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](mailto:bendor@purdue.edu)

Kenichiro Koga, Okayama University, [koga@cc.okayama-u.ac.jp](mailto:koga@cc.okayama-u.ac.jp)

Roger F. Loring, Cornell University, [roger.loring@cornell.edu](mailto: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 lie at the boarder 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, ion/surface and ion/photon 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](mailto:badu-tawiah.1@osu.edu)

Hao Chen, Ohio University, [chenh2@ohio.edu](mailto: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 chemically diverse reactions ("catalytic promiscuity"). This behavior has been argued to be crucial to the evolution of protein function, as well 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, physics and computer science. The combination of these speakers in one symposium provides a unique opportunity to bridge disciplines 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, Uppsala University, [kamerlin@icm.uu.se](mailto:kamerlin@icm.uu.se)

Qiang Cui, University of Wisconsin, [cui@chem.wisc.edu](mailto:cui@chem.wisc.edu)

Gerrit Poelarends, University of Groningen, [g.j.poelarends@rug.nl](mailto:g.j.poelarends@rug.nl)

Nobuhiko Toruriki, The University of British Columbia, [tokuriki@mssl.uba.ca](mailto:tokuriki@mssl.uba.ca)

**PHYSICAL CHEMISTRY SYMPOSIUM WORKSHOP  
FOR UNDERGRADUATE CHEM MAJORS**

The Workshop for Undergraduate Chemistry 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://phys-acs.org/ugrad\\_workshop/2017.html](http://phys-acs.org/ugrad_workshop/2017.html). The application deadline is 26 February 2017.

Casey Londergan, Haverford College, [clonderg@haverford.edu](mailto:clonderg@haverford.edu)

**PHYSICAL CHEMISTRY POSTER SESSION**

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday evening, 23 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](mailto:shea@chem.ucsb.edu)

On-Line Abstract Submission Deadline: 06 APRIL 2017

<http://abstracts.acs.org>

**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 awards, the presenting author must be a graduate or undergraduate student at the time of the poster presentation and must be present during judging.

**JOAN-EMMA SHEA, PROGRAM CHAIR**

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

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