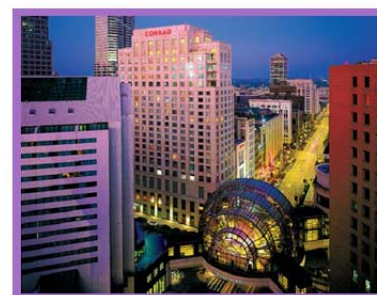




ACS DIVISION OF PHYSICAL CHEMISTRY
246TH NATIONAL MEETING
Indianapolis, Indiana
8-12 SEPTEMBER 2013



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 deadline is 18 March 2013. 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.

PHYSICAL CHEMISTRY OF SOLAR ENERGY CONVERSION

Solar energy conversion remains one of the most important scientific challenges. The overall solar-to-electricity and solar-to-fuel conversion processes involve many elementary steps, such as exciton dynamics, energy transfer, electron transfer, charge transport, and multi-electron, multi-proton chemical reactions. Fundamental understanding of these processes is essential to the design and improvement of existing solar energy conversion devices, as well as to the development of new and revolutionary concepts. Many of these processes occur in novel molecular assemblies, nano-structures, and hybrid materials. Their understanding will require state-of-the-art experimental and theoretical tools in physical chemistry. This symposium will bring together experimental and theoretical physical chemists who are investigating various fundamental processes involved in solar energy conversion. It will provide a forum for discussing the latest scientific discovery and showcase various solar-energy conversion related physical chemistry research areas.

Tim Lian, *Emory University, tlian@emory.edu*

Brian Dyer, *Emory University, briandyer@emory.edu*

COARSE-GRAINING AND MULTISCALE MODELING

The challenge in investigating the properties of complex fluids, important in many relevant applications in biology and engineering, is their development over a large range of length- and time- scales. This symposium focuses on both fundamental and theoretical approaches that bridge different length- and time-scales in complex systems, as well as on novel computational approaches developed to speed up simulations through coarse-graining and multiscale modeling. Fundamental theories for the structure and dynamics of complex systems have a long and illustrious history. Recent years have witnessed the development of numerous coarse-graining approaches to simulate both synthetic and biological systems. Theory is guiding the choice of the variables to coarse-grain and the methodology of coarse-graining. The goal of this symposium is to showcase the state-of-the-art progress in this rapidly evolving field, and to encourage discussion among the scientists working on theoretical approaches that bridge length- and time-scales for the structure and dynamics of complex macromolecular systems as well as coarse-graining methods and their applications.

Marina G. Guenza, *University of Oregon, mguenza@uoregon.edu*

Barbara Capone, *University of Vienna, barbara.capone@univie.ac.at*

MATERIALS AND MECHANISMS FOR EFFICIENT LIGHTING

About 20% of our electrical energy is consumed by lighting. Solid-state lighting (SSL), based on semiconductor light-emitting diodes (LEDs) or organic light-emitting diodes (OLED), has the potential for greatly increasing the efficiency with which we light our homes and offices. The first commercial SSL products for general illumination are now appearing. However, there is still much room for improvements and innovations in the materials, energy transfer mechanisms, and architectures for solid-state lighting. This symposium will include topics in SSL that are ripe for contributions from the Physical Chemistry community. For example, new phosphor materials, and potentially other novel wavelength down-converters such as quantum dots, are needed for efficient production of full-spectrum light by wavelength conversion from primary LED or OLED emitters. Novel SSL architectures could enable more efficient emitters, control of spatial and spectral emission properties, and improved light extraction, beyond the present SSL designs.

Mike Coltrin, *Sandia National Labs, mcoltr@sandia.gov*

Mark Thompson, *University of Southern California, met@usc.edu*

THEORY AND EXPERIMENT ON WATER AND HYDRATION

The abundance of water in nature, its function as a universal solvent, and its role in many chemical, material, and biological processes, is the driving force behind the need to understand its properties and behavior under different conditions and its function in different environments. The symposium aims at capturing recent experimental and theoretical advances in the fields of water clusters, aqueous interfaces, ions in water, water in biological systems, the structure and H-bond dynamics of liquid water, the development of interaction potentials (from classical to quantum) for aqueous solutions and the electronic structure of aqueous systems.

Sotiris Xantheas, *PNNL, sotiris.xantheas@pnnl.gov*

Richard Saykally, *UC Berkeley, saykally@berkeley.edu*

QUANTUM MECHANICS IN MANY DIMENSIONS

The quantum N -body problem at the core of chemical theory has an exponential complexity with the number of degrees of freedom. Hence all areas of first-principles chemical simulation must deal with the "curse of dimensionality" that limits the description of quantum effects to relatively simple systems. Several approaches designed to break the curse (Monte-Carlo, many-body expansion, tensor decomposition) have evolved in each domain of chemical theory, yet there are strong similarities between the seemingly domain-specific techniques. This symposium will bring together researchers from several domains of chemical theory (electronic structure, vibrational structure, dynamics) as well as related fields (physics, mathematics) in an attempt to identify and exploit the common threads of inquiry across the disciplines.

Edward Valeev, *Virginia Tech, evaleev@vt.edu*

CHEMISTRY AT THE SPACE-TIME LIMIT

This symposium aims to bring together leading efforts in pushing the horizon of joint space-time resolution of relevance to chemistry. Multiple approaches are pursued to see chemistry in the act, in real-time, and with molecular or sub-molecular spatial resolution by employing multi-dimensional (space, time, energy, momentum) measurement techniques. This is an active field that is growing with the advancement of enabling tools and theory. The methods invariably combine ultrafast laser methodologies with x-ray or electron probing and imaging, and novel approaches in nonlinear optical, nano-optical and scan-probe microscopies. The theoretical contributions focus on single-electron transport, collective plasmonic response, and nonlinear spectroscopy and scattering. A tutorial session to serve students and the broader public will be included.

Vartkess A. Apkarian, *University of California, Irvine, aapkaria@uci.edu*

Hrvoje Petek, *University of Pittsburgh, petek@pitt.edu*

ELECTROSTATICS AND POLARIZATION EFFECTS IN BIOPHYSICAL CHEMISTRY:
IN SILICO, IN VITRO, AND IN VIVO

Electrostatic forces are crucial for many key biochemical processes. For example all energy transduction processes, such as catalysis, proton transport, electron transfer and ion homeostasis involve electrostatic interactions. Similarly, all salt and pH-dependent processes are mostly driven by electrostatics. The goal of this symposium is to bring together wet- and dry-lab researchers with common interests in understanding the electrostatic effects in biological macromolecules and to forge new collaborations or strengthen ongoing collaborations between investigators. Presentations that focus on utilizing and developing different experimental and computational methods will reveal the strengths and weaknesses of these approaches and will contribute to further improvements. The symposium aims to identify important new questions for which experiment is necessary for physical insight, to guide extension of theoretical and computational models, and to provide quantitative data for benchmark of models.

Emil Alexov, *Clemson University, ealexov@clemson.edu*

Ray Luo, *University of California, Irvine, ray.luo@uci.edu*

CHEMICAL FRONTIERS IN SOLAR SYSTEM EXPLORATION

This symposium focuses on the broad interplay between space missions, telescopic observations, laboratory spectroscopy, theoretical investigations, and fundamental laboratory studies on molecular processes, which contribute to the chemical formation and evolution of distinct bodies in our Solar System. Topics will include the evolution of atmospheres of planets and their moons via gas-phase neutral and ion chemistry, surface chemistry induced by energetic photons and charged particles, spectroscopy of exotic compounds and surface ice spectroscopy, state-of-the-art analytical tools to derive the composition of meteorites, interplanetary and cometary dust, and guiding and interpretive theoretical computations and models. This symposium will bring together communities focused on space missions and terrestrial astronomical observations, with atmospheric modelers, quantum chemists, kineticists, and dynamicists, so that these communities can develop a common language and work together to identify the chemical frontiers that must be addressed and the approaches best suited to meet these challenges.

Ralf Kaiser, *University of Hawaii, ralfk@hawaii.edu*

Nadia Balucani, *University of Perugia, Italy, nadia.balucani_at_unipg.it*

PHYS DIVISION RESEARCH AWARDS AND JPC LECTURESHIPS

The PHYS Division Research Awards and Journal of Physical Chemistry Lectureship talks will take place at this one-day symposium.

UNDERGRADUATE SYMPOSIUM: BASIC RESEARCH IN PHYSICAL CHEMISTRY

The Undergraduate Symposium is targeted for current junior chemistry majors, who will be seniors at the time of the Indianapolis meeting. Up to 25 outstanding undergraduate chemistry students will be selected for a series of undergraduate-focused talks and social events during the Indianapolis 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/2013.html. The application deadline is 8 February 2013.

Carol Parish, *University of Richmond, PHYSworshop@richmond.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, 11 September 2013. See the announcement below for information about the Physical Chemistry Student Poster Awards.

Joel Bowman, *Emory University, jmbowma@emory.edu*

On-Line Abstract Submission Deadline: 18 March 2013
<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

Several 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.

Poster presenters will be contacted by e-mail and invited to declare their eligibility (student status) and desire to participate in the student poster award competition.

JOEL BOWMAN, PROGRAM CHAIR

Emory University (404) 727-6592, jmbowma@emory.edu

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