



ACS DIVISION OF PHYSICAL CHEMISTRY
244TH NATIONAL MEETING
PHILADELPHIA, PA
19-23 AUGUST 2012

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 2012.** 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.

KINETICS AND MECHANISM IN THE EARTH'S ATMOSPHERE

Observations of aerosols and their composition, of cloud and ice condensation nuclei and atmospheric oxidants continue to present intriguing physical chemistry problems. In the last few years there have been exciting advances in technologies for measuring trace gases that build on ideas from physical chemistry laboratories applied to *in situ* observations, to chamber experiments designed to mimic the atmosphere but under controlled conditions, and to observing trace gases from space. These observations have inspired new theoretical approaches to predicting oxidative mechanisms or assessing condensation and/or nucleation behavior.

Ronald C. Cohen, *University of California, Berkeley*, rccohen@berkeley.edu
Timothy H. Bertram, *University of California, San Diego*, tbertram@ucsd.edu

BRIDGING THE GAP BETWEEN AB INITIO AND CLASSICAL SIMULATIONS

The symposium offers a wide view of recent developments in the field of quantum chemistry and how quantum chemistry is combined with classical methods to address problems in chemistry and physics related to renewable energies, biological systems, and interfaces. The program will be organized in 8 sessions.

Laura Gagliardi, *University of Minnesota*, gagliard@umn.edu
Lyudmila Slipchenko, *Purdue University*, lsipchenko@gmail.com

SOLVENT DYNAMICS AT BIOMOLECULAR INTERFACES: EXPERIMENT AND THEORY

With diverse experiments and theoretical approaches developed in recent years, a vast amount of new information is now available about the role of solvation at the surface of biomolecules. In many cases, proteins, nucleic acids, lipids, and polysaccharides have been shown to modify not just the average structure but also the local dynamics of nearby solvent molecules on time scales from femtoseconds to seconds. From a physical chemistry point of view, this symposium will address these questions: What do new experimental observables say about the dynamics of the solvent around biomolecules on different time scales? Are these dynamic changes relevant or useful to biomolecular function? And how do simulations of varying levels of specificity help to understand and make connections with experiment?

Casey H. Londergan, *Haverford College*, clonderg@haverford.edu
Steven A. Corcelli, *University of Notre Dame*, scorcell@nd.edu

SYNTHESIS, SPECTROSCOPY, THEORY AND APPLICATIONS OF NANOCRYSTALS AND NANOWIRES

The symposium offers a broad view of recent development in the field of nanomaterials, focusing on nanocrystals and nanowires. The program covers synthesis and novel structures, spectroscopy and photochemistry, plasmonics, catalysis, renewable energy, and bio-nano-chemistry. It combines a blend of theory and fundamental science as well as applications and devices. A total of 8 sessions will each feature 3-4 invited speakers covering the different aspects of each sub-discipline along with 2-3 contributed talks.

Yi Cui, *Stanford University*, yicui@stanford.edu
Todd Krauss, *University of Rochester*, krauss@chem.rochester.edu
Eran Rabani, *Tel Aviv University*, rabani@tau.ac.il

DYNAMICS AND JAMMING IN COMPLEX ENVIRONMENTS

Crowding strongly influences particle dynamics in a range of physical, chemical, and biological systems. In this symposium we will bring together experimentalists and theorists from diverse communities who study the unusual relaxations, broadly termed glassy dynamics that are often found in crowded systems. Among the particular topics to be addressed are how new measurement techniques can elaborate the length and time scales associated with spatially heterogeneous dynamics and how these length scales may both be elucidated and altered using environmental perturbations such as confinement. While several sessions will include contributions from both experimentalists and theorists, two sessions devoted to theory, models, and simulations will also be featured. In these sessions, glassy dynamics will be discussed from the viewpoint of the structural glass transition, mode-coupling theories, facilitation based models, and jamming approaches. A session focused on the importance of crowding in biology will cover a broad range of topics including how crowding in the cellular milieu affects protein folding and macromolecular diffusion as well as the manifestations of crowding on longer length scales. The chief goals of this symposium are (1) exploring the commonalities in the diverse systems in which crowding is an important determinant of dynamics and (2) continuing to develop a common language with which to discuss glassy behavior, in part to facilitate experiments that may verify theoretical predictions.

Laura Kaufman, *Columbia University*, kaufman@chem.columbia.edu
Vassiliy Lubchenko, *University of Houston*, vas@uh.edu

ELECTRON AND ENERGY TRANSFER PHENOMENA: AT THE INTERSECTION OF ELECTRONIC STRUCTURE THEORY AND CHEMICAL DYNAMICS

Recent advances in quantum chemistry have made it possible to calculate *ab-initio* ground and excited-state properties of large molecules with low-lying excited states, including chromophores, conjugated polymers, and solvated multivalent clusters. With so much static *ab-initio* information available, this symposium will (i) assess what aspects of electron and energy transfer processes can be modeled accurately using current techniques and implementations, and (ii) identify what future methodological advances in quantum chemistry and chemical dynamics will be necessary to better describe these non-equilibrium processes quantitatively. Speakers will include both experimental and theoretical chemists (the latter with backgrounds in both electronic structure and chemical dynamics), with everyone focusing on the application of theoretical models to technologically as well as fundamentally interesting experimental systems.

Joseph E. Subotnik, *University of Pennsylvania*, subotnik@sas.upenn.edu
Robert J. Cave, *Harvey Mudd College*, robert_cave@hmc.edu
Marshall Newton, *Brookhaven National Laboratory*, newton1@bnl.gov

PHOTOCHEMISTRY IN BIOLOGY

Photons from the sun support nearly all life on earth, yet the same energy can cause photo-oxidation and other deleterious effects to living creatures. This symposium is motivated by key overarching questions: How do photoactive biomolecules efficiently transform photon energy to functional chemical energy or heat? What is the role of the local chromophore environment on photoreactivity? Specific topics include photosynthesis, photoreceptors, flavoproteins, photoprotection, and phototriggers. A wide range of themes centered on mechanisms and dynamics will be explored, such as mechanisms for energy transfer in light-harvesting antennae, reactions in the catalytic core of the oxygen-evolving complex, biomimetic energy harvesting, rapid conversion of light energy to protein structural changes, long-range electron transfer and charge separation, ultrafast internal conversion, and phototriggered protein dynamics. These and other topics in photobiology are investigated with a variety of optical, magnetic, and computational tools, combined with molecular biology techniques. As such, this symposium aims to assemble researchers across the disciplines of physical chemistry, biochemistry, and inorganic chemistry.

Judy Kim, *University of California, San Diego*, judyk@ucsd.edu
Mike Tauber, *University of California, San Diego*, mtauber@ucsd.edu

POSTDOCTORAL RESEARCH AWARDS

The PHYS Division will highlight leading research by postdoctoral fellows at the Fall National ACS meeting in Philadelphia through a series of special awards. Awardees will give oral presentations in a PHYS symposium and attend the PHYS executive-committee dinner. Each postdoctoral nominee should also submit the usual contributed abstract to the PHYS program when online submissions open on 23 January so he/she can present at the meeting even if not selected for the special symposium. The deadline for applications is 9 March 2012, and selections will be announced shortly after the Spring ACS Meeting in March 2012. More details on the award and application procedures may be found at <http://phys-acis.org>.

PHYSICAL CHEMISTRY SYMPOSIUM WORKSHOP FOR UNDERGRADUATE CHEMISTRY MAJORS

The Workshop for Undergraduate Chemistry Majors is targeted for current junior chemistry majors, who will be seniors at the time of the Philadelphia meeting. Up to 25 outstanding undergraduate chemistry students will be selected for a series of undergraduate-focused talks and social events during the Philadelphia 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-acis.org/PHYS_Undergraduate_Workshop.htm. The application deadline is 10 February 2012.

Carol Parish, *University of Richmond*, PHYSworkshop@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, 22 August 2012. See announcement below for information about the Physical Chemistry Student Poster Awards.

Martin Gruebele, *University of Illinois*, mgruebel@illinois.edu

On-Line Abstract Submission Deadline: 18 March 2012
<http://abstracts.acs.org>

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.

MARTIN GRUEBELE, PROGRAM CHAIR
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FOR INFORMATION ABOUT THE PHYSICAL CHEMISTRY DIVISION, VISIT OUR WEB SITE:
<http://phys-acis.org/>