



ACS DIVISION OF PHYSICAL CHEMISTRY

237th NATIONAL MEETING

Salt Lake City, Utah

March 22-26, 2009

Call for Papers

The Physical Chemistry Division has organized the following topical oral symposia, consisting of both invited and contributed papers, and also topical and general poster sessions. **The abstract deadline is October 20, 2008.** 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 presentation; contributions not selected for oral presentation will be assigned to the poster session.



NEW DEVELOPMENTS IN ENERGY CONVERSION AND LIGHT-HARVESTING

The newest developments in the field of energy conversion include low cost, solution processed solar cells utilizing semiconductor nanoparticles, organic molecules, polymers, nanowire heterostructures, etc. Advances in synthesis of novel materials combined with fundamental studies of light absorption, carrier dynamics, and electronic transport in organic and semiconductor nanostructures are the important prerequisites to novel solar cell technologies. Recent developments in photonics offer promising ideas for improved light harvesting in photovoltaic and photocatalytic systems. Improvements of thermoelectric materials are associated with nanostructured materials for optimized electronic transport and phonon scattering. All these developments require highly interdisciplinary research covering the areas from synthetic chemistry and self-assembly to ultrafast spectroscopy and theory. The goal of this symposium is to bring together scientists working in different areas related to energy research.

Dmitri Talapin, *University of Chicago*, dvtalapin@uchicago.edu

John Lupton, *University of Utah*, lupton@physics.utah.edu

David Ginger, *University of Washington*, ginger@chem.washington.edu

ADVANCES IN ELECTRONIC STRUCTURE THEORY AND FIRST PRINCIPLES DYNAMICS

This symposium will explore the interface between electronic structure theory and first principles dynamics, with particular emphasis on development and applications related to excited states, liquids and solvated species, charge transport and molecular electronics, and nanomaterials.

The symposium will bring together the local orbital and plane wave communities and will examine problems from the gas phase to condensed phases.

C. David Sherrill, *GeorgiaTech*, sherrill@gatech.edu

Giulia Galli, *UC, Davis*, gagalli@ucdavis.edu

ATTOSECOND SCIENCE- THE NEXT FRONTIER

Investigations of laser-matter interactions have entered a new spatio-temporal regime, the regime of "attosecond science", where matter structure and evolution can be measured on spatial and temporal scales natural to electron motion in molecules. The attosecond pulse is a spin-off from strong field physics in which nonperturbative effects are fundamental. Whereas previous applications of ultrashort laser pulse technology led to femtosecond measurement and control of atom movement in molecules, attosecond science will lead to measuring and perhaps even controlling electron motion inside molecules! The purpose of this symposium will be to bring together the experts, both experimental and theoretical to explore and thus advance exploitation of the new attosecond technology for chemistry.

Andre Bandrauk, *Sherbrooke*, Andre.Dieter.Bandrauk@usherbrooke.ca

Steve Leone, *UC, Berkeley*, srl@berkeley.edu

ONVERGENCE BETWEEN THEORY AND EXPERIMENT IN SURFACE CHEMISTRY AND CATALYSIS

Advances in both experimental surface science measurements and computational techniques for treating solids, molecules and the solid-gas interface are enabling a new level of synergy between experiment and theory in this area. The implications for increased physical understanding will be explored in this symposium, with examples drawn not only from surface science in ultra-high vacuum, but also systems under catalytically relevant pressures and temperatures.

John Yates, *University of Virginia*, johnt@virginia.edu

Jens Norskov, *Technical University of Denmark* norskov@fysik.dtu.dk

FUNCTIONAL MOTIONS IN ENZYME CATALYSIS

This symposium will explore experimental and theoretical progress in understanding links between dynamics in the form of functional motions, and enzyme catalysis. Particular topics to be addressed include: dynamic enigmas in enzyme catalysis, theoretical aspects of enzyme structure-motion-function relationship, calculations and simulations of enzyme chemical activity and relevant motions, and combinatorial and bioinformatic tools for identification of functional motion. Further aspects of the problem will include dynamical information from kinetic experiments, probing functional motions in enzymes by NMR relaxation and other spectroscopies. Current assessment of the implications of protein motions on enzymology will be discussed.

Amnon Kohen, *University of Iowa*, amnon-kohen@uiowa.edu

Arieh Warshel, *University of Southern California*, warshel@usc.edu

MOLECULAR HYDROGEN IN NANOPOROUS MATERIALS: MEETING GROUND FOR THEORY AND EXPERIMENT

Storing hydrogen by encapsulating hydrogen molecules in nanoporous materials, e.g., clathrate hydrates, nanostructured carbon materials, and metal-organic frameworks, has attracted a great deal of interest in recent years. Consequently, quantitative understanding of the behavior of molecular hydrogen inside the nanospaces of such materials is of great practical, as well as fundamental, significance. The topics covered by the symposium include, but are not limited to, first-principles characterization of the interactions between hydrogen molecules and the host materials, quantum dynamics of the nanoconfined hydrogen molecules and its spectroscopic signatures, molecular dynamics and Monte Carlo simulations of hydrogen adsorption, diffusion, and storage capacity, and the ways to include quantum effects in these simulations. The participants will describe the progress made to date, identify the main challenges, and present state-of-the-art methods, electronic structure and dynamics, suitable for microscopic description of these systems. The emphasis of the symposium will be on theory, but several invited talks will be devoted to experimental studies of the structural and dynamical properties of hydrogen molecules in nanoporous materials by a variety of spectroscopic techniques, such as inelastic neutron scattering, neutron diffraction, Raman and infrared spectroscopy.

Zlatko Bacic, *New York University*, zlatko.bacic@nyu.edu

FROM CLUSTERS TO THE CONDENSED PHASE: PROGRESS IN POLARIZABLE FORCE FIELDS AND SIMULATION

The allure of molecular simulation is that observables of a chemical or biological system can be calculated at one time, in the context of a molecular model that can provide insight and new hypotheses on a range of experiments. Given the demands of sampling, potential energy surfaces for many molecular simulations rely on approximations and empirical input in order to formulate tractable descriptions of the potential energy surface. The current consensus is that fixed charge models are robust for equilibrium properties for homogeneous systems, while evident discrepancies are identified away from ambient conditions, for dynamical properties, and for heterogeneous chemical systems in general. Polarizable empirical force fields, which offer a clear systematic improvement in functional form by including many body effects, are now more ubiquitous in the molecular simulation community. This symposium concerns whether polarizable force fields have successfully reached a new level of predictive power over their non-polarizable predecessors.

Teresa Head-Gordon, *UC, Berkeley*, TLHead-Gordon@lbl.gov

Vijay Pande, *Stanford University*, pande@stanford.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, March 25, 2009. See announcement below for information about the Physical Chemistry Student Poster Awards.

Martin Head-Gordon, *UC, Berkeley*, mhg@cchem.berkeley.edu

On-Line Abstract Submission Deadline:

October 20, 2008

<http://oasys.acs.org/oasys.htm>

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

At the meeting in Salt Lake City, 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 Head-Gordon, PROGRAM CHAIR
UNIVERSITY OF CALIFORNIA, BERKELEY