ACS DIVISION OF PHYSICAL CHEMISTRY
234th NATIONAL MEETING
Boston, MA
August 19-23, 2007

Call for Papers

The Physical Chemistry Division has organized the following topical oral symposia, consisting mainly of invited papers, and also a general poster session. **The abstract deadline is April 2, 2007**. 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.

SINGLE MOLECULE SPECTROSCOPY AND NOVEL IMAGING TECHNIQUES FOR BIOMOLECULAR SYSTEMS

This symposium will highlight recent advances in single-molecule detection and live-cell imaging. These methods have changed the way many biological problems are addressed. They reveal intricate biomolecular dynamics rendering them particularly powerful in elucidating mechanisms of molecular machineries. Single-molecule approaches have revolutionized our understanding of ion channels and molecular motors. They are now making significant contributions in new biological areas such as nucleic acid protein interactions, macromolecule folding, and cellular dynamics. In the mean time, chemists are developing ever more specific and powerful reporters and physicists are pushing the envelope of instrumentation and technology towards higher sensitivity and higher spatial and temporal resolution.

Xiaowei Zhuang, *Harvard University, zhuang@chemistry.harvard.edu*
Haw Yang, *U. C. Berkeley, hawyang@berkeley.edu*
Paul Selvin, *University of Illinois, Urbana Champaign, selvin@uiuc.edu*

EMERGENCE OF FUNCTION IN MOLECULAR ASSEMBLIES

Since P. W. Anderson's article in Science (1972), there has been recognition that complex systems may differ dramatically from the linear limit of their components. In thermodynamics, such observables would be characterized as containing (possibly extreme) nonadditive contributions. From a dynamic (or nonequilibrium) perspective, such behavior "emerges" in an unexpected fashion in the sense that it is not readily apparent when investigating smaller components of the complex system. The application of these concepts from physics to materials science has recently been recognized in molecular-scale assemblies. Material nanoscience research is often based on a molecular level description that does not fully account for a system's emergent properties. This symposium will bring together experimentalists and theoreticians in material science, physics and physical chemistry in order to integrate their efforts towards the understanding of the emergence of function (at whatever length scale) due to the collective nonlinear interactions within molecular assemblies.

Rigoberto Hernandez, *Georgia Tech*, *Hernandez@gatech.edu*
Deborah Evans, *University of New Mexico, debi@unm.edu*
Nadrian Seeman, *New York University, ned.seeman@nyu.edu*

COMPUTATIONAL ELECTROCHEMISTRY FOR NEW ENERGY

Future advances in several areas of alternative energy will rely upon a detailed understanding of electrochemistry. The control of chemical transformations in these and other technologies remains a central challenge. These processes involve bond breaking/formation and/or electron/hole transfer in the complex environment of a solid-liquid interface in the presence of a current potential. Computer simulations and molecular modeling methods offer the opportunity to characterize, understand, and predict the many aspects of chemical reactivity. The nature of these problems creates a demand for new theories, methods, and algorithms. This symposium will highlight the significant progress made by the computational chemistry community in addressing this challenge.

Michel Dupuis, *Pacific Northwest National Laboratory, michel.dupuis@pnl.gov*
Donald Truhlar, *University of Minnesota, truhlar@umn.edu*

HYDRATION: FROM CLUSTERS TO AQUEOUS SOLUTION

Significant progress has been made in our experimental and theoretical understanding of hydration phenomena in clusters, interfaces, and bulk water. However, the relationship between results obtained in these various environments is sometimes ambiguous and controversial. This symposium will bring the different communities together in an attempt to clarify common ground and outstanding problems.

Daniel Neumark, *U. C. Berkeley, dneumark@berkeley.edu*
Kenneth D. Jordan, *University of Pittsburgh, ken@visual1.chem.pitt.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, August 22, 2006. See the announcement below for information about the Physical Chemistry Student Poster Awards.
Gregory A. Voth, *University of Utah, voth@chem.utah.edu*

STRUCTURAL DETERMINATION, REFINEMENT, AND MODELING OF LARGE BIOMOLECULAR COMPLEXES

Biological functions occur in a wide range of time and length scales from the formation of a chemical bond in enzyme catalysis, to large-scale conformational changes in allosteric regulation and protein folding, to the complex inter-protein dynamics of molecular machines. It is a challenge for both experimental and theoretical researchers to cope with such a wide range of scales, and even more challenging to bridge the information between scales. This symposium will bring together computational and experimental experts from diverse fields to discuss these challenges, especially in relation to large molecular complexes.

Jianpeng Ma, *Baylor College of Medicine, jpma@bcm.tmc.edu*
Michael Diehl, *Rice University, diehl@rice.edu*
Shuanghong Huo, *Clark University, shuo@clarku.edu*

EXCITED ELECTRONIC STATES IN CHEMISTRY AND BIOLOGY: THEORY AND EXPERIMENT

Recent theoretical advances in modeling electronic structure of excited states and dynamics including quantum mechanical effects have opened the door to detailed treatments of photochemical and photobiological processes. Simultaneously, advances in crystallographic and spectroscopic methods are providing new data which can both test and challenge theory. This symposium will cover new developments in theory and experiment in the chemistry and dynamics of excited electronic states. Advances in theoretical and experimental methods will be included, as well as applications to photochemical and photobiological processes.

Todd J. Martínez, *University of Illinois, tjm@spawn.scs.uiuc.edu*
Spiridoula Matsika, *Temple University*, *smatsika@temple.edu*

QUANTUM MECHANICS AND STATISTICAL MECHANICS: CAN ONE AVOID THE OTHER?

Although quantum mechanics and statistical mechanics have progressed relatively independently, they share the goal of understanding and predicting the structures and activities of complex systems. Statistical mechanics has been developed with the assumption that the potential energy surface for a condensed phase system is available such that dynamic and thermodynamic quantities can be evaluated. Quantum chemical methods, once largely limited to the gas phase, necessitated an intermediate step of fitting analytical potential functions to quantum mechanical data. However, the development of ab initio molecular dynamics and combined quantum mechanical and molecular mechanical (QM/MM) methods offers the opportunity to move quantum mechanics from the gas phase realm to the condensed phase reality. This symposium will bring together theoretical and computational chemists to showcase the latest development of theories and methods that may help bridge the realms of quantum and statistical mechanics.

Jiali Gao, *University of Minnesota, gao@chem.umn.edu*
Sharon Hammes-Schiffer, *Penn State, shs@chem.psu.edu*

BIOLOGICAL ION CHANNELS: FROM MOLECULAR STRUCTURE TO CELLULAR FUNCTION

The past decade has seen tremendous strides in our understanding of the structure and function of ion channels. These proteins embed in lipid bilayers to allow the passage of ions and play a critical role in many physiological functions, including energy and signal transduction. The determination of the crystal structures of several ion channels, as well as advances in cryomicroscopy, NMR and other spectroscopic techniques, have provided insights into mechanisms of their motions and function, including ion permeation kinetics and channel gating in response to channel-specific stimuli. In this symposium recent progress in both experimental and theoretical/computational aspects of ion channel science will be explored from a physico-chemical perspective. Central themes will include how individual ion channel protein molecules interact with i) the embedding lipid bilayer membrane, ii) external stimuli such as solution pH and ligand molecules, and iii) signaling proteins both in and outside of the cell.

Rob D. Coalson, *Univ. of Pittsburgh, coalson@pitt.edu*
Maria G. Kurnikova, *Carnegie Mellon University, kurnikova@cmu.edu*

On-Line Abstract Submission Deadline:
April 2, 2007
http://oasys.acs.org/oasys.htm

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.

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