

# ACS DIVISION OF PHYSICAL CHEMISTRY 235<sup>th</sup> NATIONAL MEETING New Orleans, LA April 6-10, 2008



# **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 28, 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.

## PHYSICAL CHEMISTRY OF ATMOSPHERIC PROCESSES

This symposium is dedicated to an examination of the use of physical chemistry concepts and methods in the study of various atmospheric processes. From a topical point of view, issues related to climate change and air quality will be discussed through the investigation of the fundamental physical chemistry of the relevant atmospheric gas phase, particle-phase, and heterogeneous interaction phenomena. From a methods point of view, field observations, laboratory experiments, and theoretical and computational results will be represented. Invited speakers will provide either a broad overview of a certain research area or a focused presentation of the most current aspects of their work.

Matthew Elrod, Oberlin College, matthew.elrod@oberlin.edu

Joel Thornton, University of Washington, thornton@atmos.washington.edu

## **OPTICAL PROBES OF DYMANICS IN COMPLEX ENVIRONMENTS**

This symposium explores the latest experimental and theoretical studies on complex dynamics in chemical systems and biophysical environments. Particular emphasis is placed on new experimental methods being used to probe molecular, atomic, and electronic dynamics in liquids, solids, proteins, and clusters. It also addresses theoretical efforts to understand these experiments and the revealed by them. Specific topics dynamics of interest include multidimensional spectroscopies, ultrafast x-ray and electron diffraction, time-resolved structure determination, optical control, energy and charge transfer, chemical reaction dynamics, and timeresolved imaging.

Andrei Tokmakoff, MIT, tokmakof@MIT.EDU Roseanne Sension, University of Michigan, rsension@umich.edu

#### MULTISCALE MODELING IN BIOPHYSICS

This symposium will involve scientists with expertise in the modeling, analysis and computation of biophysical processes that span length and time scales of many orders of magnitude. Linking together those vastly different scales presents one of the main challenges in modern biophysics. Important problems that are intrinsically multiscale in nature include: 1) protein dynamics and folding, and its role in processes such as the assembly of super-molecular complexes, signaling, binding 2) DNA replication/transcription, where modeling data obtained with electron force microscopy involves bridging atomistic and continuum models, and 3) transport through ion channels. In the last few years promising multiscale methods have emerged to characterize the dynamics of large molecular systems on biologically relevant timescales. This symposium brings together researchers from different communities, representing a range of modeling and computational techniques, in order to identify and address multiscale problems in modern biophysics and to advance the development of multiscale methods.

Cecilia Clementi, Rice University, cecilia@rice.edu Gregory Voth, University of Utah, voth@chem.utah.edu

## **COMPUTATIONAL SPECTROSCOPY**

Modern computational tools (quantum chemistry + dynamics) have made it possible to evaluate spectroscopic properties of molecules and materials with ever-increasing accuracy. We plan to have nine halfday sessions in this symposium to highlight the dramatic impact of computational techniques to the important field of spectroscopy. The symposium will include both methodological developments and applications to a wide range of chemical systems, with the aim to crossfertilize ideas and techniques from a variety of areas. A part of the symposium will honor the accomplishments of Prof. Rod Bartlett, a pioneer in the field of Theoretical Chemistry.

Krishnan Raghavachari, Indiana University, kraghava@indiana.edu H. B. Schlegel, Wayne State University, Hbs@chem.wayne.edu

#### NANOSTRUCTURED MATERIALS

The symposium focuses on research in nanostructured materials. The impact on both fundamental science and the potential industrial applications have been tremendous and are still growing. There are many exciting examples of nanostructured materials including colloidal nanocrystals, C<sub>60</sub>, carbon nanotubes, semiconductor nanowires, and nanocomposite and porous materials. The field is quickly evolving and is now interfacing with many different scientific disciplines, from chemistry to physics, to materials science, engineering and to biology. The research on nanostructured materials has been highly interdisciplinary because of the different synthetic methodologies involved, as well as the many different physical characterization techniques used. This symposium provides opportunities for intensive discussions and exchange of ideas by bringing together experts working on the synthesis of nanofunctional materials, nanostructural fabrication, novel physical and chemical property characterization as well as nanoscale device fabrication and testing.

Peidong Yang, University of California Berkeley, p\_yang@berkeley.edu Xiaogang Peng, University of Arkansas, xpeng@uark.edu Christopher Murray, Univ. of Pennsylvania, cbmurray@sas.upenn.edu

## **ELECTRONIC STRUCURE AND REACTION DYNAMICS OF OPEN-SHELL SPECIES**

Open-shell species play important roles in many reactive environments (atmosphere, combustion, plasma, interstellar space, etc.), and yet it is challenging to investigate reaction dynamics of free radicals at the molecular level. This symposium highlights recent advances in experimental and theoretical studies of both the fundamental and applied aspects of open-shell species. The topics include spectroscopy and potential energy surfaces, photochemistry, and reaction dynamics of free radicals in gas phase, clusters, and condensed phase, as well as in atmospheric applications and other chemical processes.

Jingsong Zhang, Univ. of Calif. Riverside, jingsong.zhang@ucr.edu Martin Head-Gordon, Univ. of Calif. Berkeley, mhg@cchem.berkeley.edu

## SPECTROSCOPY, CHEMISTRY, AND IMAGING **THROUGH NANOPHOTONICS**

#### PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday evening, April 9, 2008. See announcement below for information about the Physical Chemistry Student Poster Awards.

Laurie J. Butler, University of Chicago, L-Butler@uchicago.edu

Nanophotonics is the study of the interaction of light with nanostructured systems. Over the past few years remarkable advances have been made in this area, with significant implications for spectroscopy, chemistry, and imaging. Systems of interest to this symposium include, but are not limited to, metal, semiconductor and hybrid nanoparticles and nanostructures. This six session symposium will report on recent major theoretical and experimental developments.

Stephen K. Gray, Argonne National Laboratory, gray@tcg.anl.gov Gary P. Wiederrecht, Argonne National Laboratory, wiederrecht@anl.gov

# **On-Line Abstract Submission Deadline:**

October 28, 2007

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

## PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

At the meeting in New Orleans, 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.

> Laurie J. Butler, PROGRAM CHAIR DEPARTMENT OF CHEMISTRY, UNIVERSITY OF CHICAGO, CHICAGO, IL 60637