



ACS DIVISION OF PHYSICAL CHEMISTRY

236th NATIONAL MEETING

Philadelphia, PA

August 17-21, 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 March 17, 2008.** For those interested in an oral presentation, please submit abstracts to the appropriate 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.

WATER MEDIATED INTERACTIONS

This symposium focuses on theoretical, simulation and experimental studies of the role of water in mediating interactions between molecules, nano-particles and macroscopic interfaces. This broad area includes the structure, dynamics, spectroscopy and thermodynamics of water and its role in mediating hydrophobic, polar and ionic interactions between small molecules and biological macro-molecules, as well as nano-materials and interfaces. Topical sessions include hydrophobic interactions, ionic interactions, biological water, aqueous interfaces, and structure and dynamics.

Dor Ben-Amotz, *Purdue University*, bendor@purdue.edu

Hank Ashbaugh, *Tulane University*, hanka@tulane.edu

ADVANCES IN THE ELECTRONIC STRUCTURE OF TRANSITION METAL SYSTEMS AND ORGANOMETALLICS

Transition metals play a dominant role as catalysts in biological and industrial processes. Understanding the properties and reactivity of systems containing transition metals is difficult and poses a number of unique challenges. Electronic structure calculations, most notably studies based on density functional theory, have made substantial contributions to understanding and sometimes to rationally designing new systems of interest. This symposium will review and discuss how the key problems in understanding the electronic structure of systems containing transition metals are being addressed. The topics discussed will include (a) transition metals in biological systems, (b) reaction mechanisms and catalysis, and (c) structure and bonding.

Mu-Hyun Baik, *Indiana University*, mbaik@indiana.edu

Christopher Cramer, *University of Minnesota*, cramer@umn.edu

SPECTROSCOPIC PROBES OF CHEMICAL DYNAMICS IN GASEOUS AND CONDENSED PHASES

This symposium highlights experimental and theoretical advances in our molecular-level understanding of how the quantum behavior of isolated systems manifests as bulk properties of the condensed phase. For small systems, emphasis will be on defining the signatures of conical intersections in the eigenstate-resolved spectra of small, isolated molecules, and the elucidation of the structures of floppy biopolymers with vibrational spectroscopy. Unifying themes include ultrafast kinetics of photoinduced chemistry and energy transfer in complex molecules, in clusters, at the air/water interface and in the condensed phase.

Steven Corcelli, *University of Notre Dame*, scorcell@nd.edu

Mark Johnson, *Yale University*, mark.johnson@yale.edu

CENTENNIAL OF THE PHYSICAL DIVISION: CELEBRATING THE PAST, EMBRACING THE FUTURE

This symposium will celebrate the Centennial of the Physical Division with a series of invited talks which will present a broad overview of modern physical chemistry. Presentations will be made by some of the most important figures in the field, including several Nobel Prize winners. The presentations will cover historical developments and current research in a variety of subdisciplines including chemical reaction dynamics, molecular beams, surface science, catalysis, atmospheric chemistry, femtochemistry, nanoscience, biophysical chemistry and molecular spectroscopy. (Invited papers only.)

George C. Schatz, *Northwestern University*, schatz@chem.northwestern.edu

Steven J. Sibener, *University of Chicago*, s-sibener@uchicago.edu

PROTEIN FOLDING DYNAMICS: EXPERIMENTS AND THEORY

The last few years have witnessed tremendous progress in the field of protein folding, ranging from probing the earliest conformational dynamics to the development of advanced theoretical and simulation methods to describe atomistic details of the folding process. The goal of this symposium is to bring together scientists with interests in understanding protein folding dynamics and mechanisms. Our primary objective is to provide an interdisciplinary forum for the sharing and synthesis of new ideas. The symposium will highlight many of the new frontier areas in the folding field, including (but not limited to) 1. Atomistic viewpoints on folding and dynamics; 2. Submillisecond folding and dynamics; 3. Folding and misfolding routes; and 4. Energy landscape perspective on folding. Both experimental and theoretical contributions in these and related areas are welcome.

Feng Gai, *University of Pennsylvania*, gai@sas.upenn.edu

Angel Garcia, *Rensselaer Polytechnic Institute*, angel@rpi.edu

RECENT ADVANCES IN BIOPHYSICAL CHEMISTRY OF TRANSPORT BY BIOMOLECULAR MOTORS AND MACHINES

This symposium focuses on recent theoretical and experimental advances toward a complete description of different processes of biomolecular directed transport and biomolecular machines. Understanding mechanisms of these phenomena presents a fundamental challenge in modern chemistry and biology. Topics include 1) mechanisms and dynamics of molecular motors; 2) protein interactions and their effect on biophysical and chemical processes in cells; 3) growth dynamics and force production by cytoskeleton filamentous proteins such as actin filaments and microtubules; and 4) transport of molecules across biological and synthetic nanopores. This symposium brings together experimental and theoretical researchers from different areas of chemistry, physics and biology in order to identify and address multi-disciplinary problems in the biophysical chemistry of transport processes.

Alan J. Hunt, *University of Michigan*, ajhunt@umich.edu

Anatoly B. Kolomeisky, *Rice University*, tolya@rice.edu

FUNDAMENTAL ADVANCES IN CONTEMPORARY NMR SPECTROSCOPY

The symposium surveys the exciting advances that NMR spectroscopy has experienced in recent years, ranging from structure determination of protein fibrils and membrane proteins, to new sensitivity-enhancement techniques for liquid and solid samples. Major emphasis will be placed on exploring the latest structural frontiers in solid- and solution-state biomolecular NMR, on the uses of NMR to follow protein folding and mis-folding, on new techniques for using NMR in drug discovery and organic analyses processes, on the uses of NMR for inorganic and polymeric materials investigations, and on ongoing developments for expanding the NMR sensitivity envelope. Major players in these areas of research have agreed to present their latest advances in this vibrant field; we look forward to your participation in this stimulating environment.

Mei Hong, *Iowa State University*, mhong@iastate.edu

Lucio Frydman, *Weizmann Institute*, lucio.frydman@weizmann.ac.il

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 20, 2008. See announcement below for information about the Physical Chemistry Student Poster Awards.

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

On-Line Abstract Submission Deadline:

March 17, 2008

<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

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