ACS DIVISION OF PHYSICAL CHEMISTRY
245th NATIONAL MEETING
New Orleans, Louisiana
7-11 April 2013

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 15 October 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.

EMERGING TECHNIQUES FOR STRUCTURE DETERMINATION OF NON-CRYSTALLINE PROTEINS

Many macromolecules of biological interest do not readily form large, well-ordered crystalline arrays. Thus, their three-dimensional structure, necessary for a molecular or chemical understanding of their function, cannot be obtained using X-ray crystallography. Solid-state NMR and cryo-electron microscopy have emerged as the techniques of choice for elucidating the molecular-level organization of these proteins and assemblies. These methods probe different length and time scales and provide complementary information. This symposium seeks to bring together researchers working on similar systems using these different approaches.

Rachel Martin, *University of CA, Irvine, rachel.martin@uci.edu*
Andres Leschziner, *Harvard University, aleschziner@mcb.harvard.edu*

FRONTIERS IN REACTION DYNAMICS

The field of Reaction Dynamics, which probes the intimate details of molecular interactions at the highest level allowed by quantum mechanics, is a robust and growing field of chemical inquiry. This is being driven by technological advances and advances in computational power and tools. The Symposium will cover frontier topics, in all cases highlighting the importance of the synergy between theory and experiment. Topics will include nonadiabatic dynamics and the role of excited electronic states in reaction; quantum state resolved photodissociation dynamics; novel reaction mechanisms; unique properties of molecular clusters; bimolecular reactions affording universal or state-resolved probing of chemical reactions; dynamics at interfaces and in solution; and photoionization dynamics and photoelectron spectroscopy. These topics will be seen in application to a broad range of subjects from combustion to astrochemistry to biochemistry, and theory and experiment will work hand-in-hand in every session.

Arthur G. Suits, *Wayne State University, asuits@chem.wayne.edu*
William L. Hase, *Texas Tech University, Bill.Hase@ttu.edu*

COMBUSTION CHEMISTRY

This symposium will cover all aspects of modern combustion research, including both experiment and theory. This is an exciting time for combustion research, with new experimental techniques revealing unprecedented information about combustion intermediates and with theory having progressed to the point where it competes successfully with experiment on many aspects. Progress is rapid on both conventional fuels and new fuels, including new formulations and biofuels for transportation and propulsion. Topics covered in the symposium include: measurements of kinetics, collisional energy transfer, and reaction intermediates; master equations, mechanisms, and combustion models; thermochemistry of combustion; oxidation, ring opening, and radical chemistry; reactions via conical intersections; optical diagnostics and sensors, laser probes and photoionization mass spectrometry; chemistry in flames and engines; aerodynamics and simulations of laminar and turbulent flames; heat and mass transfer in combustion; nanoparticle fuels; and soot.

Don Truhlar, *University of Minnesota, truhlar@umn.edu*
William H. Green, *MIT, whgreen@mit.edu*

LIPOSOMES, LIPID BILAYERS AND MODEL MEMBRANES: FROM BASIC RESEARCH TO APPLICATION

One of the main building blocks of cellular membranes is lipids, which form a two-dimensional (2D) fluid matrix and in which membrane-associated proteins are enabled to carry out their various functions. Over the years, basic studies of model membrane systems have led to the development of a number of technologies, for example, biocompatible carriers of large biomolecules, such as drugs, proteins and DNA. Dispersions of naturally derived lipid surfactants find application in a number of colloid technologies, in the fabrication of 1D, 2D and 3D nanoscale materials. Tethered membranes have been in recent years shown to be a powerful and flexible biomimetic platform. The symposium's goal is to bring together diverse communities of lipid researchers. The sessions will include leading experts in the basic and applied fields of lipid/model membrane research, and will cover topics of interest to the biomedical, food and textile communities.

John Katsaras, *Oak Ridge National Laboratory, katsarasj@ornl.gov*
Paul Butler, *National Institute of Standards and Technology, butler@nist.gov*

NEW ADVANCES IN UNDERSTANDING PROTEIN FOLDING

There has recently been a renaissance in protein folding experiment and theory, with new methods leading to new insights into the problem of how proteins self-assemble, or "fold," as well as applications to new, emerging important areas in biology. This symposium brings together key leaders in the field and focuses on the following topics: 1) new methodology in simulations and experiments; 2) intrinsically disordered proteins and 3) protein folding in the cell (including chaperone-mediated folding, membranes mediated folding, crowding, and aggregation).

Vijay Pande, *Stanford University, pande@stanford.edu*
Joan-Emma Shea, *Univ. of California, Santa Barbara, shea@chem.ucsb.edu*

ACCURATE CHARACTERIZATION OF NONCOVALENT INTERACTIONS: FROM SMALL MOLECULES TO SUPRAMOLECULAR CHEMISTRY

Noncovalent interactions govern a wide range of chemical phenomena from the energetics of small molecular clusters to the folded structures of proteins and the stability of condensed phases. Thus the ability to quantitatively characterize and accurately predict these interactions is a central theme of chemistry. This symposium will cover recent advances in the understanding and characterization of intermolecular forces. Specifically, the symposium will focus on recently developed and state-of-the-art techniques for treating intermolecular interactions; dispersion interactions; hydrogen bonding and solvation; molecular clusters, molecular aggregates and materials; and biomolecular and synthetic macromolecular interactions. In summary, this symposium is intended to connect researchers working across a variety of length scales to review where we are at the moment and to plan the next steps required to improve our understanding of noncovalent forces in chemistry.

Greg Tschumper, *University of Mississippi, tschumpr@olemiss.edu*
Troy Van Voorhis, *MIT, tvan@mit.edu*

CONFINEMENT EFFECTS IN BIOLOGY AND BIOMIMETIC SYSTEMS

This symposium will cover macromolecular recognition, binding, and adhesion at membrane interfaces; the effects of crowding on binding, chemical reactivity, and macromolecular stability; and the properties of confined water and macromolecules at surfaces, in nanopores, and in dense solutions. We seek both theoretical and experimental contributions.

Deborah Leckband, *University of Illinois, leckband@illinois.edu*

FRONTIERS IN RNA STRUCTURE AND MECHANISM: INTERFACE OF THEORY AND EXPERIMENT

Recent advances in theory and experiment have allowed new insights into the structure, function, dynamics and catalytic mechanisms of RNA molecules. This symposium will bring together experimental and theoretical researchers from a broad range of disciplines focused on complex problems involving RNA. Emphasis will be placed on bridging the gap between theory and experiment: what insights can theory provide the experimental community, and what experimental benchmarks can be used to validate and improve computational models? Catalytic RNAs are rich with compelling mechanistic questions, the answers to which can only be discovered by a coordinated, highly integrated effort between theory and experiment. This symposium provides a forum that brings together theoreticians and experimentalists to discuss key open questions in the field. A main objective of the symposium is to stimulate discussions aimed at developing innovative strategies that integrate theory and experiment to solve long-standing problems in our fundamental understanding of RNA systems at the molecular level. In this way, we hope to facilitate new science at the interface of theory and experiment, aimed at providing deeper insight into RNA catalysis.

Philip C. Bevilacqua, *The Pennsylvania State University, pcb@chem.psu.edu*
Darrin M. York, *Rutgers University, york@biomaps.rutgers.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, 10 April 2013. See announcement below for information about the Physical Chemistry Student Poster Awards.

Joel Bowman, *Emory University, jmbowma@emory.edu*

On-Line Abstract Submission Deadline: 15 October 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.

JOEL BOWMAN, PROGRAM CHAIR
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http://phys-acs.org/