ACS DIVISION OF PHYSICAL CHEMISTRY
241st NATIONAL MEETING
Anaheim, CA
March 27-31, 2011

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 18, 2010**. 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.

MEMBRANE PROTEIN STRUCTURE AND FUNCTION

Membrane proteins play vital physiological roles, such as pumps, channels, carriers, receptors, enzymes and energy transducers, and make up a third of the human genome and two thirds of drug targets. Recent progress in membrane protein structural determination has provided a springboard for obtaining structure-function relationships using experimental and theoretical techniques. This symposium will explore recent developments in describing the interplay between membranes of different composition, phase state and mechanical properties, as well as membrane proteins and membrane-active peptides. A range of biophysical techniques, such as X-ray crystallography, solution and solid-state NMR, EPR, FRET, site-directed mutagenesis, single molecule fluorescence and intracellular fluorescence microscopy, will be showcased. This symposium will also cover modern computer simulation, which is aiding elucidation of atomic-level mechanisms for important membrane protein systems.

Toby W. Allen, *University of California, Davis, twallen@ucdavis.edu*
Frances Separovic, *University of Melbourne, fs@unimelb.edu.au*

FRAGMENT AND LOCAL ORBITAL METHODS IN ELECTRONIC STRUCTURE THEORY

The past few years have seen remarkable progress in fragment or local-orbital, linear-scaling, electron-correlation methods for large molecules and solids. These methods, while differing in the details, operate under the same physical principle, namely, the truncation of long-range interactions at some distances measured in the basis of spatially localized functions, to dramatically accelerate electronic structure calculations. They hold great promise in broadening the utility of accurate electronic structure theory to the condensed phases, where, traditionally, computational studies are limited to more approximate models. This symposium will focus on the development of these methods and their application to synthetic and biological macromolecules, molecular clusters, surfaces, solids, and even liquids.

So Hirata, *University of Florida, hirata@qtp.ufl.edu*
John Z. H. Zhang, *East China Normal University and New York University, john.zhang@nyu.edu*

20 YEARS OF TUNNELING PATHWAYS

2011 marks twenty years since tunneling pathway analysis was first established to compute, analyze, and design electronic interactions in electron-transfer systems. The model relates structure to function in small molecules and proteins alike, unifies a large body of experimental data, and has proven to be an enduring tool in electron-transfer research. Recent developments in pathway theory reveal the influence of bridge dynamical effects, multiple pathway interferences, hopping-tunneling transitions, and pathway phase effects. Design principles derived from the approach are finding use in molecular materials and bio-inspired energy harvesting systems. This symposium will bring together the broad community of theoretical and experimental researchers exploring electron tunneling interactions mediated by chemical and biochemical scaffolds, in order to assess the status of the field, identify opportunities, and define frontiers.

David N. Beratan, *Duke University, david.beratan@duke.edu*
José N. Onuchic, *University of California, San Diego, jonuchic@ucsd.edu*

CHEMICAL REACTIONS AND DYNAMICS AT SURFACES: ADVANCES IN EXPERIMENT AND THEORY

The interactions between gases and surfaces are of paramount importance in a variety of fields, ranging from atmospheric chemistry to catalysis and interstellar chemistry. However, many of the details governing the reactivity and dynamics between gases and surfaces remain elusive. This symposium will present recent advances in the fundamental understanding of chemical reactions and dynamics at a variety of surfaces using both experiments and theory. The overarching goal is to provide an overview of the state of the art in gas/surface phenomena, with particular emphasis on environmental surfaces, heterogeneous catalysis, gas scattering, adsorbate dynamics, and non-adiabatic effects. Interplay between measurements and simulations will be made prominent throughout the symposium.

Diego Troya, *Virginia Tech, troya@vt.edu*
John R. Morris, *Virginia Tech, jrmorris@vt.edu*

CHEMICAL CARBON MITIGATION: A PHYSIOCHEMICAL APPROACH

An intriguing carbon mitigation strategy to combat greenhouse gas atmospheric concentrations is the chemical conversion of CO_2 to liquid phase organic products of value. This symposium will focus on endoenergetic chemical processes that lead to the capture/storage and reductive transformation of CO_2 to potential fuels. While there is a growing body of literature that outlines the chemistry of CO_2 to produce fuels via low energy routes, consideration of key intermediates, the electronic properties of such species and essential reaction dynamics are just now being studied. This symposium will focus on transformations that lead to utilitarian reduction products of CO_2. Approaches of interest include electrochemical, photo-electrochemical, thermochemical, molecular (photo or thermal) and biomimetic studies, along with theoretical investigations that evaluate existing reaction chemistry or suggest novel approaches to the chemistry of interest.

Andrew Bocarsly, *Princeton University, bocarsly@princeton.edu*
Emily Carter, *Princeton University, eac@princeton.edu*

QUANTUM INFORMATION AND COMPUTATION IN CHEMISTRY: EXPERIMENT AND THEORY

This symposium will explore the exciting interface of quantum information and computation and both theory and experiment in physical chemistry. Some of the topics at the trading zone between quantum information and chemistry that will be emphasized during the symposium are: the prospects of quantum computation for the calculation of molecular properties and for the simulation of chemical reaction dynamics; the realization and characterization of non-trivial entanglement and coherence properties of chemical systems; the use of new tools from quantum information such as tensor networks for the simulation of atoms and molecules using classical computers; the use of molecules as quantum information processors; and finally the use of quantum information concepts such as entanglement for the understanding of chemical concepts such as the chemical bond or non-covalent interactions.

Alán Aspuru-Guzik, *Harvard University, aspuru@chemistry.harvard.edu*
Ken Brown, *Georgia Institute of Technology, ken.brown@chemistry.gatech.edu*

INFRARED SPECTROSCOPY OF GAS AND CONDENSED PHASE BIOMOLECULES

This symposium will bring together gas and condensed phase spectroscopists who are working to develop infrared spectroscopy as a means of probing biomolecular structure and dynamics. Infrared spectroscopy is sensitive to biomolecular structures through couplings that depend on conformation and lineshapes that reflect the electrostatic environment. It also can provide insight into the time-scales, energy-flow, and reaction pathways. However, the intellectual understanding necessary to convert between structure and spectroscopy is lacking. In the condensed phase, spectral congestion limits tests to well-defined structural models. Gas phase experiments provide well-resolved infrared spectra, but are often modeled using methods not applicable to the condensed phase. The goal of this symposium is to bring together experimentalists and theoreticians from both fields to discuss this common interest and further develop models that could be used to study the structural dynamics of new and interesting gas and condensed phase biomolecules.

Timothy S. Zwier, *Purdue University, zwier@purdue.edu*
Martin T. Zanni, *University of Wisconsin, Madison, zanni@chem.wisc.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 30, 2011. See announcement below for information about the Physical Chemistry Student Poster Awards.

Sharon Hammes-Schiffer, *Pennsylvania State University, shs@chem.psu.edu*

On-Line Abstract Submission Deadline:
October 18, 2010
http://abstracts.acs.org

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

At the meeting in Anaheim, CA, 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.

SHARON HAMMES-SCHIFFER, PROGRAM CHAIR
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