ACS DIVISION OF PHYSICAL CHEMISTRY
238th NATIONAL MEETING
Washington, DC
August 16-20, 2009

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 16, 2009**. 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.

MOLECULAR BASIS OF PROTEIN AGGREGATION AND AMYLOID FILBRIL FORMATION

Protein aggregation refers to the incorrect folding and subsequent self-assembly of proteins into aggregate species ranging from small soluble oligomers to large fibrillar structures. These fibrils can deposit on organs and tissue in the body in the form of amyloid plaques. A number of diseases, including Alzheimer's, Parkinson's and Type II Diabetes, are associated with this pathological process. Interestingly, proteins not implicated in any disease can also form amyloid fibrils, intimating that aggregation is an intrinsic property of polypeptide chains. This symposium will explore the molecular basis of protein aggregation and amyloid fibril formation from theoretical and experimental standpoints. Specific topics will include 1) Computational and experimental investigations of the early stages of aggregation (the kinetics and thermodynamics of formation of small oligomers), 2) Computational and experimental studies of the structure of amyloid fibrils and 3) Computational and experimental strategies to inhibit aggregation. Novel theoretical and experimental approaches to tackle these problems will be highlighted.

Joan-Emma Shea *University of California, Santa Barbara*, *shea@chem.ucsb.edu*
Ehud Gazit, *Tel Aviv University, ehudg@post.tau.ac.il*

NEW DEVELOPMENTS IN STRONGLY CORRELATED ELECTRONS

Strongly correlated electrons represent one of the key challenges of modern electronic structure in chemistry and physics. Many molecular processes involving energy transfer through excited states or transition metal catalysis, as well as exotic materials phenomena such as high temperature superconductivity, have an underlying physical origin in the behavior of strongly correlated electrons. Recent years have seen substantial progress in this area with contributions from a diverse set of communities in quantum chemistry and condensed matter physics. This symposium aims to survey the latest developments relevant to strongly correlated electrons across the range of electronic structure methods, including (i) single- and multi-reference configuration interaction, perturbation theory, and coupled cluster methods (ii) Greens function theories (iii) dynamical mean-field theory (iv) density matrix renormalization group (v) quantum Monte Carlo methods, and (vi) density functionals. A major goal of this symposium will be to facilitate cross-talk and cross-fertilization between these different communities and between the chemistry and physics fields.

Garnet Kin-Lic Chan, *Cornell University, gc238@cornell.edu*
Steven White, *University of California, Irvin, srwhite@uci.edu*

25 YEARS OF ZEKE

2009 represents the 25th anniversary of ZEKE (zero electron kinetic energy) spectroscopy. Moreover, it's the year in which the key developer of ZEKE, Klaus Muller-Dethlefs, turns 60. This symposium celebrates both events. It will focus on ZEKE spectroscopy but will also cover related processes in photoionization and photodetachment, including photoelectron imaging, ion-electron coincidence techniques, spectroscopy and dynamics of highly excited Rydberg states, and time-resolved photoelectron spectroscopy.

Dan Neumark, *University of California, Berkeley, dneumark@berkeley.edu*
Masaaki Fujii, *Tokyo Institute of Technology, mfujii@res.titech.ac.jp*

PROTECTED METALLIC CLUSTERS, QUANTUM WELLS AND METAL-NANOCRYSTAL MOLECULES IN FUNDAMENTAL AND APPLIED CHEMISTRY

Rapid recent advances in the molecular modification, selection and protection of metallic clusters, nano-crystals and quantum-well films will be presented and discussed in this symposium. When restricted to a diameter below ~3-nm, the "good metals" (including alloys and inter-metallic compounds) have characteristic capacities (e/C) on the order of hundreds of millivolts, and characteristic electronic excitations in the 0.5-2.0 eV range, both scales being of perennial interest to fundamental and applied chemistry. Nonetheless, the "molecular science of the metallic state" had to await developments in preparative surface and inorganic chemistry, molecular beam spectroscopy, and especially in analytical and theoretical-computational methods. The recent total-structure determinations, and their theoretical-conceptual treatments, are the new benchmarks stimulating expanded chemical interest in the field. This symposium features lectures from pioneering researchers, organized so as to illuminate the issues for chemists of diverse backgrounds.

Robert L. Whetten, *Georgia Institute of Technology, whetten@chemistry.gatech.edu*
Ignacio Garzón, *Universidad Nacional Autonoma de Mexico, garzon@fisica.unam.mx*
Theodore Goodson, *University of Michigan, tgoodson@umich.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 19, 2009. See announcement below for information about the Physical Chemistry Student Poster Awards.

Martin Head-Gordon, *UC, Berkeley, mhg@cchem.berkeley.edu*

THE PHYSICAL CHEMISTRY OF PHOTON TO FUEL CONVERSION

This symposium will explore mechanistic and theoretical studies that will form the basis for rationally designing efficient photon to fuel conversion systems. Topic areas will include:

A. Fuel forming steps:
- Spectroscopic and theoretical studies for elucidating mechanisms of complex, coupled reactions for H_2O oxidation, H^+ reduction and CO_2 reduction.
- Theory and spectroscopy of excited state bond making and bond breaking processes (emphasis on inorganic and organometallic catalysts)
- Spectroscopic and theoretical studies of chemical reactions at interfaces and on surfaces relevant to fuel formation

B. Assembly of integrated systems:
- Dynamic multi-D spectroscopy, X-ray diffraction, scattering and theory/modeling of the directional transport of ions, redox equivalents, and molecules across soft or hard phase boundaries; separation of final product molecules
- Hierarchical organization of molecular components through self assembly: Multi-scale theories, physico-chemical tools for monitoring assembly process in real time with atomic precision

C. Light capturing mechanisms: Harvesting and delivering photons in a molecular energy conversion machine

Heinz Frei, *Lawrence Berkeley National Laboratory, hmfrei@lbl.gov*
David Chandler, *University of California, Berkeley, chandler@cchem.berkeley.edu*
Elaine Chandler, *Lawrence Berkeley National Laboratory, EAChandler@lbl.gov*

GRAPHITIC MATERIALS

Graphitic materials are structures based on graphene, a single layer of carbon atoms arranged in a hexagonal honeycomb lattice. Graphitic materials span a wide range of dimensionality starting from 0D fullerenes, to 1D carbon nanotubes (CNTs) and graphene nanoribbons (GNRs), 2D single-layered (or few layered) graphene, up to 3D graphite, their derivatives, and intercalated compounds. Graphitic materials are interesting both from a basic research viewpoint and for its important technological applications in energy, health, and environmental issues. As examples of fundamental research opportunities, fullerenes serve as an ideal model system for the study of quantum confinement effects, CNTs allow for the study of the characteristics of Luttinger liquid behavior, and GNRs serve as a condensed matter platform for the study of quantum electrodynamics effects. The chemistry of graphitic materials is very rich but poorly understood. Besides the traditional application of graphite as pencil "lead", diverse technological applications of graphitic materials have been suggested and developed within the past decade. These and numerous further applications are being explored at different development stages all the way from the laboratory up to full scale commercial production. This symposium will bring together experimentalists and theoreticians with diverse backgrounds (Chemistry, Physics, Materials Science and Chemical Engineering) to explore the various facets of this field.

Gustavo Scuseria, *Rice University, guscus@rice.edu*
Yael Hanein, *Tel-Aviv University hanein@eng.tau.ac.il*

FLUORESCENCE MICROSCOPY BEYOND THE DIFFRACTION LIMIT

Recent technical advances in fluorescence microscopy enable imaging of labeled proteins with spatial resolution far better than the 200-nm resolution of diffraction-limited imaging by visible light. These sub-diffraction-limit methods involve "structured illumination" of the sample or successive imaging of photoactivatable labels one molecule at a time. For example, in favorable cases multiple copies of the same genetically labeled protein in a fixed cell can be located with 2-5 nm accuracy, providing qualitatively new information about the architecture of multi-protein machinery at a length scale approaching the size of the constituent proteins themselves. This symposium will explore the new sub-diffraction methods and their biological applications and compare capabilities with electron tomography and other ultra-high resolution electron microscopy techniques.

James Weisshaar, *University of Wisconsin, weisshaar@chem.wisc.edu*
Jan Liphardt, *University of California, Berkeley, Liphardt@berkeley.edu*

CHEMICAL REACTION DYNAMICS IN GASEOUS AND CONDENSED PHASES

The study of chemical reaction dynamics stands at the forefront of modern physical chemistry with applications in biophysics, atmospheric chemistry, combustion, energy transfer, and interstellar chemistry. Tremendous progress has been marked by the convergence of theory and experiment at an unprecedented level of detail. This symposium will highlight recent advances in the study of reaction dynamics in both gaseous and condensed phases. Topics to be covered include dynamics on multiple electronic states, novel experimental probes of dynamics, and recent theoretical developments.

Simon W. North, *Texas A&M University, swnorth@tamu.edu*
David A. Blank, *University of Minnesota, blank@umn.edu*

SPECIAL SYMPOSIUM FOR POSTDOCTORAL PRESENTERS

Contributions from all areas of physical chemistry are highly encouraged for this symposium. The presenter must be a post doctoral researcher at the time of the presentation and must apply to present in this session by Friday March 6, 2009. Details on the application process can be found on the PHYS website (http://hackberry.chem.trinity.edu/PHYS/postDocAward.html).

Martin Head-Gordon, *UC, Berkeley, mhg@cchem.berkeley.edu*

On-Line Abstract Submission Deadline:
March 16, 2009
http://oasys.acs.org/oasys.htm

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

At the meeting in Washington, DC, 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