Division of Chemical Physics

The American Physical Society

A Message from the Chair

The Division of Chemical Physics (DCP) of the American Physical Society is an organization representing a broad range of research interests and activities historically across the boundaries of physics and chemistry, and today extending to fields in biology, materials science, environmental and earth science, and many other disciplines. At present, DCP's functions include the organization of chemical physics programs in the annual March meeting, administering the Dependant Care Award and Graduate Student Travel Award programs for encouraging participation in the March meeting by members with child-care issues and students, and managing the process awarding APS Fellowships and the APS Prizes through the Division (Broida, Langmuir, Plyler). All these functions are aimed at promoting interactions among chemical physicists and with physicists in other fields, and continuing the development of chemical physics as a discipline of research and scientific enterprise.

The next annual March meeting will be held in Denver from March 5 through 9, 2007. Dan Neumark has assembled a dynamic program covering a wide range of timely subjects. It will be a week of interesting and stimulating science and I urge members to attend. Although the regular abstract submission deadline has passed, receipt of post-deadline abstracts is still open till Dec. 29 and early registration ends on Jan. 5.

It is important to recognize that DCP symposia in the March meeting offer great opportunities for oral contributed talks. A typical session in a symposium consists of no more than 2 invited talks (36 minutes each) and 9 contributed talks (12 minutes each). The many oral presentations provide an excellent venue not only for graduate students, postdoctorals and beginning researchers to present their research results, but also opportunities for established researchers to engage with their colleagues. Because of the many oral contributed presentations, the symposia are often well attended.

DCP is presently facing several challenges that will need the input and assistance from members. Foremost among them is to increase the size of the membership which stands at about 2,200. The size of the membership dictates the amount of resources DCP will have to support its activities, including the size of the DCP program in the annual meetings and the number of fellows it can elect. We urge you to encourage your students – student membership is free the first year – and your colleagues to sign up for APS membership. Members enjoy a variety of benefits including networking opportunities, low premium life insurance, and reduced meeting fees. Also, if you know someone who is an APS member with interests in chemical physics but belongs to another division, please encourage them to sign up for DCP when they renew their annual membership.

DCP greatly appreciates the input from its members on the topics that are addressed in the annual meeting. While the Executive Committee does its best to name challenging and interesting symposium topics, some of the best ones are suggested by the membership. Please forward your ideas for focused topics for the 2007 March meeting to any of the officers of the Division. Better yet, please join us in the Division meeting in Denver to voice your ideas.

It gives me great pleasure to announce that Dan Neumark will assume the Chair position and Wil Castleman the Chair-Elect of DCP after the March meeting. They will be continually assisted by the excellent effort of Council Member Charlie Parmenter, and the Division Executive Committee. I am also grateful to past chairs Mark Ratner and Emily Carter for their efforts in affording a vibrant DCP.

Wish you a happy and successful 2007 and see you in Denver,

Hai-Lung Dai

• **Post-deadline abstracts:** December 29, 2006

• Early registration for March meeting: January 5, 2007

• **APS Fellowship nominations for DCP:** February 9, 2007

March APS Meeting, Denver, CO, March 5-9, 2007

The March APS 2007 meeting will be held March 5-9 in Denver, CO. Information about the meeting is available on the APS web site at http://www.aps.org/meet/MAR07/index.cfm. The deadline for early registration at the reduced fee is January 5, 2007.

The annual DCP business meeting is also part of the March meeting and will include short reports of DCP activities, presentation of Certificates of Fellowship to new APS Fellows from the DCP, and introduction of student travel fellowship awards. All members are invited to attend. The date of the general business meeting will be published in the January newsletter.

The DCP Special Focus Topics for the March 2007 meeting include the following.

11.8.1. Electron and Ion Solvation in Clusters and the Condensed Phase

Organizer: Peter J. Rossky

Description: The symposium will bring together a critical mass of leading individuals who share as a common focus the understanding of solvation effects on electronic processes in solvated ionic species. The symposium will feature many of the foremost theoretical and experimental research efforts currently being pursued. By this means, one goal of the symposium is to develop a deeper understanding of the connections among such processes taking place in cluster and condensed phase environments.

11.8.2. New Frontiers in Imaging

Organizers: Thomas Meersman and Warren Warren

Description: This symposium will focus on new fundamental advances in imaging technology for a broad range of diagnostic applications ranging from material sciences and engineering to in vivo medical research. Chemical physics will be the common denominator for this symposium that intends to foster synergy between various areas of expertise in imaging technology. Some emphasis will be on magnetic resonance imaging (MRI) and to a somewhat lesser extent on optical imaging. The presentations will cover novel combinations of existing technology, fundamental physical and technological developments in imaging technology and new areas of applications.

11.8.3. Nonadiabatic Molecular Dynamics and Control at Conical Intersections

Organizers: Todd J. Martínez and Albert Stolow

Description: The nonadiabatic coupling of electronic and nuclear motion in molecules is a general and fundamental aspect of their dynamics, underlying both photochemistry and photobiology. Conical intersections (true degeneracies of two or more electronic eigenstates) play a key role in electronic transitions and the breakdown of the Born-Oppenheimer adiabatic approximation. A detailed understanding of these processes will lead to the development of simple rules governing dynamics at conical intersections, and new strategies for controlling charge flow and reactivity in molecules. There are many opportunities to exploit our understanding of conical intersections in order to control molecular dynamics with laser fields. Conversely, the form of these fields might be used to better understand the details of dynamics around

conical intersections. This focus session brings together researchers in the fields of nonadiabatic dynamics, conical intersections, and control in order to foster further cross-fertilization between these fields.

11.8.4. Charge Transport through Nanostructures

Organizers: Hongkun Park and Barry Dunietz

Charge transport plays a crucial role in determining many of the functional properties of nanometer-sized structures. Therefore, although the task of engineering nano-scale devices is highly challenging, their prospect has drawn considerable attention from the scientific and engineering communities. This symposium will provide a forum to discuss this important research subject and to share recent related developments, in both theory and experiment. Topics of the symposium will include charge and spin transport through molecules, carbon nanotubes, nanowires, polymers, and other nanometer-sized structures.

11.8.5. Protein folding theory and simulations

Organizer: William Eaton

Understanding how proteins fold from the myriad conformations of the denatured state to the unique, biologically-functioning conformation of the native state is one of the great challenges to biophysical science. The introduction of new physical techniques, the application of modern statistical mechanics, and advances in computer simulations have all contributed greatly to this problem. This symposium focuses on the theory and simulation of protein folding, which have played a major role in both interpreting and synthesizing experimental results and in providing new directions for experimental research.

11.8.6. Ultrafast dynamics with X-rays and electrons

Organizers: Christoph Rose-Petruck and R. Dwayne Miller

The symposium brings together colleagues who are using electron or x-ray pulses to measure the structural dynamics of molecules or crystals as well as the electronic structure of molecules during chemical and physical processes. The purpose of the symposium is to provide a forum for presentations and discussions of recent results and to describe promising future methods and applications. Experimental and theoretical research based on accelerator as well as laboratory radiation sources is covered. The symposium additionally includes novel methods some of which might, for instance, rely on optical pulses for the generation of the structure-probing electrons inside of the studied molecules.

11.8.7. Frontiers of electronic structure theory

Organizer: Martin Head-Gordon

The principal aim of this focus session is to explore topics at the forefront of electronic structure theory, with particular emphasis on novel developments, including those where chemists and physicists often do not interact. New ideas in density functional theory, wavefunction-based methods, reduced density matrices and other distribution functions will be covered. Complementing these developments will be new algorithms for large-scale applications and selected applications to problems ranging from the molecular to the nanoscale to the solid state.

Congratulations to APS Prize Winner

The Division of Chemical Physics extends its congratulations to the 2007 awardee of the APS Earl K. Plyler Prize. The Plyler Prize is administered by the DCP and funded by generous contributions from the George E. Crouch Foundation and Spectra-Physics (http://www.spectra-physics.com/).

Timothy S. Zwier, Purdue University, was awarded the Earl K. Plyler Prize for the design and implementation of multiple resonance methods that elucidate the potential energy landscapes of flexible biomimetic molecules and their hydrates by optical control of isomer populations.

More information about winners of APS prizes and awards in 2006 is available on the web at http://www.aps.org/praw/06winners.cfm

Congratulations to 2005 APS Fellows

The Division of Chemical Physics extends its congratulations to the following individuals who were nominated by the Division of Chemical Physics and elected to Fellowship in the American Physical Society. Only 1/2 of 1% of the total APS membership is selected for Fellowship in the Society each year.

Louis John Allamandola, NASA Ames Research Center

For his seminal contributions in astrochemistry that have forever revolutionized our understanding of interstellar molecules, interstellar ices, and the chemical physics of the interstellar medium.

Bernard T. Delley, Paul Scherrer Institute, Switzerland

For his pioneering contributions to density functional methodology and helping to establish density functional theory as a major tool for academic and industrial chemistry.

Sabre Kais, Purdue University

For the development of a finite size scaling approach to calculate quantum critical parameters for atomic, molecular and quantum dot systems.

Shashi P. Karna, US Army Research Laboratory

For contributions to the theory and understanding of the mechanism of nonlinear optical phenomena in molecules and nanoscale atomic nanoclusters.

Stephen Jacob Klippenstein, Argonne National Laboratory

For fundamental contributions to the development and application of quantative theoretical methods for predicting the kinetics of chemical reactions in the gas phase.

Richard Martel, Universite de Montreal, Canada

For seminal advances in understanding and exploiting the electrical and optical properties of individual carbon nanotubes.

Andrew Marshall Rappe, University of Pennsylvania

For contributions to electronic structure methodology, understanding mechanisms of chemisorption bonding and energy exchange with surfaces, and for relating chemical identity to material response in ferroelectric oxides.

Michael Springborg, University of Saarland, Germany

For his seminal contributions to the development of density-functional methods exploiting helical symmetry of one-dimensional systems and their application to the polymers and chain compounds.

Arthur G. Suits, Wayne State University

For pioneering work in the application of state-resolved and "universal" ion imaging techniques to a broad range of problems in chemical physics and reaction dynamics.

Xueming Yang, Chinese Academy of Sciences

For his contributions to the study of reaction dynamics of elementary chemical reactions using the state-of-the-art crossed molecular beam methods.

Fellowship Committee and Nominations

Nominations for APS Fellowship to be considered by the DCP Fellowship Committee should be made before February 9, 2007. Thanks go to this year's committee, Jim Lisy (chair), Marsha Lester, and Al Wagner. Instructions for submitting a nomination for consideration next year are included on the APS web site (http://www.aps.org/fellowship/fellinfo.html).

DCP Membership

Membership in the American Physical Society's Division of Chemical Physics allows you to directly support a primary forum for chemical physics research. The status and influence of the DCP within the APS is dependent on the number of DCP members. Increasing DCP membership is crucial to preserving this important professional asset. If you are not a DCP member, we encourage you to join on the web (http://www.aps.org/memb/unitapp.html) or by phone (301-209-3280).