

A Message from the Chair, John C. Tully

The interdisciplinary field of chemical physics is a fertile source of new concepts and discoveries. Nanoparticles, molecular electronics, femtosecond spectroscopy, quantum control, and single-molecule imaging are but a few of the exciting frontiers of chemical physics that are impacting both science and the public at large. The APS Division of Chemical Physics (DCP) provides a forum for researchers to present ideas, compare approaches and otherwise join forces to enhance progress. The mission of the officers of DCP is to make this forum as useful as possible to the widest possible audience of chemical physicists. We welcome input from all members of the Division.

The major event of the DCP each year is the APS March Meeting. This year's meeting in Seattle was well attended, featuring a number of standing-room-only sessions. (Most sessions required the presence of a fire marshal at the door to limit attendance). I wish to thank the organizers of the sessions, Ara Apkarian, Dan Auerbach, Eric Bittner, Steve Buratto, Gustavo Scuseria and Bob Wyatt. Next year the March Meeting will be held in Indianapolis from March 17-22. Laurie Butler is the Program Chair for the DCP sessions. She has put together an exciting program, as described below in this Newsletter.

I wish to thank the following retiring officers for their outstanding contributions to the DCP: Charles Harris (past Chair) and Thom Dunning (past Secretary-Treasurer). I also welcome their replacements, Roger Miller (Vice-Chair) and Bruce Garrett (Secretary-Treasurer), and Peter Rossky (Member-at-Large). Finally, I thank the APS staff for their continuing support and assistance.

March APS Meeting, Indianapolis, Indiana, March 18-22, 2002

This Division of Chemical Physics Program at the March meeting will consist of eight (8) sessions. Laurie Butler (DCP Program Chair) organized a program that encompasses a broad range of topics in chemical physics. Invited and contributed papers will be combined in these sessions. Information on the March 2001 meeting is available at (<http://www.aps.org/meet/MAR02/>). Instructions for submitting abstracts can be found at <http://www.aps.org/meet/meet-abstract.html> (includes instructions for online submission of abstracts). The deadline for abstracts is December 7, 5 PM EST.

The annual DCP business meeting is also part of the March meeting. The business meeting is tentatively scheduled for Tuesday, March 19, 2002 after the afternoon sessions and is open to all DCP members. The business meeting will include short reports of DCP activities, presentation of Certificates of Fellowship to new APS Fellows who are DCP members, and introduction of student travel fellowship awards.

Important Deadlines

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| • Graduate Student Travel Award applications: | December 1, 2001 |
| • Abstracts for contributions to the March meeting: | December 7, 2001 |
| • Ballots for new DCP officers: | December 14, 2001 |
| • APS Fellowship Nominations: | February 15, 2001 |

The DCP Special Focus Topics for the March 2002 meeting include the following.

11.9.1. Protein Dynamics (joint with DBP)

Organizer: Norbert Scherer, Department of Chemistry and Institute for Biophysical Dynamics, The University of Chicago, 5735 South Ellis Avenue, Chicago, IL 60537, Telephone: (773) 702-7069, FAX: (773) 702-0805, E-mail: nfschere@uchicago.edu; Joan-Emma Shea, Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106, Telephone: (805) 893-5604, FAX: (805) 893 4120, E-mail: shea@chem.ucsb.edu

A full understanding of protein function and molecular recognition requires a description of the system or complex that extends beyond the static three-dimensional picture provided by "traditional" structure determination approaches. This Symposium concentrates on experimental, theoretical and computational studies and approaches that are at the forefront of probing and analyzing the dynamic behavior of proteins and protein-ligand complexes. The individual sessions are organized around the following broad topics: Quantum dynamics and electron transfer processes; Long time dynamics; Time-resolved folding; Protein-Ligand dynamics including single molecule behavior; Ion Channel dynamics. Papers are solicited in all areas related to protein dynamics.

11.9.2. The Physical and Electronic Structure of Conjugated Polymers: From Photophysics to Devices

Organizer: Benjamin J. Schwartz, Department of Chemistry and Biochemistry, 2077A Young Hall, University of California, Los Angeles, Los Angeles, CA 90095-1569, Telephone: (310) 206-4113, FAX: (310) 206-4038, E-mail: schwartz@chem.ucla.edu

Conjugated polymers are remarkable materials that combine the electrical properties of semiconductors with the mechanical properties and processing advantages of plastics. As a result, these materials show great promise for use in a variety of optoelectronic applications, including LEDs, displays and photovoltaic devices. This focused session will provide a broad overview on the current state-of-the-art for what is known concerning the critical relationship between the physical properties of conjugated polymers (e.g. chain conformation and orientation) and the electronic properties of conjugated polymers (e.g. presence of interchain electronic species, behavior in optoelectronic devices). Experimental and theoretical papers are solicited on a wide variety of phenomena, including but not limited to: processing effects on conjugated polymer solutions or films, spectroscopy of conjugated polymer solutions or films, the nature of conjugated polymer interchain species, carrier recombination and transport properties in conjugated polymers, the relationship between film morphology and device performance, properties of conjugated polymer/metal interfaces, studies of single conjugated polymer molecules. Authors are encouraged to stress the relationship between their work and the applications of these materials in practical devices. Contributions based on all experimental, theoretical and computational methodologies are welcome.

11.9.3. Chemical and Physical Properties of Supported and Isolated Metal Nanoclusters

Organizer: Scott L. Anderson, Department of Chemistry, University of Utah, 315 S. 1400 E. Room 1216, Salt Lake City, UT 84112, Telephone: (801) 585-7289, FAX: (801) 581-8433, Email: anderson@chem.utah.edu

Supported metal nanoclusters are important in many catalysts and in other materials applications. It is known that the chemical and materials properties of supported clusters depend strongly on parameters such as cluster size, morphology, and oxidation state, and also on support properties such as defect structure and redox behavior, however, the origin of the effects is not understood. Recently, there have been major advances in the study of supported clusters using both

deposition of size-selected clusters and controlled nucleation of clusters on supports. Simultaneously, new spectroscopic, diffraction, and imaging methods have been developed that allow detailed study of isolated clusters. This focus session will provide a forum for discussion and comparison of different approaches to probing the relationships between the physical, chemical, and materials properties of metal nanoclusters. Experimental and theoretical papers are solicited in any related area, including, but not limited to:

- Deposition of energy and/or mass-selected clusters
- Growth, mobility, properties of cluster on surfaces
- Physical and chemical properties of isolated metal clusters
- Nanocluster-based catalysts or materials
- Theory on clusters or cluster-support interactions

11.9.4. Vibronic Chemistry in Isolated Molecules, at Surfaces, and in Solution

Organizers: Martin Gruebele, Departments of Chemistry and Biophysics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, Telephone: (217) 333-1624, FAX: (217) 244-3186, E-mail: mgruebel@uiuc.edu; Alec M. Wodtke, Department of Chemistry and Biochemistry, University of California, Santa Barbara, Santa Barbara, CA 93106, Telephone: (805) 893-8085, E-mail: wodtke@chem.ucsb.edu

The breaking and making of chemical bonds involves the intricate and coordinated motion of electrons and nuclei. How vibrational motion of reactants and products relates to electronic reorganization is a forefront topic of modern chemical research, spanning topics of importance to isolated molecules in the gas-phase and to the complex environments of condensed phase. Surfaces, especially molecules at metals and semiconductors, are another important venue for chemistry where electronic interactions are critically important. This symposium seeks to provide avenues for exchange between scientists working in all of these diverse areas.

11.9.5. Nonlinear Spectroscopy and Molecular Choreography (DCP)

Organizer: David M. Jonas, Department of Chemistry and Biochemistry, University of Colorado at Boulder, 215 UCB, Boulder, CO 80309-0215, Telephone: (303) 492-3818, FAX: (303) 492-5894, E-mail: jonas@colorado.edu

The term molecular choreography is borrowed from spin choreography in NMR and emphasizes the control we exert over the molecular dance we see in a nonlinear spectroscopic experiment. These sessions about making and watching molecules dance cover both experimental and theoretical aspects of nonlinear molecular spectroscopy, coherent molecular control, and the molecular dances in the elementary steps of chemical reactions.

11.9.6. New Techniques, Applications and Instruments in X-Ray Absorption Spectroscopy (joint with GIMS)

Organizers: Ting Guo, Chemistry Department, University of California, One Shields Ave., Davis, CA 95616, Telephone: (530) 754-5283, FAX: (530) 752-8995, E-mail: tguo@ucdavis.edu; Robert Schoenlein, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, Telephone: (510) 486-6557, FAX: (510) 486-5530, E-mail: rwschoenlein@lbl.gov; John Rehr, Department of Physics, University of Washington, Seattle, WA 98195-1560, Telephone: (206) 543-8593, FAX: (206) 685-0635, E-mail: jjr@phys.washington.edu

X-ray absorption spectroscopy (XAS) has been instrumental to the advancement of many fields, including biology, chemistry, physics, and materials science. Recent developments in XAS have enabled researchers in these fields to investigate phenomena that would otherwise be impossible to study. This call-for-abstracts solicits reports in all areas

related to new developments in both experimental and theoretical aspects of x-ray absorption spectroscopy. Results on x-ray absorption near edge spectroscopy or extended x-ray absorption fine structure investigations of nanoparticles, improved multiple scattering theories, new ultrafast x-ray sources and time-resolved absorption techniques and applications, and the high spatial resolution x-ray microscopy are particularly encouraged. This symposium draws attention to the combined strength of new technologies and new theories, and is sponsored by both the Division of Chemical Physics (DCP) and the Instrumentation and Measurement Science Topical Group (GIMS).

11.9.7. Progress in Heterogeneous Catalysis, Fuel Cells, and Chemical Sensors (joint with FIAP)

Organizers: Alexander Bogicevic, Scientific Research Laboratories, Ford Motor Company, P.O. Box 2053, MD 3083 SRL, Dearborn, MI 48121-2053, Telephone: (313) 845-8625, FAX: (313) 594-2923, E-mail: abogicev@ford.com; Jennifer J. Zinck, HRL Laboratories, 3011 Malibu Canyon Road, Malibu, CA 90265, Telephone: (310) 317-5913, FAX: (310) 317-5483, E-mail zinck@hrl.com; D. Wayne Goodman, Department of Chemistry, Texas A&M University, College Station, TX 77840-3012, Telephone: (409) 845-0214, FAX: (409) 845-6822, E-mail: goodman@mail.chem.tamu.edu

While the areas of catalyst, fuel cell (both PEM and SOFC), and gas sensor development are perhaps not normally grouped together, they actually have several key issues in common. All three areas rely on complex catalytic reactions on one or two separate electrodes, atomic and molecular transport on surfaces and in the bulk, and are all faced with issues of thermal and chemical stability under harsh oxidizing/reducing environments and large temperature variations. This focus session will provide an overview of the current state of the art in these fields, and a forum for comparisons of different approaches to common problem formulations. Experimental and theoretical papers are solicited on a wide variety of phenomena, including (but not limited to) the following areas:

- Structural (e.g., microstructure, mechanical properties, durability)
- Chemical (e.g., surface chemistry, micro- and macrokinetics, triple-point boundaries)
- Transport (e.g., bulk and surface diffusion, ionic transport, dopant interactions)
- Electronic (e.g., band-gap engineering, optical properties, nanostructures)
- Methodology (e.g. combinatorics, computation, nanotechnology)

Authors are encouraged to stress the relevance of their work to technological and industrial problems. Materials of interest include metals, semiconductors, and ceramics, either in bulk or at surfaces or interfaces. Contributions based on all experimental, theoretical, and computational methodologies are welcome.

11.9.8. Physics of Chemically Modified Interfaces (joint with DCMP and DMP)

Organizer: Eric Borguet, Department of Chemistry & Surface Science Center, University of Pittsburgh, 219 Parkman Avenue, Pittsburgh PA 15260, Telephone: (412) 624-8304, FAX: (412) 624-8611, E-mail: borguet@pitt.edu

Chemical modification of interfaces is a means to many ends including molecular electronics, ultrathin gate dielectrics, and tribology. Recently, there has been considerable effort to use the methods of synthetic chemistry to modify the properties of interfaces, leading to the creation of new systems and the observation of novel physical phenomena. Our goal is to foster interactions and exchange between members of this diverse community, as well as between theorists and experimentalists. Experimental and theoretical papers in all areas related to physics of chemically modified interfaces are solicited, including (but not limited to) the following areas:

- Novel probes of chemically modified interfaces
- Dynamics of charges at chemically modified interfaces
- Electron transmission through chemically modified interfaces

- Devices based on chemically modified interfaces
- Nanostructured chemically modified interfaces
- Chemically modified nanoparticle interfaces
- Biological surfaces

Graduate Student Travel Awards

DCP sponsors travel awards for graduate students who present a paper or a poster at the March or April meetings. Eligible expenses include reduced rate airfare or car travel, registration, economy room and board for the duration of the meeting. Awards can range from \$250 to \$400. As many as twelve awards will be made. Criteria:

1. The work must be of significance suitable for a National APS meeting. The work would be presented as a poster at a DCP poster session or in a DCP sponsored oral session.
2. The applicant cannot have previously received a DCP-GSTA award.
3. The student must be a member of DCP. Students who are not currently members can still apply, but they must join both APS and DCP before their check will be issued.

Application:

1. The graduate student should submit an abstract directly to APS (see meeting information above) as well as a copy to the DCP-GSTA committee chair listed below. In addition, the graduate student should send a list of estimated expenses to the DCP-GSTA committee chair.
2. The faculty advisor of the student must write a nomination letter specifying the student's role in the research and explaining the significance of the work. Normally, only one applicant from any research group will be selected.

The application deadline is December 1. This is a rigid deadline for when applications must be received. Decisions will be made quite quickly so that any unsuccessful applicants may, if they wish, withdraw their abstract before it is published in the APS bulletin. The amount of individual awards will be based on total available funds and estimated expenses. Send applications to Bruce Garrett.

Applications may be sent by:

E-mail: bruce.garrett@pnl.gov

FAX: 509-376-0420

Postal: Pacific Northwest National Laboratory, P.O. Box 999, Mail Stop K8-91, Richland, WA 99352

If you know a student who would benefit from this opportunity, please bring this to her or his attention.

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).

New DCP Web Site

The DCP web site has been overhauled. You can see the new web site at <http://www.aps.org/units/dcp>. Thanks go to Tara Hoyem and Amanda Kissire at Pacific Northwest National Laboratory for their help it designing and laying out the web pages. We are soliciting graphics and images for the home page and plan to rotate them periodically. If you have an image or artwork you would like to see featured, please send a jpeg file and caption to Bruce Garrett (bruce.garrett@pnl.gov).

Fellowship Committee and Nominations

Nominations for APS Fellowship to be considered by the DCP Fellowship Committee should be made before February 15, 2002. Thanks go to Mark Ediger for chairing the committee this year, and to Joel Bowman and Mary Mandich for their service on the committee. Instructions for submitting a nomination are included on the APS web site (<http://www.aps.org/fellowship/fellinfo.html>).

Election of New DCP Officers

John Tully will retire as DCP Chair and Roseanne Sension will be leaving her position as a Member-at-Large of the Executive Committee in March. Our current Chair-Elect, Laurie Butler, will then become Chair, and Roger Miller will advance from Vice-Chair to Chair-Elect. The main duties of the Chair are to provide general leadership for the Division, to make sure that the various Division committees are staffed, and to preside at the business meetings of the Division. The most time-consuming job of the Chair-Elect is to organize the DCP symposia for the upcoming National meeting. The duties of the Member-at-Large are less well defined, other than to attend the March meeting. In the past they have organized the student fellowship program, assisted in membership recruiting, and helped with the organization of National meetings. All members of the Executive Committee, which includes the DCP Officers as well as the Members-at-Large, meet at the March APS meeting to help plan DCP activities for the coming year. At this time we must elect a new Vice-Chair and one Member-at-Large.

This year the election will be conducted electronically. DCP members with email addresses on file will be emailed a ballot. Paper ballots and candidate information will be mailed to those members who cannot be reached by email. The deadline for returning ballots (electronically and by mail) is December 14, 2001.

The Nominating Committee, consisting of Paul Barbara (chair), James Skinner, and Bruce Kay, has convinced the following individuals to stand as candidates.

Candidates for Vice-Chair

EMILY A. CARTER. Professor, Department of Chemistry and Biochemistry, University of California, Los Angeles. B.S., University of California, Berkeley, 1982. Ph.D., California Institute of Technology, 1987. APS Fellow, 1998.

RESEARCH INTERESTS: General - quantum chemistry, theoretical solid state physics, materials science, surface science, and mechanical engineering models of materials failure. Specific - ab initio energetics, kinetics and dynamics of gas-surface reactions and interface formation for metals and metal oxides, including design of protective ceramic coatings for metals; ab initio structure, dynamics and reactions of gaseous species; development of new electron correlation,

density functional, condensed matter quantum embedding, and ab initio molecular dynamics methods, and simulation tools to bridge atomistic-mesoscopic length scales to couple chemistry with engineering models.

Web site: <http://www.chem.ucla.edu/carter/>

SHAUL MUKAMEL. C.E Kenneth Mees Professor, Department of Chemistry, University of Rochester. B.Sc., Tel Aviv University, 1969. M.Sc., Tel Aviv University, 1971. Ph.D., Tel Aviv University, 1976. APS Fellow, 1987.

RESEARCH INTERESTS: Theoretical studies of ultrafast nonlinear optical spectroscopy in condensed phases; multidimensional coherent spectroscopy of biomolecules and liquids; electronic excitations of molecular aggregates, dendrimers and semiconductor nanostructures; single molecule spectroscopy.

Web site: <http://mukamel.chem.rochester.edu/>

Candidates for Member-at-Large of the Executive Committee

MARK MARONCELLI. Professor, Department of Chemistry, Pennsylvania State University. B.A., Williams College, 1979. Ph.D., University of California, Berkeley, 1983.

RESEARCH INTERESTS: Structure and dynamics of liquids and solutions, solvation and solvent effects on chemical reactions, supercritical fluids, ultrafast spectroscopy, and computer simulation.

Web site: <http://maroncelli.chem.psu.edu/>

TIMOTHY S. ZWIER. Professor, Department of Chemistry, Purdue University. B. S., Calvin College, 1977. Ph.D., University of Colorado, Boulder, 1981. APS Fellow, 2000.

RESEARCH INTERESTS: laser spectroscopy and dynamics of isolated molecules and molecular cluster; hydrogen bonding; mode-specific processes; photochemistry.

Web site: <http://www.chem.purdue.edu/zwier/>

Meetings of Possible Interest to DCP Members

American Conference on Theoretical Chemistry (ACTC-2002)

July 14-18, 2002

Seven Springs Resort, Pennsylvania

Organizer: Kenneth D. Jordan, Department of Chemistry, University of Pittsburgh

Email: actc@imap.pitt.edu

Web site: <http://pro3.chem.pitt.edu/actc2002/>

Gordon Research Conference on Molecular and Ionic Clusters

January 6-11, 2002

Ventura, CA

Organizer: James Lisy

E-mail: J-LISY@UIUC.EDU

Web site: <http://www.grc.uri.edu/programs/2002/molionic.htm>

If you would like to have information about any future meetings included in a future DCP Newsletter and/or on the DCP web site, send the information to Bruce Garrett (bruce.garrett@pnl.gov).