DCP News

November 2004

Division of Chemical Physics

The American Physical Society

A Message from the Chair, Emily A. Carter

The Division of Chemical Physics (DCP) represents a unique niche in the APS, one that bridges across other divisions of the APS in ways that other divisions often do not. While one may argue our central focus is molecules, we also cross into DAMOP (atomic and molecular physics), DCMP (condensed matter physics), DMP (materials physics), and DBP (biological physics), just to name a few. As a result, we are deeply relevant to the March Meeting of the APS, which has historically been mainly the venue of the DCMP. I strongly encourage you to participate in the 2005 March Meeting and to send your students and postdocs, which will help the DCP to continue to grow and thrive. Mark Ratner and his focus session organizers have put together compelling symposia in some traditional, some controversial, and some truly cross-cutting areas of chemical physics, as described below. I expect our DCP program this year will be very stimulating and will attract people from many other divisions. The March meeting emphasizes contributed talks, offering an excellent opportunity for younger scientists to gain much needed experience and exposure. I urge you to contribute a talk yourself as well as to give your students and postdocs the opportunity to share their work. This year's meeting is in Los Angeles, California. I can personally attest to what LA has to offer: beautiful scenery, excellent cuisine, and diverse culture (and the weather isn't too bad either!). Don't miss this chance to experience Southern California. Let me also call your attention to graduate student travel awards to help defray the costs of attending the conference (see below for details). Lastly, I want to personally thank all of my March 2004 APS DCP focus session organizers who made the DCP symposia in Montreal so successful and DCP committee members who gave so generously of their time this past year to keep DCP going strong. I'd particularly like to thank Sylvia Ceyer for so ably representing DCP as Councilor for the last four years. I'd like particularly to thank Sylvia Ceyer for so ably representing DCP as Councilor for the last four years; her term ends on December 31.

March APS Meeting, Los Angeles, March 21-25, 2005

The APS March 2005 meeting will be held March 21-25 in Los Angeles, CA. Information about the meeting is available on the APS web site at http://www.aps.org/meet/MAR05/ and instructions for submitting abstracts can be found at http://www.aps.org/meet/MAR05/abs.cfm. The deadline for abstracts is December 1, 2004 at 5 PM EST and the deadline for early registration at the reduced fee is January 14, 2005.

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.

• **Graduate Student Travel Award applications:**	November 26, 2004
• **Abstracts for contributions to the March meeting:**	December 1, 2004
• **On-line ballots for new DCP officers:**	December 17, 2004
• **Early registration for March meeting:**	January 14, 2005
• **APS Fellowship nominations for DCP:**	February 11, 2005

The DCP Special Focus Topics for the March 2005 meeting include the following.

11.8.1. Biophysical Dynamics

Organizers: David Reichman & Andrei Tokmakoff

This symposium aims to bring together experimentalists and theoreticians concerned with investigations of the dynamics and non-equilibrium behavior of biological systems including (but not limited to) proteins, nucleic acids, and ion channels. Topics to be covered include time-dependent fluctuations and conformational changes, dynamics of heterogeneous ensembles, protein RNA folding and hydrophobicity in a biological context. Featured methods include single molecule investigations and force microscopies, transient spectroscopies, and molecular dynamics and Monte Carlo simulation techniques.

11.8.2. Molecular Electronics Science and Technology: Pros, Cons, and Issues

Organizers: Cherie R. Kagan & Edwin A. Chandross

Molecular electronics is the science of electronic devices made from molecular materials, ranging from individual molecules to assemblies of many molecules. It continues to receive much attention both scientifically and technologically as traditional semiconductor devices approach performance limits and fabrication becomes more difficult as they are scaled to nanometer size. Measurements of molecular charge transport are exceptionally challenging because test structures are much larger than individual molecules. Mating molecules to metal or semiconductor surfaces presents practical problems as well as issues in understanding structure and properties of interfaces, and in the theory used to model their very different characteristics.

This symposium will address the physics and chemistry of molecular materials and the practical fabrication and characteristics of devices for electronics, (processors and memory), and sensor applications. We will focus on the scientific understanding of both materials and devices. Topics include: synthesis and self-assembly; structural, microscopic, spectroscopic, electrochemical, and electronic characterization of molecules and their assemblies; the mechanistics of charge transport and storage, switching; the interfacial physics of molecules and semiconductors or metals; and the fabrication and theory of test structures and devices. The possibility and probability of technology derived from these devices will be included.

11.8.3. Energy Landscapes of Clusters, Materials and Biomolecules

Organizers: David M Leitner & Martin Gruebele

The study of energy landscapes provides key insights into a broad range of systems ranging from proteins to metal clusters to glasses. This symposium aims to bring together researchers who use energy landscapes to understand the systems they study. A variety of theoretical, computational and experimental techniques that characterize and probe energy landscapes will be represented, including clusters in beams, statistical mechanics, protein binding and folding, glasses, and magnetic materials. We welcome experimental and theoretical papers in all aspects of the study and application of energy landscapes to biomolecules, liquids and glasses, clusters and materials.

11.8.4. Environmental Interfaces

Organizer: Franz Geiger

It is now well known that surface and interfaces play a key role in chemical and physical processes that are important in the environment. Studying this special role that "Environmental Interfaces" play is an area that is only just emerging, in part because appropriate laboratory and computational techniques have not been available until recently. Researchers in geochemistry and atmospheric chemistry are often not aware of the common challenges that both fields face in terms of understanding how surfaces and interfaces control chemical binding and chemical transport. A similar disconnect exists in studying the impact of environmental surfaces and interfaces on the chemical composition of the aqueous and solid (geochemistry) and the gas phase (atmospheric chemistry). Identifying these overlaps, and beginning a dialog among the two disciplines will have direct implications for improving our understanding of pollutant transport, contaminant remediation, aerosol physics, atmospheric radiative forcing, and fundamental surface and interfaces science. The "Environmental Interfaces" focus session at the 2005 APS March Meeting will bring together leading experts in atmospheric chemistry and geochemistry to exchange new experimental and theoretical findings and to foster communication among current and future leaders in this emerging field.

11.8.5. Nanophotonic materials, nonlinear optics and spectroscopy

Organizers: Michael D. Barnes, Robert M. Dickson, & John T. Fourkas

This focus session will address the creation, understanding, and utilization of nanophotonic and nonlinear optical materials and their emerging applications in nanotechnology and biophysics. This session will combine experiment, theory, and device applications of new optical and electroluminescent nanomaterials, linear and nonlinear optical microscopies, and light-based fabrication methods. Applications involving nanoscale light sources, high resolution optical and nonlinear spectroscopies or microscopies, and their application to characterization of nanoscale dynamics, nanoscale and quantum light emitters, and microfabrication are all strongly encouraged.

Graduate Student Travel Awards

DCP sponsors travel awards for graduate students who present a paper or a poster at the March meeting. 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 November 26. This is a rigid deadline for when applications must be received. Decisions will be made 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 Professor Michael A. Duncan.

Applications may be sent by:
E-mail: maduncan@uga.edu
FAX: 706-542-1234
Postal: Department of Chemistry, University of Georgia, Athens, Georgia 30602-2556

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

Important Changes to Earle K. Plyler Prize

DCP is pleased to announce that beginning in 2005 the Earle K. Plyler Prize will be awarded at the $10,000 level. This is thanks to an increased annual gift from the George E. Crouch Foundation (sponsor of the prize since it inception in 1976) coupled with new annual co-sponsorship by Spectra-Physics. This effort was spearheaded by a DCP fund raising committee composed of Timothy Zwier (chair), Fleming Crim, Michael Fayer, Bob Field, Bill Klemperer, David Pratt, and Roger van Zee. The committee is particularly grateful to Michael Fayer for his successful negotiations with Spectra-Physics. The 2005 recipient will be Robert Tycko (see below).

Congratulations to APS Prize Winners

The Division of Chemical Physics extends its congratulations to awardees of APS prizes administered by the DCP.

Hanna Reisler, University of Southern California, was awarded the Herbert P. Broida Prize for theoretical insights and carefully executed experiments on the detailed dynamics of small molecules. The prize was established in 1979 as a memorial to and in recognition of the accomplishments of Herbert P. Broida, late Professor of Physics at the University of California, Santa Barbara, and it is supported by his friends and colleagues.

David Chandler, University of California, Berkeley, was awarded the Irving Langmuir Prize for the creation of widely used analytical methods and simulation techniques in statistical mechanics, with applications to theories of liquids, chemical kinetics, quantum processes, and reaction paths in complex systems. The prize was established in 1964 by the General Electric Foundation (now the GE Fund & GE R&D) as a memorial to and in recognition of the accomplishments of Irving Langmuir.

Robert Tycko, National Institute of Health, was awarded the Earl K. Plyler Prize for the development of novel techniques in NMR spectroscopy and their application to a wide range of fundamental problems including work on Berry's phase, fullerenes, quantum wells, and amyloid fibrils.

More information about winners of APS prizes and awards in 2005 is available on the web at http://www.aps.org/praw/05winners.cfm.

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).

Fellowship Committee and Nominations

Nominations for APS Fellowship to be considered by the DCP Fellowship Committee should be made before February 11, 2005. Thanks go to Terry Miller for chairing the committee this year, and to David Beratan and Jim Lisy 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

We are fortunate to have an excellent slate of candidates for the positions of Vice-Chair and Member-at-Large of the Executive Committee. These positions are for three-year terms. The Vice-Chair becomes the Chair-Elect in the second year of the term and Chair in the final year. 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. We are indebted to the Nominating Committee, consisting of Mark Johnson, Daniel Neuhauser, and Casey Hynes, for their efforts to enlist the following candidates.

Sylvia Ceyer ends her four-year term as DCP Councilor in December. We appreciate the time and effort that Sylvia devoted to this task. The DCP Executive Committee has nominated two excellent candidates for this position. The Division Councilor serves as liaison between the APS Council and the DCP Executive Committee of the Division and reports on any Council actions that affect the Division.

The election will be conducted using the APS web-based voting system. DCP members will be emailed a voting announcement with a link to the voting system. The deadline for casting your on-line ballot is December 17, 2004.

Candidates for Vice-Chair

DANIEL NEUMARK. Professor of Chemistry, University of California, Berkeley, CA. B.A., M.A. Harvard University, 1977; Ph.D., Physical Chemistry, University of California, Berkeley, 1984; Postdoctoral Fellow, JILA, University of Colorado, 1984-86; Fellow, American Physical Society, 1993; Fellow, American Association for the Advancement of Science, 1994; Fellow of the American Academy of Arts and Sciences, 2000; American Chemical Society Nobel Laureate Signature Award (with Martin Zanni), 2000; Bomem-Michelson Award, 2001, Chairman of the ACS Division of Physical Chemistry, 2001.

RESEARCH INTERESTS: Our research focuses on three areas in chemical dynamics and spectroscopy: (i) studies of reaction dynamics through a combination of transition state spectroscopy with state-resolved photodissociation experiments on stable molecules and reactive free radicals, (ii) size-dependent spectroscopy and dynamics of semiconductor clusters, and (iii) the effect of clustering and solvation on fundamental chemical processes. Novel experiments involving photodetachment of negative ion beams have been developed to address several of these issues.

Web site: http://chem.berkeley.edu/people/faculty/neumark/neumark.html

PETER J. ROSSKY. Collie-Welch Regents Chair in Chemistry, Professor of Chemical Engineering, and Director, Institute for Theoretical Chemistry, The University of Texas at Austin. B.A. 1971, Chemistry, Cornell University; Ph.D. 1978, Chemical Physics, Harvard University. Fellow of the American Physical Society, 1994, Fellow of the American Academy of Arts & Sciences, 2004.

RESEARCH INTERESTS: Published approximately 200 articles primarily in the area of theory and simulation of liquids; areas of emphasis including the behavior of aqueous systems and the treatment of quantum effects on condensed phase structure and dynamics. Current focus areas include solvation in biopolymer materials, chemistry in supercritical fluids, electronically non-adiabatic processes in amorphous materials, and quantum simulation of nuclear dynamics in liquids.

Web site: http://www.cm.utexas.edu/faculty/Rossky.html

Candidates for Member-at-Large of the Executive Committee

BRANKA LADANYI. Professor, Department of Chemistry, Colorado State University, Fort Collins, CO. B.S., McGill University, 1969. Ph.D., Yale University, 1973. APS Fellow, 1997. Associate Editor, Journal of Chemical Physics.

RESEARCH INTERESTS: Statistical mechanics, structure and dynamics of molecular fluids, liquid interfaces and clusters. Theoretical and computational studies of chemical reactions in solution, dielectric relaxation, neutron scattering, light scattering, nonlinear optical phenomena and vibrational relaxation.

Web site: http://www.chm.colostate.edu/bl/

MITCHIO OKUMURA. Professor, Department of Chemistry, California Institute of Technology, Pasadena, CA. B.S./M.S., Yale University, 1979. Churchill Scholar, Cambridge University, 1980. Ph. D., University of California, Berkeley, 1986. Postdoctoral Research Fellow, University of Chicago, 1987-8.

RESEARCH INTERESTS: Spectroscopy, kinetics, and reaction dynamics of free radicals, clusters, and transient intermediates; atmospheric chemistry; tropospheric ozone chemistry and hydrocarbon oxidation; vibrational dynamics of weakly bound species; Jahn-Teller and nonadiabatic effects; photochemistry and dissociation dynamics; cavity ringdown and cavity enhanced spectroscopies.

Web site: http://www.its.caltech.edu/~mo/

Candidates for Division Councilor

CHARLES S. PARMENTER. Distinguished Professor of Chemistry, Department of Chemistry, Indiana University. B.A. University of Pennsylvania. Ph.D. University of Rochester, 1962. Research Fellow, Harvard University 1962-64. APS Fellow 1984

RESEARCH INTERESTS. Experimental molecular dynamics with emphasis on how molecules acquire vibrational and rotational energy in collisions and how energy subsequently flows among vibrational modes of energized molecules and clusters. Vibrational and rotational state resolution is achieved with various forms of laser-excited fluorescence, sometimes used with single or crossed molecular beams or with high pressures of added gases.

Web site: http://www.chem.indiana.edu/

JACK SIMONS. Henry Eyring Scientist and Professor of Chemistry, Department of Chemistry, University of Utah. B.S., Case Institute of Technology, 1967. Ph.D., University of Wisconsin, 1970, Postdoctoral Fellow, MIT, 1971.

RESEARCH INTERESTS: Theoretical studies of negative molecular ions. The goals are to understand the properties of novel anions and to predict new such species. The species include dipole-bound, cluster, and solvated anions as well as biological ions involving DNA fragments and peptides and include both stable and electronically metastable states.

Web sites: http://simons.hec.utah.edu and http://simons.hec.utah.edu/TheoryPage

Meetings of Possible Interest to DCP Members

American Conference on Theoretical Chemistry
July 16-21, 2005
UCLA, Los Angeles, CA
Chair: Emily A. Carter
Vice-Chair: Mark Ratner
Email: eac@princeton.edu
ratner@chem.northwestern.edu
URL: http://www.conferences.ucla.edu/actc

Gordon Research Conference on Chemical Reactions At Surfaces
February 13-18, 2005
Ventura Beach Marriott, Ventura, CA
Chair: Charles T Campbell
Vice Chair: Cynthia M Friend
Email: campbell@chem.washington.edu
cfriend@deas.harvard.edu
URL: http://www.grc.org/programs/2005/chemreac.htm

Gordon Research Conference on Gaseous Ions: Structures, Energetics & Reactions
February 27 - March 4, 2005
Ventura Beach Marriott, Ventura, CA
Chair: William L Hase
Vice Chair: Vicki H Wysocki
Email: BILL.HASE@TTU.EDU
VWYSOCKI@U.ARIZONA.EDU
URL: http://www.grc.org/programs/2005/gaseous.htm

GRC Graduate Research Seminar: Molecular Energy Transfer
January 8-9, 2005
Santa Ynez Valley Marriott, Buellton, CA
Chairs: Anne B McCoy & Alec Wodtke
Email: MCCOY@CHEMISTRY.OHIO-STATE.EDU
WODTKE@CHEM.UCSB.EDU
URL: http://www.grc.org/programs/2005/gradmet.htm

Gordon Research Conference on Molecular Energy Transfer
January 9-14, 2005
Santa Ynez Valley Marriott, Buellton, CA
Chairs: Alec Wodtke & Anne B Mccoy
Email: MCCOY@CHEMISTRY.OHIO-STATE.EDU
WODTKE@CHEM.UCSB.EDU
URL: http://www.grc.org/programs/2005/molenerg.htm

Gordon Research Conference on Quantum Control Of Light And Matter
July 31 - August 5, 2005
Colby College, Waterville, ME
Chair: Paul Corkum
Vice Chairs: Philip H Bucksbaum & David Tannor
Email: PAUL.CORKUM@NRC.CA
PHB@UMICH.EDU
DAVID.TANNOR@WEIZMANN.AC.IL
URL: http://www.grc.org/programs/2005/quantcon.htm