

A Message from the Chair, Charles B. Harris

Highlighting the DCP activities in 2000 was the March APS meeting in Minneapolis. The scientific presentations formed the basis for four focus sessions or symposia centered about a topic or theme. My thanks go to the organizers of the four symposia who did a great job putting together an exciting and stimulating program. They were: James Heath and Mark Ratner (Molecular Scale Electronics); Paul Alivisatos and Mostafa El-Sayed (Nanocrystals from Scaling Laws to Applications); Ken Eisenthal and Tony Heinz (Structure and Dynamics at Liquid and Solid Interfaces); Paul Barbara and Peter Rossky (Experimental and Theoretical Frontiers in Molecular Quantum Dynamics) and Shaul Mukamel (Multidimensional Optical Spectroscopes). Without exception all symposia were filled to capacity or more, even through the end of the week. Thanks also goes to John Tully (Chair elect) for putting together as exciting a program for the March 2001 meeting in Seattle. These symposia are briefly described below.

As a final note, I'd like to congratulate and thank Laurie Butler from the University of Chicago for becoming the chair elect following John Tully. Additional thanks go to the new members at large, Roseanne Sension from the University of Michigan and Martin Gruebele from the University of Illinois. Congratulations also go to Sylvia Ceyer from MIT who will be DCP's new councilor. Finally, I would personally like to thank out-going Secretary-Treasurer, Thom Dunning, for all the service he gave the division over the past three years. I would also like to thank many members of Division and also the staff at the APS Washington offices for their help and guidance.

March APS Meeting, Washington State Convention Center, Seattle, Washington, March 12-16, 2001

This Division of Chemical Physics Program at the March meeting will consist of five (5) sessions which encompass a broad range of topics in chemical physics. John Tully (DCP Program Chair) organized these sessions. Invited and contributed papers will be combined in these sessions. Information on the March 2001 meeting is available at (<http://www.aps.org/meet/MAR01/>). Instructions for submitting abstracts can be found at <http://www.aps.org/meet/meet-abstract.html> (includes instructions for online submission of abstracts).

CONDENSED PHASE DYNAMICS

Organizer: Ara Apkarian, Department of Chemistry, University of California-Irvine, 516 Rowland Hall, Irvine, CA 92697-2025; Telephone: 949-824-6851, Facsimile: 949-824-8571; E-mail: aapkaria@uci.edu.

Molecular transformations that take place in the condensed phase—liquids, solids, glasses, interfaces, polymers and biological systems—are of central importance in chemical physics. Because they are more difficult to study, however, our understanding of dynamical events in the condensed phase lags behind

that of gas-phase dynamics. This symposium will highlight recent experimental and theoretical progress in condensed phase dynamics. New experimental methods include femtosecond and coherent spectroscopies. Computational advances in molecular simulation methods will also be included.

DYNAMICS AT SURFACES

Organizer: Daniel Auerbach; IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, CA 95120-6099; Telephone: 408-927-2432; Facsimile: 408-927-4180; E-mail: dja@almaden.ibm.com.

Chemical physics at the gas-solid interface combines the richness of the condensed phase with the simplicity of the gas phase. For example, the exquisite control of gas-phase reactants now achievable and the state-selective detection of products are revealing definitive information about reaction and energy transfer at surfaces. Scanning probe methods have revolutionized the study of clean, adsorbate-covered and defective surfaces. Nonlinear spectroscopies provide interface-selective probes, not only at the gas-solid interface but at the gas-liquid, liquid-solid and buried interfaces as well. Many examples of non-thermal laser-induced chemistry at surfaces have been achieved. This symposium will focus on recent advances in our atomic-level understanding of structure and chemistry at interfaces.

NANOSCALE SPECTROSCOPY AND IMAGING

Organizer: Steven Buratto; Department of Chemistry, University of California-Santa Barbara, Santa Barbara, CA 93106; Telephone: 805-893-3393; Facsimile: 805-893-4120; E-mail: buratto@chem.ucsb.edu.

Our ability to fabricate materials of nanometer dimensions, combined with an amazing array of spatially-resolved spectroscopic probes, has opened up a myriad of new scientific and technical opportunities. One example is single-molecule spectroscopy which has revealed that molecules of the same nominal composition are neither identical nor static. Another is the demonstration of quantum size effects that can drastically alter materials properties as a result of electron confinement. This symposium will focus on advances in both the techniques for studying nanometer sized objects as well as what we have learned about their physics and chemistry.

MATERIALS THEORY AND SIMULATION

Organizer: Gustavo Scuseria; Chemistry Department, Rice University, 6100 Main Street, MS 60, Houston, TX 77005-1892; Telephone: 348-527-4746; Facsimile: 348-285-5155; E-mail: guscus@katzo.rice.edu.

Our ability to synthesize and deploy both traditional and exotic materials is limited by our current experimental and computational capabilities for understanding materials properties and growth mechanisms. Ab initio electronic structure methods have advanced considerably in the last few years, particularly their applicability to large systems and to electronic excited states. Computer simulation methods, including on-the-fly ab initio approaches have also progressed. New spectroscopic and imaging methods have added greatly to our characterization toolbox. This symposium will focus on electronic structure, simulation and experimental methods for elucidating the growth and properties of inorganic and organic materials.

QUANTUM DYNAMICS, CONTROL, AND COMPUTING

Organizers: Eric Bittner; Department of Chemistry, University of Houston; 4800 Calhoun; Houston, TX 77204-5641; Telephone: 713-743-2775; Facsimile: 713-743-2709; E-mail: bittner@uh.edu. Robert Wyatt; Department of Chemistry and Biochemistry; University of Texas at Austin; Austin, TX 78712; Telephone: 512-471-3114; Facsimile: 512-471-8696; E-mail: wyatt@quantum.cm.utexas.edu.

The ability to prepare and interrogate coherent excited states of isolated molecules or ensembles using magnetic resonance or laser techniques is opening up new possibilities for study. Coherent steering of chemical reaction pathways has been achieved. Though still in its infancy, there has been progress towards developing quantum computers. Our understanding of decoherence processes is evolving. This symposium will include invited and contributed experimental and theoretical papers in the areas of quantum dynamics, coherence, decoherence, quantum control and quantum computing.

Graduate Student Travel Awards

Information on the Graduate Student Travel Awards can now be obtained from the DCP website, see:

http://www.cchem.berkeley.edu/~rjsgrp/APS_CPD/travel_awards.html

Election of New DCP Officers

Charles Harris will retire as DCP Chair in March, Roseanne Sension will be leaving her position as a Member-at-Large of the Executive Committee, and Thom Dunning will retire as Secretary-Treasurer. Our current Chair-Elect, John Tully, will then become Chair, and Laurie Butler 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 Vice-Chair organizes and edits the DCP contribution to *Physics News*. Activities of the members of the Executive Committee include administering the Graduate Student Travel Awards, Administering the DCP Web Site, and helping 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, one Member-at-Large, and the Secretary-Treasurer. The Nominating Committee, chaired by Mark Ratner, have convinced the following individuals to stand as candidates.

Candidates for Vice-Chair

ROGER E. MILLER. Professor, Department of Chemistry, University of North Carolina-Chapel Hill. B.S., University of Waterloo, 1975. M.S., University of Waterloo, 1977. Ph.D., University of Waterloo, 1980.

RESEARCH INTERESTS: Development of new laser spectroscopic and molecular beam techniques; spectroscopy and dynamics of clusters; high resolution infrared spectroscopy of molecules in superfluid liquid helium droplets; photochemical reactions at the state to state level; spectroscopy of aerosols-application to atmospheric chemistry; combustion chemistry-laser detonation of aerosols; rotational and vibrational energy transfer at surfaces by laser spectroscopy.

Website: <http://www.unc.edu/depts/chemistry/faculty/miller/index.html>

KRISHNAN RAGHAVACHARI. Distinguished Member of Technical Staff, Bell Laboratories, Lucent Technologies. B.Sc., Madras University (India), 1973; M.Sc., Indian Institute of Technology (India), 1975; Ph.D., Carnegie-Mellon University, 1981,

RESEARCH INTERESTS: Theoretical developments and applications in quantum chemistry; electronic structures of materials; atomic scale interactions and vibrations on silicon surfaces; chemical reactions on semiconductor surfaces; defects and doping in silicate glasses; electron correlation methods in quantum chemistry; accurate methods for theoretical thermochemistry; electronic structures of clusters and fullerenes.

Candidates for Secretary-Treasurer

BRUCE C. GARRETT. Group Leader; Theory, Modeling and Simulation; Environmental Molecular Sciences Laboratory; Pacific Northwest National Laboratory. B.S., University of California-Irvine, 1973; Ph.D., University of California-Berkeley, 1977.

RESEARCH INTERESTS: Development and application of reaction rate theories, particularly variational transition state theory; studies of quantum mechanical effects on chemical reaction rates; studies of solvent effects on chemical reactions; solvation structure and dynamics in supercritical fluids; solvation energetics and dynamics at gas/liquid interfaces important in heterogeneous atmospheric processes; Molecular theories for vapor-to-liquid nucleation.

Website:

<http://pnlxnotes3.pnl.gov/bios/Biosketch.nsf/All+Public+Documents/Garrett,+Bruce+C?Opendocument>

ALBERT F. WAGNER. Group Leader, Chemistry Division, Argonne National Laboratory. B.S., Boston College, 1966; Ph.D., California Institute of Technology, 1972.

RESEARCH INTERESTS: Application and extension modern dynamics and kinetics theories to elementary reactions of interest in combustion; parallelization of chemical dynamics codes.

Website: <http://chemistry.anl.gov/staff/chem-dyn/wagner.html>

Candidates for Member-at-Large of the Executive Committee

SHIRLEY CHIANG. Professor, Department of Physics, University of California-Davis. B.S., Harvard University, 1976; Ph.D., University of California-Berkeley, 1983.

RESEARCH INTERESTS: Study of nucleation and growth phenomena of thin metal films on clean single crystal substrates and observation of small molecules on metal surfaces, with the goal of observing chemical reactions on a surface.

Website: <http://www.physics.ucdavis.edu/Text/Chiang.html>

PETER J. ROSSKY. Professor, Department of Chemistry, University of Texas–Austin. B.S., Cornell University, 1971; M.A., Harvard University, 1972; Ph.D., Harvard University, 1978.

RESEARCH INTERESTS: Liquid water structure, solvation structure, theory of polar liquids, ionic association phenomena, computer simulation techniques, quantum effects in condensed phases.

Website: <http://www.cm.utexas.edu/research/profiles/Rossky.html>

Meetings of Possible Interest to DCP Members

75th Colloid and Surface Science Symposium

June 10-13, 2001

Carnegie Mellon University

Pittsburgh, PA 15213

Contact: S. Garoff (sg2e@andrew.cmu.edu) or R. Tilton (tilton+@andrew.cmu.edu), Carnegie Mellon University, Pittsburgh,

Web site: <http://colloids2001.cheme.cmu.edu/>

If you would like to have information about any future meetings included in the Spring DCP Newsletter, send the information to Thom Dunning before April 1, 2001 (thom.dunning@pnl.gov). You can add information on future meetings at any time to the DCP Web Site:

http://www.cchem.berkeley.edu/~rjsgrp/APS_CPD/