

American Chemical Society
Division of Physical Chemistry

Theory Subdivision
Winter Update
December, 2004

IBM Graduate Student Awards in Computational Chemistry:

There are two awards in Computational Chemistry that are open to current graduate students. We are grateful to IBM for their support of these awards. The competition is open to any graduate student (regardless of citizenship) who began graduate study after August 1, 2000 and who is an ACS member (or whose advisor is an ACS member). These awards are designed to encourage graduate work in computational chemistry, to recognize research accomplishments, and to stimulate interest in the Subdivision of Theoretical Chemistry and the Physical Chemistry Division of the ACS.

These two awards, supported by IBM, will provide one-time cash stipends of \$2500 and \$1000 as supplements to normal financial aid to doctoral candidates in the research-dissertation stage in 2005. Awardee selection will be made on a competitive basis. Applicants should be working on new and innovative computational chemistry methods or applications in theoretical chemistry.

The complete announcement, which includes instructions for submitting an application, can be found at www.chem.missouri.edu/theory. **Please note the deadline is January 31, 2005.**

Theory Subdivision Webpage:

Visit the Theory Subdivision website at www.chem.missouri.edu/theory. Highlights included on the site are links to upcoming meetings of interest to the theoretical community. Please let us know how we can make this site more useful to you by directing your comments to the Subdivision's Webmaster, John Adams (AdamsJE@missouri.edu).

We are compiling a list of useful and interesting links to web sites for theoretical and computational chemists or for individuals who want to learn more about theoretical and computational chemistry. If you have a recommendation for a site that might be of interest to the larger community, please send the URL and a brief description of the site to the webmaster.

Theoretical Chemistry Postdoctoral Position Clearinghouse:

The Subdivision continues to run a clearinghouse for people interested in hiring postdocs and people looking for postdoc positions. Currently there is a list of those looking for a position and one for those looking to hire, both of which are available on the Subdivision web page. If you wish to be on either list, please email the webmaster at AdamsJE@missouri.edu.

ACS PRF Summer School:

Computation, Simulation, and Theory in Chemistry, Chemical Biology, and Materials Chemistry, June 11-18, 2005 (Park City, Utah) Organized by Jack Simons. <http://simons.hec.utah.edu/school/index.html>

American Conference on Theoretical Chemistry:

Emily Carter, Conference Organizer, July 16-21, 2005 (UCLA) www.conferences.ucla.edu/ACTC Invited speakers include Robert Cave, Juan de Pablo, Weinan E, Philip Geissler, Sharon Hammes-Schiffer, Martin Head-Gordon, Hannes Jonsson, Kenneth Jordan, Ronnie Kosloff, Christopher Lee, Andrea Liu, Paul Madden, Dmitrii Makarov, Todd Martinez, Andrew Rappe, Mark Ratner, David Reichman, Karsten Reuter, Peter Rossky, Steven Schwartz, David Srolovitz, Bruce Tidor, John Tully, Troy van Voorhis, Zhen-Gang Wang, Chris Wolverton, Sophia Yaliraki.

229th ACS National Meeting Preview:

March 13-17, 2005, San Diego, CA Symposia of interest include: Hydrogen Bonds: Developments in Experiment and Theory (PHYS), Biophysical Aspects of Protein and Peptide Aggregation, Experiment and Theory (PHYS), Computational Methods and Modeling in Fuel Chemistry (FUEL), Applications of Information Theory in Chemistry (COMP/CINF), John Pople Memorial Symposium (COMP/PHYS), Michael Klein 65th Birthday Symposium (COMP)

Request for Future Symposia Topics:

Members of the Theoretical Subdivision are encouraged to suggest topics of interest to the community for future symposia at American Chemical Society meetings. Suggestions for symposia topics for future ACS meetings should be sent to Krishnan Raghavachari, (kraghava@indiana.edu).

How to Join the Theory Subdivision:

You must be a member of the Division of Physical Chemistry in order to join the Subdivision. If you are already a dues-paying member of the Division of Physical Chemistry, just send a note to the Secretary of the Subdivision (Jan Steckel, steckel@netl.doe.gov) indicating your wish to join.

228th ACS National Meeting Recap:

The August, 2004, meeting of the ACS in Philadelphia was a great experience for those who attended. Theory subdivision members had a lot to choose from, with very interesting papers presented in many symposia. A few are highlighted here.

Quantum/Classical Calculations in Chemistry and Biophysics (PHYS) was an interesting series with talks on semiclassical dynamics and path integrals, mixed quantum/classical dynamics, clusters and materials and the frontiers of QM/MM potential development.

Advances in Quantum Chemistry–Theory, Algorithms and Applications (PHYS) held the interest of many. Topics included density matrix approaches, large scale methods, multireference methods, and explicit electron correlation methods. Lively forum discussions occurred at the end of each day.

High Performance Computing in Computational Chemistry (COMP) was another choice for theorists. Topics included highlights of the IBM blue gene project from William Swope, distributed computing problems, and applications of HPC to biomedicine.

The symposium in Honor of Henry F. Schaefer's 60th Birthday (COMP/PHYS) featured papers by many prominent members of the theoretical community. Topics included molecular orbital theory, accuracy, scaling of computations, simulation of spectra, and many others.

Champions Announced In The Second Industrial Fluid Properties Simulation Challenge:

Scientists and engineers from 3M, BP, Dow Chemical, DuPont, ExxonMobil, Mitsubishi Chemical, and NIST challenged the molecular modeling community to predict physical properties of industrially relevant fluid systems. Contest entrants presented their work, the champions were announced, and prizes awarded, during a special session at the AIChE Annual Meeting in Austin, TX. November 7, 2004. For more information, please see www.cstl.nist.gov/FluidSimulationChallenge/

Call for Papers:

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap. 230th National American Chemical Society Meeting, Washington, DC August 28-September 1, 2005. Sponsored by the Computers in Chemistry Division and Co-sponsored by the Physical Chemistry Division.

With increasing accuracy and applicability of molecular modeling tools, the challenge is beginning to shift to addressing how molecular modeling can help engineer materials and processes at the macro-scale. The properties at the macro-scale not only depend on the molecular arrangement, but often on how the nanoscale arrangements of these molecules themselves cluster. Thus, molecular design of macroscale properties requires increased understanding of molecular scale, nanoscale, mesoscale and macro-scale phenomena.

This symposium will focus on applications and methodology development in integrating the nano, meso and larger length scale regions. Applied large-scale atomistic molecular dynamics simulations, mesoscale simulations, and additional coarse grain methodology studies with focus on structure-property behavior as well as kinetic processes are requested. Applications in nanotechnology, biology, inorganic materials, catalysis, polymers, pharmaceuticals and additional life and materials science areas are encouraged. Contributions are solicited from academic, industrial, and the governmental research sectors.

A poster session is planned in addition to oral presentations. A panel discussion of modeling and simulation in this area is also planned. In addition, the organizers plan to publish a proceedings pending interest from contributing authors. A social event for contributing authors during the ACS meeting is also planned.

Please submit abstracts to either Sanat Mohanty or Rick Ross (email below) at your earliest convenience to aid in session planning. Please also submit abstracts directly to the American Chemical Society via the official on-line abstract submissions system when it becomes available (March 2005) for this meeting to have your presentation officially entered for the meeting. For additional information on the symposium, please contact Sanat Mohanty or Rick Ross.

Symposium Organizing Committee: Sanat Mohanty and Rick Ross 201-2E-23, Corporate Research Materials Laboratory 3M Company, St. Paul, MN 55144 smohanty@mmm.com; rbross@mmm.com

See <http://oasys.acs.org/> for abstract submission access and guidelines.

ACS Theoretical Subdivision Officers:

Chair Sharon Hammes-Schiffer, Department of Chemistry, Pennsylvania State University, shs@chem.psu.edu

Chair-Elect Krishnan Raghavachari, Department of Chemistry, Indiana University, kraghava@indiana.edu

Vice Chair Angel Garcia, Theoretical Biology and Biophysics Group, Los Alamos National Laboratory, New Mexico, angel@atlas.lanl.gov

Secretary Jan Steckel, National Energy Technology Laboratory, Pittsburgh, steckel@netl.doe.gov

Webmaster John Adams, Department of Chemistry, University of Missouri-Columbia, adamsje@missouri.edu