

American Chemical Society
Division of Physical Chemistry

Theory Subdivision Summer Newsletter August, 2006

Message from Theory Subdivision Chair, Krishnan Raghavachari:

I would like to report that a nominating committee consisting of Gustavo Scuseria, Ken Jordan, and Krishnan Raghavachari has been formed to elect the next Vice-Chair-Elect of the Theory Subdivision. We plan to announce the result at the ACS meeting in San Francisco.

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).

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.

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 an e-mail to ACS Member Services (service@acs.org) indicating your wish to join.

232th ACS National Meeting Preview:

September 10-14, 2006, San Francisco, California. There are many symposia of interest to theorists at this meeting. A few of the symposia of interest are: Frontiers in Molecular Biophysical Dynamics: Experiment and Theory (PHYS), Fundamentals of Metal Oxide Catalysis (PHYS and COLL), Theory of Rare Events and Accelerated Dynamics (PHYS), Progress in Computational and Experimental Studies of Materials for Hydrogen Storage (PHYS and FUEL) and Frontiers in Molecular Dynamics: Experiment and Theory (PHYS).

233rd ACS National Meeting Preview:

March 25-29, 2007, Chicago, IL. Some symposia of interest are: Measures of Accuracy and Reliability in Molecular Simulation (PHYS), Capturing Complexity in Physical Sciences Simulation (PHYS), Dynamics on the Nanoscale (PHYS), Implications and Applications of Chirality in Chemistry (PHYS), Vibrational Spectroscopy as a Probe of Biomolecular Structure and Dynamics: Theory and Experiment (PHYS).

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).

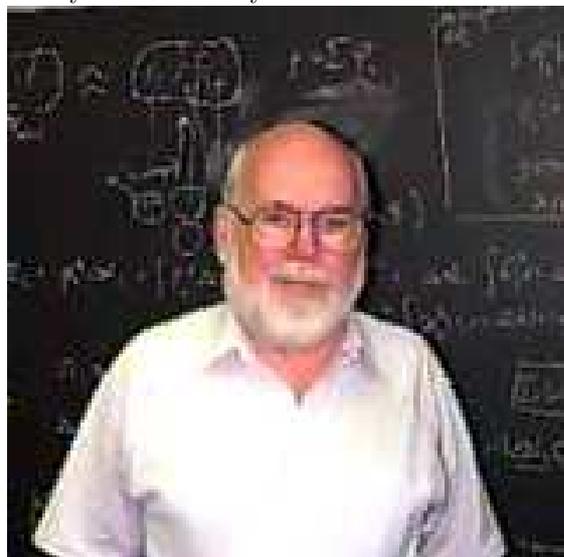
Retrospective: Density Functional Theory Symposium in Atlanta:

"Frontier Applications and Developments of Density Functional Theory: A Symposium in Honor of Robert G. Parr's 85th Birthday" was held at the Spring 2006 meeting of the ACS in Atlanta. The symposium consisted of sixty-two invited talks, beginning with Nobelist Walter Kohn, who paid tribute to the Parr's role in establishing density functional theory (DFT) as a practical tool for chemists and physicists alike before lecturing on the origin of dispersion interactions. From there, the whole gamut of recent work in density functional theory was on display, including new approaches for describing weak interactions, relativistic effects, and excited states; new density functionals and novel methods for constructing density functionals; more efficient computational strategies; innovative ideas for attacking the electron correlation problem; the interpretation of chemical reactivity; and applications to molecules, materials, surfaces, the solid state, and biology. In addition to the scientific content of their talks, the speakers discussed how Parr had influenced them either directly (as a mentor) or indirectly, through his scientific work. The latter comments attest to Parr's persistent scientific excellence: speakers cited papers ranging from his early work on Pariser-Parr-Pople theory (1952-53) to his most recent work on atoms in molecules (2005).

Participants in the symposium learned more about the origins of Pariser-Parr-Pople theory at the symposium banquet, where Rudy Pariser discussed the origins of the method in his after dinner talk. After Pariser's recounting of what it was like to work with Parr during the early days at Carnegie Institute of Technology (now Carnegie Mellon University), Nicholas Handy spoke about his studies with Parr at Johns Hopkins University. Lee Pedersen concluded by telling an anecdote from Parr's years at the University of North Carolina. Finally, the evening culminated with Prof. Parr offering some thoughts of his own, and graciously deflecting credit to his family and former students and postdoctoral associates, many of whom were in attendance.

Many speakers at the conference spoke admiringly of Parr's open-mindedness and creativity, especially his prodigious ability to generate unexpected "crazy ideas." Prof. Parr, giving a talk as the last speaker in the symposium, met these expectations. After quipping that "This is a lot more fun than a memorial symposium," he presented his recent work on determining energies by scaling the different portions of the Hamiltonian and presented a new density functional for the correlation contribution to the kinetic energy, based the value of the electron density at the atomic nucleus.

The symposium was organized by Weitao Yang of Duke University and Paul Ayers of McMaster University, and was cosponsored by the Division of Computer in Chemistry and the Division of Physical Chemistry.



This photo of Prof. Parr, from his webpage, was featured in many of the talks.

Thanks to Paul Ayers and Weitao Yang, co-organizers of the Symposium in Honor of Robert G. Parr's 85th Birthday, for contributing this description of the symposium for those who were unable to attend.

HP Scholar Program Provides Travel Awards for Outstanding Junior Faculty

Hewlett-Packard and the ACS Division of Computers in Chemistry (COMP) are pleased to announce the HP Outstanding Junior Faculty Award program that will provide \$1,000 in travel funds for each of four outstanding tenure-track junior faculty to present their work in COMP symposia at the ACS National Meeting in San Francisco. The Awards are designed to assist new faculty members in gaining visibility within the COMP community. Award certificates and \$1,000 prizes will be presented at the COMP Poster session on Tuesday evening. While special consideration will be given to Assistant Professors presenting work in the area of algorithm and methods development, applications for HP Scholar Awards are invited from all current tenure-track junior faculty who are members of ACS as well as the ACS Division of Computers in Chemistry. Selection criteria will include the novelty and importance of the work to be presented, as well as the level of Departmental support as indicated by a letter of support by the Chair or Chair designee. To apply, an extended abstract of the work (no more than 2 written pages) and the letter of Departmental support should be sent to Wendy Cornell (wendy_cornell@merck.com). The application deadline for the HP Outstanding Junior Faculty Award program for the San Francisco ACS meeting is September 1, 2006.

ACS Theoretical Subdivision Officers:

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