Nov. 30, 2010

Potential Energy Surfaces for Simulating Complex Chemical Processes

On Nov. 30, 2010, U.S. Energy Secretary Steven Chu announced the funding of a new round of cutting-edge research projects funded through the U.S. Department of Energy Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. The INCITE program gives cutting-edge research projects access to supercomputing processor hours.

The Truhlar group received a grant of 15 million hours of processor time on the IBM BlueGene/P computer at DOE's Leadership Computer Facility at the Argonne National Laboratory for research involving electronic structure calculations required for structural characterization and rate constant and dynamics calculations. The Truhlar group will look at potential energy surfaces for simulating complex chemical processes. Group members working on this research include Co-Principal Investigator Oksana Tishchenko and Boris Averkiev, Anant Kulkarni, Xufei Xu, Shuxia Zhang, and Jingjing Zheng. Also collaborating is Dr. Carlos Sosa of IBM.

Projects receiving INCITE awards utilize complex simulations to accelerate discoveries in ground-breaking technologies. The University of Minnesota researchers will apply multi-reference perturbation theory and multi-configuration quasi-degenerate perturbation theory to study three challenging classes of reactive systems in the gas phase and materials, including charge transfer coupled to magnetic spin state change in metallofullerenes and metal-doped carbon nanotubes; reactions of phenolic antioxidants with free radicals; and radical-radical and radical-molecule association reactions. The first class of problems is important for achieving a fundamental understanding of charge transfer and polarity in the context of molecular electronics and spintronics. The second class is important for understanding the cytoprotective effects of both natural agents and drugs or drug leads. The third class of problems is important for developing clean, efficient fuels and for understanding atmospheric chemistry. The project also explores density functional theory as applied to catalytic reactions at gas–solid and gas–nanoparticle–solid interfaces and to charge transfer at material interfaces.

Large-scale electronic structure theory will provide potential energy surfaces and force fields for simulating these complex chemical processes important for technology and biological chemistry. To obtain accurate

energies and stationary points for systems whose electronic structure has high multi-reference character, the researchers will use multi-reference perturbation theory (MRMP2) and multi-configuration quasi-degenerate perturbation theory (MCQDPT) as well as density functional theory. The main software packages for this project are the GAMESS, POLYRATE, and GPAW codes. Computational parallelism is exploited in both the electronic structure and dynamics steps.