Type: New
Title: "Potential Energy Surfaces for Simulating Complex Chemical Processes"

Principal Investigator: Donald G. Truhlar, University of Minnesota

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **15,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (15,000,000 processor hours)

Research Summary:
Large-scale electronic structure theory provides potential energy surfaces and force fields for simulating complex chemical processes important for technology and biological chemistry. Addressing the challenge of obtaining accurate energies and stationary points for systems whose electronic structure has high multi-reference character, researchers use multi-reference perturbation theory (MRMP2) and multi-configuration quasi-degenerate perturbation theory (MCQDPT). The team applies MRMP2 and MCQDPT to study three classes of reactive systems in the gas phase and materials: (1) charge transfer coupled to magnetic spin state change in metallofullerenes and metal-doped carbon nanotubes, (2) reactions of phenolic antioxidants with free radicals, and (3) 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.

The computer-intensive part of this research consists of electronic structure calculations required for structural characterization and rate constant and dynamics calculations. The main software packages for this project are the GAMESS, POLYRATE, and GPAW codes. Computational parallelism is exploited both in the electronic structure and dynamics steps.