Theoretical Chemistry
Code 6189

Postdoctoral Opportunities

Postdoctoral areas of emphasis include:

Theoretical Chemistry

- Theoretical methods are developed and used to study the electronic, structural and dynamic properties of a variety of solid-state and large molecular systems, particularly for low-dimensional systems such as nanowires, polymers, surfaces, and interfaces. Areas of current emphasis include: (1) electronic, structural and transport properties of nanowires including carbon nanotubes; (2) empirical simulations of surface involving metals and metal oxides; (3) semiconducting and metallic polymers; (4) many-body effects on surface states; and (5) high pressure phases of solids.

Quantum Chemistry Studies of High Energy Density Materials

- Quantum chemical electronic structure methods are used to determine the structures, energies and vibrational spectra of high energy density materials. Reaction pathways involved in the synthesis and decomposition of these compounds are characterized by locating the transition state structure separating the reactants and products. The height of the energetic barrier at the transition state is associated with the activation energy of the reaction pathway. Calculations are performed for known materials as well as for those that have not yet been synthesized.

Simulations of Chemical Reactions in Condensed Phases

- Molecular dynamic simulations of chemical reactivity in both solids and solid surfaces are currently being implemented using a variety of many-body potentials. These modeling efforts include chemistry, gas-surface chemical reactions, tribo-chemsitry, and energetic-collision-induced reactive cluster scattering. On a microscopic scale, results of these simulations are used to study such processes as the propagation of chemically sustained shock waves, atomic scale adhesion and friction, and shock-induced reactions in molecular solids.

Density Functional Theory in Chemistry

- The applicability of density-functional approaches to theoretical studies of chemical reactions and processes is being established. The linear-combination-of-Gaussian-type-orbitals density functional method is being developed and applied to clusters and to clusters as models of surfaces and interfaces. Variational fitting is used to make these calculations more efficient without loss of accuracy. Current interests include magnetic clusters, fullerenes, and first-principles molecular-dynamic simulations of chemical reactions.

All information was taken from:

Cooperative Research Associateships,
Attainable at the Naval Research Laboratory:
Washington, D.C.
Monterey, California
Stennis Space Center, Mississippi

The postdoctoral program at the Naval Research Laboratory is restricted to U.S. citizens. Initial appointments are for one year and are routinely renewable for a second year.

The applicant is responsible for selecting a research project and writing a research proposal in collaboration with a prospective advisor. The fellowship is administered through the National Research Council. Deadlines for application material are January 15 for the February review and April 15 for the June review.

For more information please contact:

Dr. Carter White
Theoretical Chemistry
Code 6189 Navy Technology Center for Safety and Survivability