



**NRL BAA Announcement
#61-09-07**

COMPUTATIONAL CHEMISTRY

First-principles and semi-empirical simulations are increasingly important computational and theoretical tools for understanding and predicting chemistry at surfaces, interfaces, and in solids, as well as identifying new materials of potential importance to the Navy.

The Theoretical Chemistry Section of the Naval Research Laboratory (NRL) is interested in receiving proposals to perform first-principles and semi-empirical simulations of solid-state and materials-related chemistry using high-performance computing. Specific problems of interest include: developing fast, scalable, zero- and one-dimensional, electronic structure and chemical dynamics using Gaussian-based density-functional theory; transport properties of nanostructures including nanowires; shock-induced chemical reactions in energetic materials; the dynamics of chemical vapor deposition; and materials processing and growth via cluster-surface collisions. Also of interest to the Theoretical Chemistry Section are simulations of friction and adhesion at the atomic-scale, molecular dynamics simulations of structural and elastic properties of bulk systems, surfaces, and interfaces composed of metals, metal-oxides, and related materials, and molecular dynamics simulations of hypervelocity cluster-surface impacts and carbon nanostructures. It is anticipated that projects might span two years. Proposals for lesser periods and/or stand-alone subsets of the effort, each individually priced, are encouraged.

Address White Papers (WP) to Code 6189, or [E-mail](#), telephone (202) 767-3270. Allow one month before requesting confirmation of receipt of WP, if confirmation is desired. Substantive contact should not take place prior to evaluation of a WP by NRL. If necessary, NRL will initiate substantive contact.