

# First Principles Modeling of Nanostructures

Serdar Ögüt

*Department of Physics, University of Illinois at Chicago*

Among the various theoretical tools for investigating microscopic material properties, *ab initio* (first principles) methods based on density functional theory and pseudopotentials have had a very good track record over the last two decades in terms of accuracy, reliability, and efficiency. The application of these methods to nanostructures to investigate their structural, electronic, and optical properties has, however, not been quite straightforward due to the large computational demand and new physics inherent in the nanometer and sub-nanometer size region. One particularly useful extension to overcome the computational demand imposed by localized nanostructures has been the introduction of methods based on a real-space implementation, such as the higher order finite difference pseudopotential method.

In this talk, after reviewing the basic theoretical tools of density functional theory, *ab initio* pseudopotentials, and higher-order finite difference method, I will present various applications of the method to different properties of various nanostructured materials. These applications include (i) structural and electronic properties of small semiconductor (Si, Ge, GeTe) clusters, (ii) calculation of quasiparticle and exciton binding energies in Si quantum dots containing up to 1,000 atoms, and (iii) a new efficient real-space approach for calculating the microscopic dielectric screening matrix, its inverse, and the resulting exciton Coulomb energies in hydrogenated Si clusters up to  $\sim 1$  nm diameter in size.