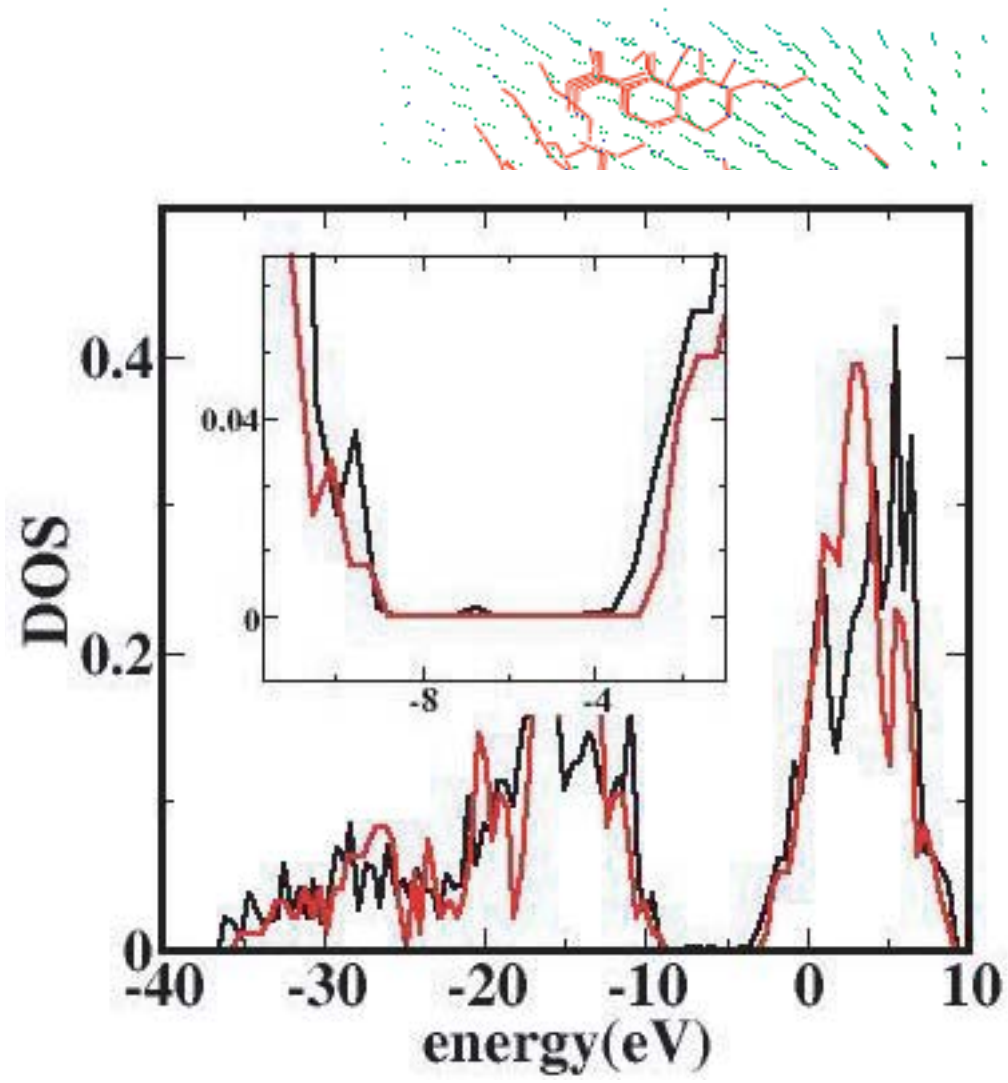
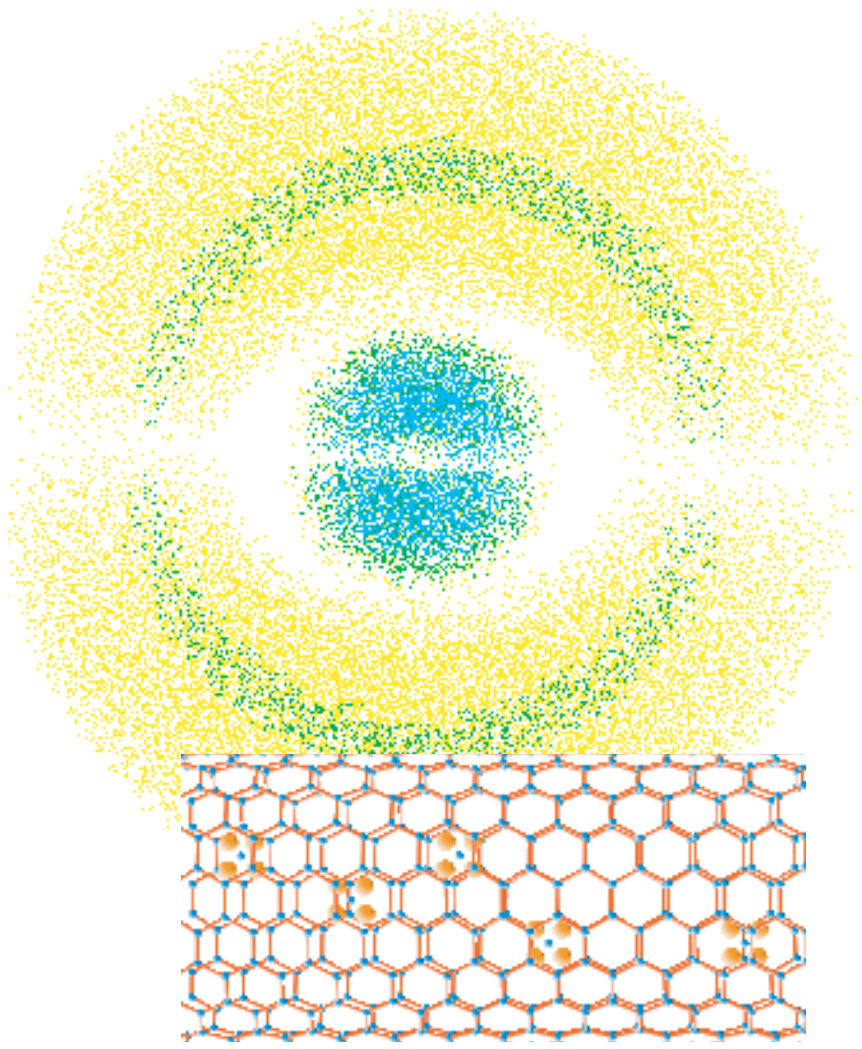
Boston University Physics Colloquium





Atomistic simulation and visualization: modeling in the world of condensed matter

Numerical modeling of condensed matter systems is a rapidly developing field of both intrinsic and technological interest. Nanoscale systems are natural candidates for such studies. Schroedinger's equation can only be solved analytically for the hydrogen atom. Helium, or the hydrogen molecule already require a numerical solution, and even nanoscale condensed matter systems require sophisticated numerical methods.

Modeling in tandem with laboratory experiments is the ideal. In principle, the application of Newton's equations of motion to potentials generated from the solution of Schroedinger's equation can model any process that can occur, and generate any measurement that can be made in the laboratory. In practice, computational shortcuts are required even for picoseconds at the nanoscale.

I will give an introduction to atomistic simulation and visualization with examples from our models of carbon allotropes such as nanotubes and nanodiamonds and compare the results with laboratory experiments.

Joan Adler

Technion - Israel Institute of Technology

January 29, 2008 (Tuesday) at 3:30 pm (Refreshments at 3:15 pm)
SCI 107, Metcalf Science Center, Boston University

Call: Winna Somers (wsomers@bu.edu) (617)353-9320
Host: William Klein