

# Physics Colloquium

## Michigan Technological University

Thursday, January 31th, 2008, 4:00 pm

Room 139, Fisher Hall

### Enhanced Implicit Solvation Model for Bio-molecular Simulation

Parimal Kar

Advisor: Ulrich H.E. Hansmann

**Abstract:** Reliable consideration of the effect of water on structure and dynamics of biomolecules is among the key factors governing accurate descriptions of biological matter. Within a series of individual refinement steps we demonstrate that a general purpose Poisson-Boltzmann approach can be fine-tuned to a stage where semi-quantitative model description is not completely out of reach. These refinement steps take into account the analogous classical terms introduced in the Polarizable Continuum Model (PCM) which is a powerful implicit solvation method in Quantum Mechanics. Within this present work we summarize the kernel of these individual contributions, discuss parameterization data obtained recently, outline the remaining technical challenges, and provide a series of example studies that underline the current stage of development and hint at future activities.

### Boron Nitride Nanotubes: Synthesis, Characterization, and Functionalization

Chee Huei Lee

Advisor: Dr. Yoke Khin Yap

**Abstract:** We have succeeded for the first time on direct growth of boron nitride nanotubes (BNNTs) on substrates. These BNNTs can be effectively synthesized by a simple thermal CVD technique. Our experiments provide some new understanding on the growth mechanism of BNNTs. Some of the critical growth parameters have been identified and will be discussed in the talk. Dense BNNTs can now be consistently deposited on various types of substrates including Si, oxidized Si, quartz, and sapphire. Furthermore, by carefully control the amount of precursors, it is able to adjust the diameters of these BNNTs. We think that our work representing an important pathway for direct growth of BNNTs on substrates for future device applications. The success of this high yield synthesis has also lead to the study of functionalization of BNNTs with polymer by means of  $\pi$ - $\pi$  interaction. Finally, preliminary data on the doping of BNNTs will also be presented.