

# Physics Seminar

Michigan Technological University

Friday, January 11, 2008

11:00 am

Room 130, Fisher Hall

## ***Ab initio* Optical Spectra of ZnSe clu**

**Sachin Nanavati**

Centre for Development of Advanced Computing (C-DAC),  
Pune University Campus,  
Pune 411 007, India

### **Abstract:**

In the present work, simulations have been carried out to obtain the optical absorption spectra of semiconductor clusters like ZnSe and compare them with experiments. These calculations were carried out within the time dependent density functional theory (TD-DFT) formalism.

We employed a pseudopotential based "real space" method where the Kohn-Sham equations were directly solved at each point on a 3 dimensional grid, constructed around the cluster. This procedure avoids the usage of conventional "supercell method" employed in all Fourier space technique, to account for a non-periodic structure like quantum dot. Further, partially charged Hydrogen atoms were used to passivate the unsaturated dangling bonds on the cluster surface, to reproduce the experimental condition.

The present talk will give an overview of the pseudopotential based real space DFT method and discuss the results obtained. It will also address the practical computational issues involved in porting the code across different operating systems and enhancing the performance of the simulation by using efficient numerical library.