

Physics Colloquium

Michigan Technological University

March 3 (Thursday) 4:00 to 5:00 pm
Room 139, Fisher Hall

Theoretical Study of Gallium Oxide Clusters

S. Gowtham

Adviser: Professor Ravindra Pandey

Gallium oxide is an important semiconducting material with applications in the areas of optics and micro-electronics. Considerable efforts have been made in the past to understand the structural, optical and electronic properties of gallium oxide. On the other hand, interest in studying the properties of this material at the cluster level is relatively recent. Small clusters of gallium oxide can be taken as a prototype to understand the Physics and Chemistry of surfaces and nanostructures. Equilibrium structure, bonding and electronic properties computed under the framework of Density Functional theory will be discussed.

A Hydrophobic scoring of Proteins

Vasyl Aleksenko

Advisor: Professor Ulrich Hansmann

We propose a simple measure that allows profiling protein configurations. It is based on calculation of a restricted radius of gyration evaluated only between the centroids of hydrophobic residues and measures the formation and compactness of the hydrophobic core. Some preliminary results for applications of the new score in generalized-ensemble simulations will be presented.