

# Physics Colloquium

## Michigan Technological University

Thursday, January 24th, 2008, 4:00 pm

Room 139, Fisher Hall

### Replica Exchange Aided Wang-Landau Algorithm For Protein Folding by Liang Han

Advisor: Ulrich Hansmann

#### Abstract:

The Wang-Landau algorithm, first introduced by Wang and Landau in the spin glass system in 2001, has sparked great interest in many computational physics problems. Unlike conventional Monte Carlo algorithms, the Wang-Landau algorithm takes the density of states as its goal of simulation. Many thermodynamic properties can be determined from the derivatives of the partition function that can be calculated directly from the density of states. This method decreases the relaxation time of a system with a rough energy landscape. The original idea of the Wang-Landau algorithm is based on discrete systems while the all-atom representation of the protein is a continuous system. In order to apply this algorithm in the protein folding problem, we tested a continuous representation of the entropy with the statistical temperature in a small protein, Met-enkephalin. The second step of our project is to parallelize our modified Wang-Landau algorithm. Our approach is to combine the modified algorithm with the replica exchange method that has demonstrated to be one of the most powerful methods to overcome the broken ergodicity problem.

### The Oxidation of Atomic Boron Clusters: Gaining Insight into Experimental Results via *ab initio* Electronic Structure Calculations by Wil Slough

Engineering Physics

Advisor: Warren Perger

#### Abstract:

Atomic clusters created from bonding together like-atoms define a transitory position between the more familiar states of matter. They exist as possible energetically favored structures arising along the transition from gases to denser phases (liquids and solids). Clusters generated solely from boron atoms have been studied experimentally and theoretically for the past two decades. In addition, experimental work on the chemical reactivity of bare boron clusters with a variety of gas phase molecules has produced interesting results that have yet to be fully explained. In this talk I will discuss some experimental results, and offer some explanation derived from *ab initio* electronic structure computations for one specific test case--the interaction of a  $B_{13}$  cluster (anion, neutral, and cation) with molecular oxygen.