Physics Colloquium
Michigan Technological University

April 13 (Thursday) 2006, 4:00 to 5:00 pm
Room 139, Fisher Hall

Atomic clusters: Seeking structure at the nanoscale

Koblar Jackson

Physics Department
Central Michigan University

Atomic clusters exist in a size range where "size matters", i.e. where physical and chemical properties can change dramatically with the addition of even a single atom. This makes clusters fascinating from a fundamental point of view, but it also makes them potentially very useful, as careful size selection may result in properties that are optimal for applications such as nanocatalysis. A major problem in studying clusters is determining the structures they adopt. The atomic arrangements are generally unlike those in bulk materials, and in some cases very much so. Furthermore, the number of possible arrangements grows explosively with cluster size, making it very challenging to find the most stable isomer for all but the smallest clusters. In this talk, I will discuss a method we have developed to find the most stable structure for clusters containing up to around 50 atoms. The method is completely unbiased, and employs a hierarchy of approximations that results in the ground state structure determined at a first-principles level of theory. I will illustrate the use of the method through applications to Si_n and Cu_n. I will also show how using experimental data such as ionization potentials, ion mobilities, vertical detachment energies and photoelectron spectra, is an essential part of making definitive structural assignments. Finally, I will briefly present a new method we are developing to investigate the dielectric properties of clusters.

Prof. Jackson maintains an active research program in computational materials physics, focusing on the electronic structure of disordered systems. His work has involved both developing state-of-the-art molecular-modeling tools and applying those tools to various problems of both fundamental and applied interest. Recent applications involve studying the properties of materials at the nanoscale, exploring the small-size limits of such technologically important materials as silicon and iron. He is also interested in the atomic-scale structure of network glasses.