Physics Colloquium
Michigan Technological University

April 7 (Thursday) 2005, 4:00 to 5:00 pm
Room 139, Fisher Hall

A Theoretical Study of Spin-Polarized Electron Tunneling along a Molecular Wire

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Understanding of the "controlled transport of spin-polarized electrons" through a molecular spacer has been an ultimate goal and has attracted much attention in recent years for its potential applications in spin-based molecular electronic devices. In this talk, I will present the results of a theoretical study of the spin-polarized electron tunneling in a configuration involving a non-bonded magnetic probe tip and a molecular wire consisting of a self-assembled monolayer of benzene 1,4-dithiol on the Ni(111) substrate. A periodic, gradient-corrected density functional method together with Bardeen, Tersoff and Hamann formalism is employed for electron transport calculations. The electron tunneling is found to be strongly dependent on both structural and magnetic configurations of the probe tip. A significant higher tunneling current is obtained for the configuration in which the spin of the non-bonded magnetic tip is aligned parallel to that of the magnetic substrate than for the configuration with anti-parallel alignment — an effect prerequisite for the *molecular spin valve*.

First-Principles Study of Elemental Boron Nanoclusters & Nanotubes

Kah Chun Lau
Advisors: Dr. Ravindra Pandey and Dr. Ranjit Pati

Current trends in miniaturization of electronic devices have triggered an intense research in various nanoscale structures. Besides carbon nanotubes, boron nanotubes are believed to be another stable ``homonuclear'' nanotubes, which has recently been synthesized. Understanding of the structural stability, electronic properties and chemical bonding of boron nanotubes can be set as another baseline for the evolutionary changes from carbon nanotubes to hybrid $B_xC_yN_z$ nanotubes to boron-nitride nanotubes. I will present the results on structural stability, electronic properties and chemical bonding of boron nanotubes obtained using first principles periodic density functional approach. Specifically, the size-dependent structural transition of boron nanoclusters and their physical properties will be discussed.