

Physics Colloquium

Michigan Technological University

October 20 (Thursday) 2005, 4:00 to 5:00 pm
Room 139, Fisher Hall

Theory and Modeling of Molecular Electronics

Hong Guo

*Department of Physics
McGill University, Montreal, Canada*

Abstract

Significant progress has been made in quantum transport measurements of molecular scale nanoelectronic systems. These systems represent perhaps the ultimate size limit of functional devices. In this talk, I will review some important issues of molecular electronics theory. I will then present a first principles self-consistent formalism for theoretical modeling of quantum transport properties at molecular scale under external bias and gate potentials. This formalism is based on performing density functional theory (DFT) analysis within the Keldysh nonequilibrium Green's functions (NEGF) framework. I will report our recent investigations using the NEGF-DFT formalism on resistance of several molecular wires and compare results with the corresponding experimental data. I will also report our investigations on electron-phonon coupling during nonequilibrium charge transport, and transport properties of molecular spintronics.

Biography

Prof. Hong Guo completed his undergraduate degree in Sichuan Normal University in China, and Ph.D in theoretical condensed matter physics at University of Pittsburgh in 1987. In 1990, he joined the faculty of the Department of Physics, McGill University in Montreal, Canada. He is now a James McGill Professor of Physics and serves as the Director, Centre for the Physics of Materials, McGill University. He is a Fellow of the American Physical Society. Prof. Guo's research is in the field of quantum transport theory and mesoscopic physics, computational physics and device modeling, as well as materials physics.