McGill Computational Science and Engineering Seminar

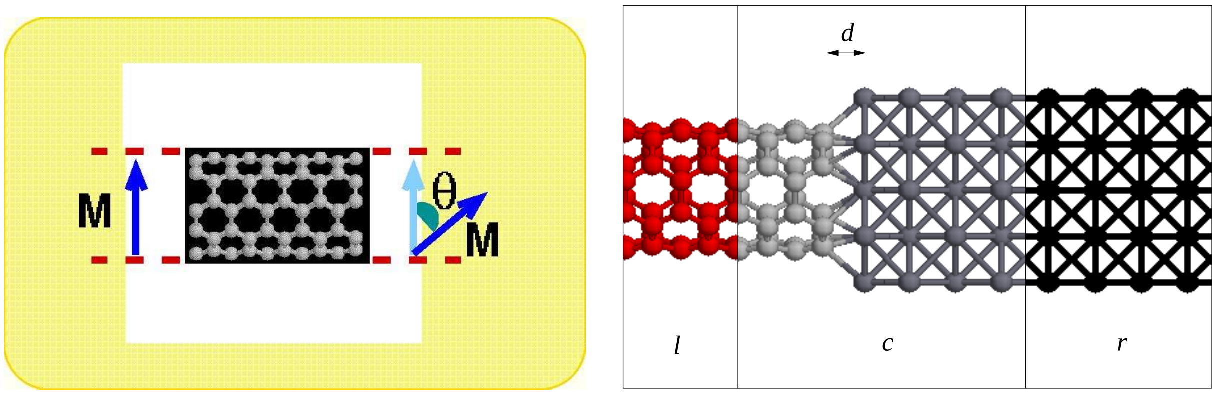
Friday October 20th at 14:00 in Burnside Hall room 1205

Nanoelectronics: Theory and Computation

Hong Guo

Center for the Physics of Materials & Department of Physics McGill University

Nanoelectronics is an exciting area of condensed matter research which may well play an important role for the search of a new generation of functional devices. At truly nanometer scale, electrical conduction can however be dominated by quantum phenomena for which some of the classical understanding of device physics need to be extended. In this talk I will discuss theoretical and computational issues concerning prediction of quantum transport properties of conductors at atomic and molecular scale, where such effects as the device-electrode interaction, the atomic/molecular orbitals, electron-electron interactions, etc., must be treated from first principles. Specific examples of charge transfer doping induced molecular current switching and anomalous quantum contribution to capacitance will be reported.



On the left a Nanotube TMR (tunneling magneto-resistence junction) and on the right a nanotube-metal interface.

Coffee and desserts are served after the seminar at 15:00 in the lounge, Burnside Hall 1024