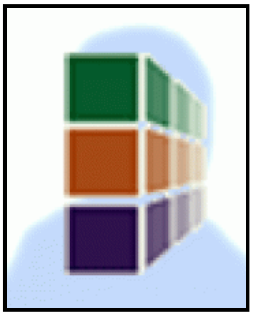

Special Guest Lectures

On the Role of Defects and Single Molecules Embedded in Low Dimensional Systems: a Computational Nanoscience Study

Vincent Meunier, Oak Ridge National Laboratory

Nicholson Hall 435
April 21, 2008 - 03:40 pm

Abstract:
Nanoscale electronic structures have been extensively investigated as a new frontier beyond traditional material science. At the same time as the relevant size of practical systems is shrinking, there is a tremendous expansion of the available computational resources, in terms of scalability and speed. The consequence is that we are now rapidly approaching the point where the typical length scales of systems available experimentally are becoming comparable to the ones that can be treated accurately on state-of-the-art large-scale computers. As a result, combining theoretical and experimental research is expected to yield more accurate understanding of fundamental mechanisms at the atomic level. In this talk, I will present two recent examples where large-scale calculations have been used to understand and predict novel phenomena at the molecular and nano-scales. In the first illustration, I will show how a combination of scanning tunneling microscopy measurements and large-scale density functional theory calculations can be used to elucidate the fundamental role and formation process of defects on TiO2 (110) surface. In the second part of the talk, I will show how it is possible to couple large-scale quantum electronic structure calculations with non-equilibrium Green function formulation of electronic transport to design new paradigms for nano devices. In particular, I will present recent findings on a nano-switch based on the encapsulation of a donor/acceptor molecule within a carbon nanotube. The switching behavior is analyzed in detail and a novel model for nanoscale non-volatile memory element is presented.

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