

SES07-2007-000085

Abstract for an Invited Paper
for the SES07 Meeting of
the American Physical Society

A computational study of the role of defects and single molecules on transport properties in low dimensional systems

VINCENT MEUNIER, ORNL

Nanoscale electronic devices have been extensively investigated as a new frontier beyond conventional microelectronics. At the same time as the typical size of practical devices is shrinking, there is a tremendous expansion of the available computational resources, in terms of scalability and speed. The result is that we are now rapidly approaching the point where the typical length scales of systems available experimentally are becoming similar to the ones that can be treated accurately on state-of-the-art computers. 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 nanoscale. 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 TiO_2 (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 for determining the quantum conductance of a number of molecular systems. The switching behavior in systems based on individual molecules embedded in a conducting nanotube is analyzed in detail and a novel paradigm for nanoscale non-volatile memory element is presented.