Using large-scale computing for the simulation and prediction of novel phenomena at the nanoscale

Vincent Meunier

Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN USA

Abstract. Nanoscale electronic devices have been extensively investigated as a new frontier beyond conventional microelectronics. In this regime, the size scaling that has effectively taken device features from the microscopic scale to the nanoscale is no longer valid. New alternative materials and device structures are required and the need for highly accurate and large scale (in terms of approaching the actual number of actives sites in a working device) modeling and computational tools has become acute. 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 net effect is that we are now rapidly approaching the point where the typical length scales of systems studied in the lab and the ones that can be modeled on state-of-the-art computers are finally meeting. While the molecular-electronics revolution calls for new computational models that account for fundamental physical interactions that take place at the quantum mechanical level, the confluence of the experimental and simulation worlds is largely due to the development of new computational infrastructures, which enable simulations at unprecedented scale.

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 [1], 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. The effect of the presence of the defect on chemical reactions on the surface will also be demonstrated. 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, thereby allowing for a detailed understanding of the processes governing exotic behavior in molecular-based nanodevices. In particular, the switching behavior in systems based on individual molecules embedded in a conducting nanotube will be analyzed in detail and a novel paradigm for nanoscale non-volatile memory device will be proposed [2].

REFERENCES

1. K. Park, M. H. Pan, V. Meunier, and E.W. Plummer, *Phys. Rev. Lett.* **96**, 226105 (2006).
2. V. Meunier, S. K. Kalinin, B.G. Sumpter, *Phys. Rev. Lett.* **98**, 056401 (2007).