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Nicholas Metropolis Award for Outstanding Doctoral Thesis Work in Computational Physics Talk: Understanding Nano-scale Electronic Systems via Large-scale Computation

CHAO CAO, University of Florida

Nano-scale physical phenomena and processes, especially those in electronics, have drawn great attention in the past decade. Experiments have shown that electronic and transport properties of functionalized carbon nanotubes are sensitive to adsorption of gas molecules such as H2, NO2, and NH3. Similar measurements have also been performed to study adsorption of proteins on other semiconductor nano-wires. These experiments suggest that nano-scale systems can be useful for making future chemical and biological sensors. Aiming to understand the physical mechanisms underlying and governing property changes at nano-scale, we start off by investigating, via first-principles method, the electronic structure of Pd-CNT before and after hydrogen adsorption, and continue with coherent electronic transport using non-equilibrium Greens function techniques combined with density functional theory. Once our results are fully analyzed they can be used to interpret and understand experimental data, with a few difficult issues to be addressed. Finally, we discuss a newly developed multi-scale computing architecture, OPAL, that coordinates simultaneous execution of multiple codes. Inspired by the capabilities of this computing framework, we present a scenario of future modeling and simulation of multi-scale, multi-physical processes.