

UNIVERSITY OF TEXAS AT DALLAS - DEPARTMENT OF PHYSICS
PHYSICS COLLOQUIUM

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Wednesday, June 7, 2006; 11:00 AM - 12:00 PM
Founders North 2.104

**Multiscale Modeling of Nanowire-Molecule
Interactions**

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At nanometer scale, materials behave differently from their bulk properties. Material properties become a function of their size and shape at 1-100 nm scale due to strong quantum mechanical effects and surface effects. For practical applications of nanomaterials, it is desirable to identify their functional properties based on the *structure-property relationship* before fabricating them. However, such relationship is not intuitively simple so that it is not easy to identify the target material structures (e.g., size, shape, and composition) corresponding to the target functional properties. Computational modeling of the atomic and electronic structures of nanomaterials can provide a rational understanding of nanomaterials' structure-property relationship, and a *rational design* method can be used to guide the experimental development process. In this talk, I will apply multiscale modeling methods (atomistic and quantum simulations) to study the structure-property relationship of nanoscale wires (carbon nanotubes and silicon nanowires) and their interaction with molecular species. The nanowire-molecule interaction is the key process in sensor application of nanowires and developing a nanomaterial for hydrogen storage applications. In both applications, the key question is how molecules interact with nanowire surface and modify the physical properties of nanowires. We will discuss the reactivity and sensing mechanisms of carbon nanotubes sensors and how one can apply modeling method to design improved sensors. The surface reactivity of carbon nanotubes also provides a critical insight on the controversial problem of hydrogen storage capacity of carbon nanotubes. We have systematically investigated the hydrogen-nanotube interaction to elucidate the source of diverse experimental data based on rational understanding of nanotube-molecule interactions. We will discuss broader implications of the nanowire-molecule interaction study in developing novel device systems and nanomaterials for clean energy technology.