

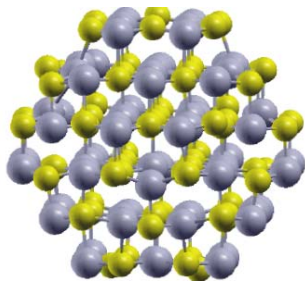
THE GEORGE WASHINGTON UNIVERSITY
Department of Physics
Summer Colloquium

DYNAMICS ON THE NANOSCALE:

Time-domain ab initio studies of quantum dots and molecule-semiconductor interfaces.

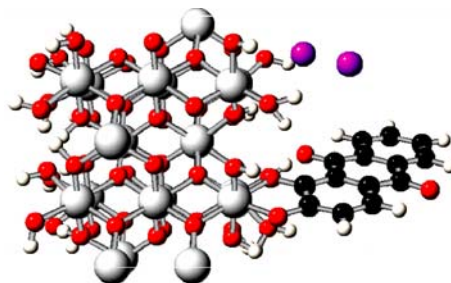
Prof. Oleg Prezhdo,
University of Washington, Seattle

Design of novel materials for energy harvesting and storage requires an understanding of the dynamical response of the materials on the nanometer scale. A great deal of experimental and theoretical work has been devoted to characterizing the excitation, charge, spin, and vibrational dynamics in quantum dots, conducting polymers, carbon nanotubes, inorganic semiconductors and molecular chromophores. We have developed state-of-the-art non-adiabatic molecular dynamics techniques and implemented them within time-dependent density functional theory in order to model the ultrafast processes in these materials at the atomistic level and in real time.



The colloquium will focus on quantum dots and chromophore-semiconductor interfaces that form the basis of new generations of solar cells. Quantum dots (QD) are quasi-zero dimensional structures with a unique combination of molecular and bulk properties. As a result, QDs exhibit new physical phenomena such as the electron-phonon relaxation bottleneck and efficient carrier multiplication, which have the potential to greatly increase the efficiency of solar cells.

Photo-induced charge separation across molecular/bulk interfaces drives the dye-sensitized semiconductor solar cell. A subject of active research, it creates many challenges due to the stark differences between the quantum states of molecular and periodic systems, as well as the different sets of theories and experimental tools used by physicists and chemists.



Our time-domain atomistic simulations create a detailed picture of these materials. By comparing and contrasting their properties, we provide a unifying description of quantum dynamics on the nanometer scale, resolve several highly debated issues, and generate theoretical guidelines for development of novel systems for energy harvesting and storage.

TIME: 11:00-12:00 am, Monday, June 22, 2009

PLACE: 104 Corcoran Hall, GWU

725 21st Street, N.W. (Between G and H Streets)

METRO STATION: GWU/FOGGY BOTTOM (BLUE & ORANGE LINES)