Quantum dots (QD) are quasi-zero dimensional structures with a unique combination of solid-state and atom-like properties. Unlike either bulk or atomic materials, QD properties can be modified continuously by changing QD shape and size. Often, the bulk and atomic viewpoints contradict each other, leading to differing predictions about the behavior of QDs. For example, the atomic view suggests strong electron-hole and charge-phonon interactions, as well as slow energy relaxation due to mismatch between electronic energy gaps and phonon frequencies. In contrast, the bulk view advocates that the kinetic energy of quantum confinement is greater than electron-hole interactions, that charge-phonon coupling is weak, and that the relaxation through quasi-continuous bands is rapid.

QDs exhibit new physical phenomena. In particular, the so-called phonon bottleneck to the electron and hole energy relaxation and generation of multiple excitons upon absorption of a single photon can be used to improve efficiencies of photovoltaic devices. Slowing down of the energy relaxation can result in extraction of hot electrons and holes, thereby increasing the solar cell voltage. Generation of multiple electron-hole pairs can increase the current.

Our state-of-the-art non-adiabatic molecular dynamics techniques, implemented within time-dependent density functional theory, allow us to model the response of QDs at the atomistic level and in real time. The studies provide a unifying description of quantum dynamics in nanoscale materials, resolve the debated issues, and generate theoretical guidelines for development of novel systems for solar energy harvesting and other applications.

1. C. F. Craig, W. R. Duncan, O. V. Prezhdo “Trajectory surface hopping in the time-dependent Kohn-Sham theory for electron-nuclear dynamics”, *Phys. Rev. Lett.*, **95** 163001 (2005).
2. O. V. Prezhdo “Photoinduced dynamics in semiconductor quantum-dots: insights from time-domain ab initio studies”, *Acc. Chem. Res.*, 42, 2005 (2009).
3. S. A. Fischer, C. M. Isborn, O. V. Prezhdo, “Excited states and optical absorption of small semiconducting clusters: dopants, defects and charging”, *Chem. Science,* **2**, 400 (2011).
4. Kim H.-D., O. V. Prezhdo, “Time-domain ab initio study of Auger and phonon-assisted Auger processes in a semiconductor quantum dot”, *Nano Lett.*, **11**, 1845 (2011).