Time-domain ab initio studies of molecule and quantum dot sensitized TiO2

Oleg Prezhdo University of Rochester, USA

Solar energy applications require understanding of dynamical response of novel materials on nanometer scale. Our state-of-the-art non-adiabatic molecular dynamics techniques, implemented within time-dependent density functional theory, allow us to model such response at the atomistic level and in real time. The talk will focus on photoinitiated charge transfer at the interfaces of bulk TiO2 with organic molecules, water and semiconductor quantum dots (QDs). Photoinduced charge separation across molecular/bulk interfaces drives dye-sensitized semiconductor solar cells. It creates many challenges due to stark differences between molecular and periodic systems. QDs are quasi-zero dimensional structures with a unique combination of molecular and bulk properties. They exhibit new physical phenomena, including phonon bottleneck and multiple exciton generation, with the potential to increase solar cell efficiency. Our simulations provide a unifying description of quantum dynamics on nanoscale, resolve highly debated issues, and generate theoretical guidelines for development of novel systems for energy harvesting and storage.