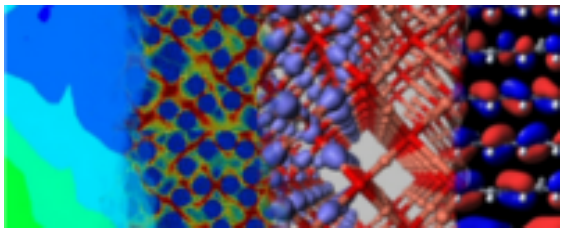

Contribution ID: **9** Type: **Talk**

Modeling Dye-Sensitized Solar Cells from First Principles: Understanding the mechanism, improving the efficiency

Friday, November 9, 2012 2:00 PM (45 minutes)

We present computer simulations on the fundamental constituents of Dye-sensitized solar cells (DSCs) and their interactions at the respective molecular/solid/liquid interfaces. Predictive dye design and modeling of realistic semiconductor (TiO2, ZnO) nanostructures enables us to investigate the structural, electronic and optical properties of dyes adsorbed onto semiconductor surfaces by means of DFT and TDDFT calculations. Thus, the alignment of ground and excited state energy levels for the interacting DSC constituents is presented and discussed in relation to experimental photovoltaic performances. Modeling of the combined dye / semiconductor / electrolyte heterointerfaces is then achieved by performing ab initio molecular dynamics simulations of semiconductor adsorbed dyes in the solution and electrolyte environments. In particular, we present the case of Ru(II)-dyes on TiO2 and their interaction with a Cobalt-based electrolytes. The nature and localization of the electronic states at the dye/semiconductor/electrolyte interface is discussed in relation to the device efficiency parameters. The mechanistic details of dye regeneration and the recombination pathways with the oxidized dye and with TiO2-injected electrons are presented. A multiscale approach to the simulation of the mesoporous TiO2 film based on a first-principle description of the individual and aggregated nanocrystals is finally presented.

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Session Classification: Session: Energy conversion: photovoltaics, dye-sensitized cells (Click for details or select 'Detailed view')

Track Classification: Energy conversion: photovoltaics, dye-sensitized cells