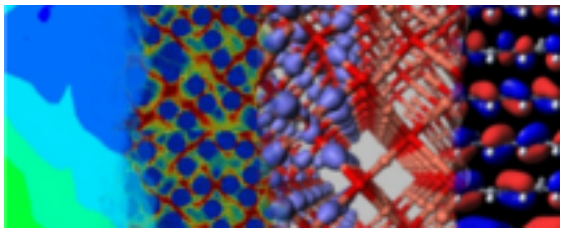

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Modeling of lateral hole diffusion on dye sensitized metal oxide monolayer.

Friday, November 9, 2012 3:10 PM (25 minutes)

In Dye Sensitized Solar Cells (DSSC), photocurrent generation results from electron injection into a nanocrystalline oxide electrode from a photo-oxidized dye molecule adsorbed on to the oxide surface while the dye is normally regenerated by a Hole Transporting Medium (HTM). In an alternative mechanism, the dye may be regenerated through the lateral transport of holes between dye molecules on the oxide surface. Such lateral transport may have application in solid state devices by providing an additional pathway for the holes to reach the solid HTM, especially when the HTM is in poor contact with the dye molecules. Although there is experimental evidence for this 'hole hopping'mechanism, the factors controlling it are not yet understood in detail. In this work we introduce a multi-scale method to model hole diffusion dynamics through a monolayer of dye molecules anchored to a nanocrystalline film. We treat the intermolecular charge transfer step as a non-adiabatic hopping process and calculate the hopping rate as a function of the electronic coupling (J) and the reorganization energy (λ). First we propose a numerical method based on quantum chemical calculations to calculate the inner- and outer-sphere reorganization energies and show that the nature of the surrounding medium dominates λ, consistent with the high values of λ observed experimentally (λ ~ 1 V). Next, we again use quantum chemical methods to study the influence of the dyes arrangement at the nanoscale on J. Finally we incorporate these parameters into a continuous time random walk (CTRW) to estimate the hole diffusion coefficient at the scale of the dyes monolayer. We randomize the waiting times distribution to treat the configurational disorder. We show how this procedure leads to anomalous diffusion of holes. The results show reasonable agreement with experimental measurements on a range of dye sensitized films. Our method provides a deeper insight on how to control the lateral hole transport between dye molecules and is expected to assist in the design of higher performance devices.

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