

# Imaging the ultrafast photoelectron transfer process in alizarin-TiO<sub>2</sub>

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In this work, we adopt a quantum mechanical approach based on time-dependent density functional theory (TDDFT) to study the optical and electronic properties of alizarin supported on TiO<sub>2</sub> nano-crystallites, as a prototypical dye-sensitized solar cell. To ensure proper alignment of the donor (alizarin) and acceptor (TiO<sub>2</sub> nano-crystallite) levels, static optical excitation spectra are simulated using time-dependent density functional theory in response. The ultrafast photoelectron transfer from the dye to the cluster is simulated using an explicitly time-dependent, one-electron TDDFT ansatz. The model considers the  $\delta$ -pulse excitation of a single active electron localized in the dye to the complete set of energetically accessible, delocalized molecular orbitals of the dye/nano-crystallite complex. A set of quantum mechanical tools derived from the transition electronic flux density is introduced to visualize and analyze the process in real time. The evolution of the created wave packet subject to absorbing boundary conditions at the borders of the cluster reveal that, while the electrons of the aromatic rings of alizarin are heavily involved in an ultrafast charge redistribution between the carbonyl groups of the dye molecule, they do not contribute positively to the electron injection and, overall, they delay the process. © 2015 by the authors.

Dye-sensitized solar cell

Electronic flux density

Optical spectra

alizarin

anthraquinone derivative

titanium

titanium dioxide

chemical structure

chemistry

conformation

electron

photochemistry

spectroscopy

thermodynamics

three dimensional imaging

Anthraquinones

Electrons

Imaging, Three-Dimensional

Models, Molecular

Molecular Conformation

Photochemical Processes

Spectrum Analysis

Thermodynamics

Titanium