Calculated Surface Electron Transfer Mechanisms in Dye-Sensitized Semiconductor Nanocrystals

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Quantum-chemical calculations have been used to study electronic properties of aromatic dye molecules anchored on semiconductor nanoparticles. This provides a theoretical perspective on the nature of surface electron transfer processes important in photoelectrochemical devices such as dye-sensitized solar cells (1, 2).

Recent advances of the modeling of nanostructured semiconductors, in particular TiO_2, enable systematic studies of the electronic structure and electron transfer mechanisms at accurate levels of theory. This includes calculations at the configuration interaction and density functional levels of theory.

As a significant breakthrough, direct comparisons between experiment and calculations have recently been used to probe ultrafast surface electron transfer processes on the few-femtosecond time-scale (3).

Here, new results will be presented on density functional calculations of aromatic adsorbates such as catechol anchored on cluster models of TiO_2 nanoctrystals.

References:

1. Quantum Chemical Study of Photoinjection Processes in Sensitized TiO2 Nanoparticles
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2. Electronic interactions at aromatic-metal oxide interfaces calculated from first principles
P. Persson, S. Lunell, and L. Ojamäe
Chem. Phys. Lett. 364, 469 (2002)

3. Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor
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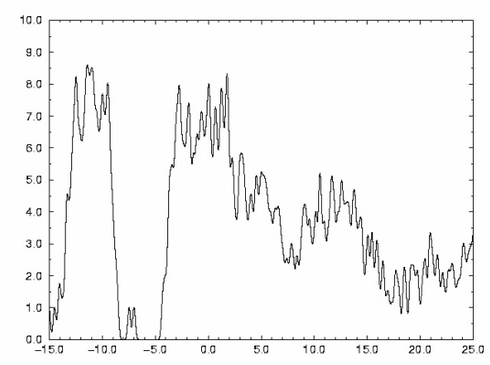

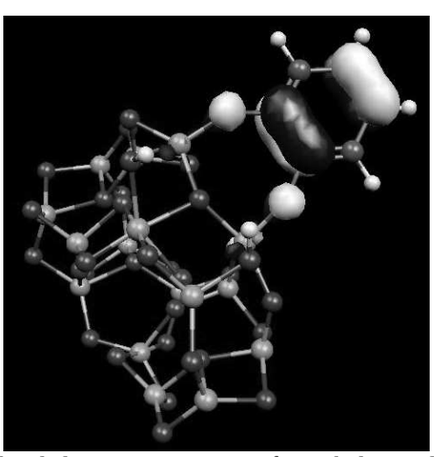

Calculated electronic properties of catechol on a cluster model of nanocrystalline TiO2. Calculated Density Of States (top) and HOMO molecular orbital from density functional calculations.