Simulation of Electron Transfer Processes at Molecule-Metal and Molecule-Semiconductor Interfaces

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Heterogeneous electron transfer (ET) in molecular systems at semiconductor or metal surfaces is a key step in many processes relevant to Chemistry, Physics and Material Science. Important applications where this process plays a fundamental role include photonic energy conversion in nanocrystalline dye-sensitized solar cells, in which photoexcitation triggers the injection of an electron from an excited electronic state of a dye molecule into the conduction band of a semiconductor, and charge transport in nanoscale molecular junctions. Recently, we have developed an approach to study the dynamics of ET in molecule-metal and molecule-semiconductor systems that combines a first-principles characterization of the systems with an accurate quantum treatment of the dynamics.[1,2] In this contribution, we present the results obtained in the simulation of ET processes in perylene-titanium dioxide dye-semiconductor systems[2] and self-assembled monolayers of nitrile-substituted alkanethiolate molecules adsorbed at metal surfaces.[3,4] In particular, we investigate the roles that the symmetry of the donor state and the molecular structure of the spacer groups have in the dynamics of the charge transfer process.

References

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