DFT description of heterogeneous electron transfer

Recent progress in the use of quantum-chemical calculations to obtain information about heterogeneous electron transfer processes in dye-sensitized semiconductor nanoparticles will be discussed. The emphasis of the talk is on explicit calculations of experimentally important systems using accurate computational methods, such as DFT. In particular, calculations of structural and electronic properties of several organic sensitizers, such as perylenes, anchored to TiO2 surfaces or nanoparticles will be presented. It is argued that such calculations provide a basis for a detailed understanding of interfacial electronic properties, such as the strength of the dye-semiconductor electronic coupling, or the ability of different anchor and spacer groups to act as barriers to, or mediators of, interfacial charge-transfer.