Interaction of YD2 and TiO<inf>2</inf> in dye-sensitized solar cells (DSSCs): a density functional theory study

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 The interaction of the dye YD2 with a cluster of (anatase-phase) TiO<inf>2</inf> (which is utilized in dye-sensitized solar cells, DSSCs) and electron injection by the dye into the cluster were studied by performing density functional theory (DFT) calculations at the B3LYP, PBE, and TPSS levels of theory, including dispersion effects. We studied and quantified the interaction of the metallomacrocycle with the TiO<inf>2</inf> cluster and the electronic spectrum of the complex. TDDFT calculations using the B3LYP functional were found to be the most suitable for describing the observed absorption energy bands of YD2 and YD2?TiO<inf>2</inf>. Our calculations show that the diarylamino groups act as electron donors in the photon-induced injection that occurs in DSSCs. The free-energy changes that take place during electron injection support the good performance of YD2 on TiO<inf>2</inf> clusters. [Figure not available: see fulltext.]