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Molecular modelling of charge transfers in hybrid organic-inorganic photovoltaic devices

We report results of computational studies investigating the electron transfer between the dye and the TiO2 nanocluster as well as between the electrolyte and the dye, to understand the mechanisms that influence the performance of dye-sensitized solar cells. By means of density functional theory calculations, we determine the parameters of Marcus'theory for charge transfer from a cobalt-based electrolyte to a sensitizing dye with a triphenylamine donor group. We also study TiO2 nanoclusters of various sizes as well as of complex systems with various molecules adsorbed onto these clusters, with the goal to understand charge transfer processes relevant not only for hybrid organic–inorganic photovoltaics but also for the photocatalytic degradation of pollutants. We find acceptable minimal sizes of the (TiO2)n (n = 14, 24, 34, 44, 54) nanoclusters, to model systems and interface processes that occur in hybrid photovoltaics. We illustrate various adsorption cases with a small rigid molecule based on coumarin, a larger rigid oligomethine cyanine dye with indol groups. We argue that cluster sizes with n ≥ 34 are necessary to provide the reliability expected from the calculations but recognize that the use of much larger clusters may bring little improvement at a significantly higher computational cost.

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