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Quantum dynamics simulations of interfacial charge-transfer in organic dye-sensitized solar cells¹ LUIS G.C. REGO, Department of Physics, Universidade Federal de Santa Catarina, R. DA SILVA, Department of Chemistry, Universidade Federal de Santa Catarina, D.A. HOFF, Department of Physics, Universidade Federal de Santa Catarina — We describe a novel time-dependent quantum-mechanics/molecular-mechanics method for studying electron transfer in dye sensitized semiconductor interfaces, that takes into account the interacting electron-hole quantum dynamics, the underlying nuclear fluctuations and solvation dynamics. We provide a comprehensive investigation of the quantum dynamics, the electronic and the structural properties of prototypical D- π -A organic dyes sensitizing the TiO₂ anatase surface, both in vacuum and solvated by liquid acetonitrile. The organic dyes are comprised of an electron donating moiety and an anchoring acceptor moiety, conjugated by thiophene bridges. Although interfacial electron transfer is very efficient, it is demonstrated that the coupling between the photoexcited electron and the hole delays the electron injection. Simulations demonstrate that the solvent screens the dye from the surface, narrowing the absorption peaks and delaying the electron injection. We have also studied several aspects that are relevant for the recombination process, such as the role played by surface defects and the interaction of redox species with the TiO₂ surface, and the effect of additives.

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