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Quantum dynamics simulations of interfacial electron transfer in sensitized TiO_2 semiconductors SABAS G. ABUABARA, Department of Chemistry, Yale University, P.O.Box 208107, New Haven, 06520-8107, U.S.A., LUIS G. C. REGO, Department of Physics, Universidade Federal de Santa Catarina, Florianopolis, SC 88040-900, Brazil, VICTOR S. BATISTA, Department of Chemistry, Yale University, P.O.Box 208107, New Haven, 06520-8107, U.S.A. — A mixed quantum-classical method combining *ab initio*-DFT molecular dynamics simulations with electronic relaxation calculations is used to investigate interfacial electron transfer in catechol/TiO_2-anatase nanostructures under vacuum conditions at finite temperature. The calculations demonstrate that the injection mechanism is accelerated by thermal nuclear motion. In particular, electron-phonon scattering leads to ultrafast adsorbate monolayer electron transfer and the disappearance of the anisotropic charge delocalization (*i.e.*, carrier diffusion) identified in frozen lattice studies, due to increased coupling between quasistationary molecular orbitals localized on the adsorbates and those orbitals delocalized throughout the semiconductor bulk. The results are particularly relevant to the understanding of surface charge separation in efficient mechanisms of molecular-based photovoltaic devices.

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