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Interficial Electron Transfer from a PbSe Quqantum Dot into the TiO_2 Surface[1] RUN LONG, Department of Chemistry, University of Rochester, NY 14627 USA; School of Chemical & Bioprocess Engineering, University College Dublin, Ireland, OLEG PREZHDO, Department of Chemistry, University of Rochester, NY 14627 — We reporte an *ab initio* nonadibatic molecular dynamics (NAMD) simulation of ultrafast photoinduced electron transfer (ET) from a PbSe quantum dot (QD) into the rutile TiO_2(110) surface. The simulation supports the obervation that the ET successfully competes with energy losses due to electron-phonon relaxation. The ET proceeds by the adibatic mechanism due to strong donor-acceptor coupling. High frequency polar vibrations of both QD and TiO_2 promotes the ET, since these modes can rapidly influence the donor-acceptor state energies and coupling. Low frequency vibrations generate a distribution of initial conditions for ET, which shows a broad variety of scenarios at the single-molecule level. The system exhibits diverse scenarios for individual electron injection events, involving a complex interplay of ET mechanims, time scales, and phonon dynamics.

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