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Ab Initio Nonadiabatic Molecular Dynamics of Wet-Electrons on the TiO_2 Surface[1] SEAN FISCHER, University of Washington, WALTER DUNCAN, Schrodinger Inc., OLEG PREZHDO, University of Washington — The electron transfer (ET) dynamics of wet-electrons on a TiO_2 surface was investigated using state-of-the-art ab initio nonadiabatic molecular dynamics, which includes electronic evolution, phonon motions, and electron-phonon coupling. Delocalized over both water and TiO_2, wet-electrons are supported by a new type of state that is created at the interface due to the strong water-TiO_2 interaction and that cannot exist separately in either material. Our simulations indicate that the ET is sub-10 fs and driven mainly by low frequency vibrational modes. The high density of TiO_2 conduction band states leads to frequent crossings of the strongly coupled donor and acceptor states, which is conducive to fast ET. The average ET dynamics for the system feature essentially equal contributions from both adiabatic and nonadiabatic transfer mechanisms. Similar states are present in a number of other systems with strong interfacial coupling, including certain dye-sensitized semiconductors. The wet-electron state may also have relevance to the electrochemical photolysis of water.

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