

A Combined Molecular Dynamics and Computational Spectroscopy Study of a Dye Sensitized Solar Cell

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An organic dye sensitized solar cell consisting of a squaraine molecule attached to a TiO₂ surface is modeled using first principles molecular dynamics and time-dependent density functional theory. The system is surrounded by solvent molecules which are treated at the same level of theory as the dye molecule and the surface. The effect of the solvent on the optical properties is investigated by computing many absorption spectra for various configurations along a molecular dynamics trajectory. It is shown that the dynamical effects induced by thermal fluctuations have a strong effect on the optical properties, and that a satisfactory agreement with experiments is only achieved if those thermal effects are accounted for explicitly.