

Abstract Submitted
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First-principles calculation of photo-induced electron transfer rate constants in phthalocyanine-C₆₀ organic photovoltaic materials: Beyond Marcus theory¹ MYEONG H. LEE, University of Michigan, Kent State University, BARRY D. DUNIETZ, Kent State University, EITAN GEVA, University of Michigan — Classical Marcus theory is commonly adopted in solvent-mediated charge transfer (CT) process to obtain the CT rate constant, but it can become questionable when the intramolecular vibrational modes dominate the CT process as in OPV devices because Marcus theory treats these modes classically and therefore nuclear tunneling is not accounted for. We present a computational scheme to obtain the electron transfer rate constant beyond classical Marcus theory. Within this approach, the nuclear vibrational modes are treated quantum-mechanically and a short-time approximation is avoided. Ab initio calculations are used to obtain the basic parameters needed for calculating the electron transfer rate constant. We apply our methodology to phthalocyanine(H₂PC)-C₆₀ organic photovoltaic system where one C₆₀ acceptor and one or two H₂PC donors are included to model the donor-acceptor interface configuration. We obtain the electron transfer and recombination rate constants for all accessible charge transfer (CT) states, from which the CT exciton dynamics is determined by employing a master equation. The role of higher lying excited states in CT exciton dynamics is discussed.

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