Abstract Submitted
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A computational study of photo-induced electron transfer rate constants in subphthalocyanine/C_{60} organic photovoltaic materials via Fermi's golden rule[1] MYEONG H. LEE, University of Michigan, Kent State University, BARRY D. DUNIETZ, Kent State University, EITAN GEVA, University of Michigan — We present a methodology to obtain the photo-induced electron transfer rate constant in organic photovoltaic (OPV) materials within the framework of Fermi's golden rule, using inputs obtained from first-principles electronic structure calculation. Within this approach, the nuclear vibrational modes are treated quantum-mechanically and a short-time approximation is avoided in contrast to the classical Marcus theory where these modes are treated classically within the high-temperature and short-time limits. We demonstrate our methodology on boron-subphthalocyanine-chloride/C_{60} OPV system to determine the rate constants of electron transfer and electron recombination processes upon photo-excitation. We consider two representative donor/acceptor interface configurations to investigate the effect of interface configuration on the charge transfer characteristics of OPV materials. In addition, we determine the time scale of excited states population by employing a master equation after obtaining the rate constants for all accessible electronic transitions.

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