

Abstract Submitted
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DFT calculation of photo-induced charge transfer in organic molecule MARK PEDERSON, Naval Research Laboratory, TUNNA BARUAH, University of Texas at El Paso — We propose a method for obtaining the charge transfer time for a chromophore-donor-acceptor system from density functional theory. Our calculations are done on a porphyrin-carotene-C₆₀ molecular triad. The geometry of the large molecular triad was optimized at the all-electron level using GGA. We are considering single electron excitations, the energies of which are obtained using a newly developed approach. The electronic dipolar transition probabilities are calculated from Einstein's A and B coefficients. However, in real systems the polarization effects play an important role in the transfer process since the charge separated states can possess huge dipole moments. The stabilization of the large dipole state can be calculated from the classical dipole-dipole interaction and the polarizability of the surrounding medium. The stabilization of the dipole states is an important aspect which dominates the charge transfer process and therefore the rise time. The efficiency of the molecule as a solar energy converter will also be discussed.

Tunna Baruah
University of Texas at El Paso

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