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Photoinduced Charge Transfer Process LUIS BASURTO, Department of Computational Science, University of Texas at El Paso, TUNNA BARUAH, RAJENDRA ZOPE, JOSE RODRIGUEZ, Department of Physics, University of Texas at El Paso — The photoinduced charge transfer process is the fundamental process in a photovoltaic system. Organic photovoltaics contain a donor-acceptor molecular system which undergoes photoinduced charge transfer leading to a large dipole moment. Often the charge transfer properties of such donor-acceptor systems are measured in solution. The dipole moments on the solvent molecules creates a reaction field. To simulate this reaction field we adopt an approach similar to the explicit solvent model proposed by Washel and co-workers. We use Monte Carlo simulations to determine various possible solvent structures. We use a carotenoid-porphyrin-C60 molecular triad as the light-harvesting system. This molecular triad has a very large dipole moment (153 Debye) in the charge separated state. The resulting solvent structures and the reaction field as a function of temperature will be presented.

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