

Abstract Submitted
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Understanding the Dielectric Response of Polar Organic Solvent in an Artificial Photosynthetic System FRANCIS DE DIOS, University of Texas — The artificial photosynthetic analogue of interest is the triad molecule composed of an organic material in fullerene (C60), and two naturally occurring compounds: porphyrin and carotene. The components of the triad are abundant in nature and the cost of its synthesis is very small relative to the expense of fabrication of inorganic solar cells. Combining the economic advantages of the triad with its ability to mimic the natural photosynthetic process, the triad promises to be a feasible basis for highly cost-effective solar energy conversion. The present work focused on the behavior of solvent molecules in the presence of both a ground state and excited state triad molecule. The solvent significantly influences the structural fluctuations of the triad and increases the lifetime of the photo-induced charge-separated state of the triad by providing an electrostatic-screening effect. The two types of organic solvents that were investigated were Tetrahydrofuran (THF), which is a polar molecule, and Toluene, which is non-polar. Reduced radial shells of the solvent were taken to observe significant large-scale variations in the dielectric constant. The results from the dielectric constant evaluation suggest a much stronger interaction between the THF solvent and the triad compared to the interaction between Toluene and the triad due to the significantly larger dipole moment of THF relative to that of Toluene. Furthermore, the interaction is very large between THF and the charge-separated excited state of the triad, meaning that the magnitude of interaction between the solvent and the triad is largely dependent on the electronic state of the triad and the dipole strength of the solvent molecules. The spatial correlations between selected solvent molecules were also analyzed to gain further insight on the solvent fluctuations.

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