

Abstract Submitted
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Understanding the influence of solvent field and fluctuations on the stability of photo-induced charge-separated state in molecular triad¹

D. BALAMURUGAN, University of Houston, ADELIA AQUINO, HANS LISCHKA, Texas Tech University, FRANCIS DIOS, LIONEL FLORES, MARGARET CHEUNG, University of Houston — Molecular triad composed of fullerene, porphyrin, and carotene is an artificial analogue of natural photosynthetic system and is considered for applications in solar energy conversion because of its ability to produce long-lived photo-induced charge separated state. The goal of the present multiscale simulation is to understand how the stability of photo-induced charge-separated state in molecular triad is influenced by a polar organic solvent, namely tetrahydrofuran (THF). The multiscale approach is based on combined quantum, classical molecular dynamics, and statistical physics calculations. The quantum chemical calculations were performed on the triad using the second order algebraic diagrammatic perturbation and time-dependent density functional theory. Molecular dynamics simulations were performed on triad in a box of THF solvent with the replica exchange method. The two methods on different length and time scales are bridged through an important sampling technique. We have analyzed the free energy landscape, structural fluctuations, and the long-range electrostatic interactions between triad and solvent molecules. The results suggest that the polarity and re-organization of the solvent is critical in stabilization of charge-separated state in triad.

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