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Density functional study on a light-harvesting carotenoid-porphyrin-C_{60} molecular triad in explicit solvent CARLOS DIAZ, TUNNA BARUAH, RAJENDRA ZOPE, University of Texas at El Paso — We investigate the effect of solvent on the electronic structure of a biomimetic molecular triad that shows photoinduced charge transfer in laboratory. The supramolecular triad contains three different units - C60, porphyrin, and beta-carotenoid. We have performed classical molecular dynamics simulation of the triad surrounded by 15000 water molecules using NAMD for 20 nanoseconds. Subsequently, we performed an all-electron density functional calculations (DFT) using large basis sets on the 50 snap-shots taken from the molecular dynamics simulation. The solvent effects in the DFT calculations are treated using both the explicit water molecules as well as using the point charge representation of water. The excitation energies and absorption spectra show that the polar solvent induces significant changes in the electronic structure of the triad.

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