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Electronic structure of electron donor-acceptor complexes in solution[1] CARLOS DIAZ, SUHUA ZHU, University of Texas at El Paso, TUNNA BARUAH, tbaruah@utep.edu, RAJENDRA ZOPE, University of Texas at El Paso
— We investigate the effect of solvent on the electronic structure of donor-acceptor complexes relevant in light harvesting. The model complexes we are studying are a porphyrin-fullerene dyad, a carotene-porphyrin-fullerene triad, a multichromophoric hexad molecule that consists of BDPY, Zn-tetraphenyl porphyrin, bis-phenyl anthracene, and fullerene. We first performed classical molecular dynamics simulation of the systems in explicit solvent. Subsequently, all-electron density functional calculations (DFT) using large basis sets is performed on the snap-shots taken from the molecular dynamics simulations. The solvents effects in the DFT calculations are treated using the explicit solvent or using their point charge representation. The effect of the solvents on the electronic properties will be discussed.

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