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DFT study of a carotenoid-porphyrin-C_{60} light-harvesting molecular triad[1]

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The abundance of solar energy reaching the earth presents an attractive alternative energy source. Nearly 75% of the solar energy striking the upper atmosphere reaches the earth in the form of photons of energies typically higher than 1 eV. Biological light-harvesting systems are highly efficient in utilizing the solar radiation. Bio-mimetic molecules are investigated to mimic the photosynthesis process efficiently in laboratory. We present a computational study of the process in a bio-mimetic carotenoid-porphyrin-C_{60} molecular triad which is about 5 nm long. The description of the photo-induced charge separation process requires accurate excited state energies and coupling between electrons and the phonons of the system. Since charge-transfer excitations create large changes in a molecular dipole moment, changes in excited-state energies due to coupling between a 5 nm molecular photovoltaic and the surroundings (solvent and spectator molecules) also has to be taken into account. A density functional theory based method including all these effects to describe the photo-induced charge separation process will be presented.

[1]ONR, UTEP, NSF