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First-Principles Simulation of a Light Harvesting Molecular Triad
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We investigate the properties of a recently synthesized light harvesting molecular triad containing a diaryl-porphyrin, carotenoid and a C_{60} fullerene which act as a chromophore, electron donor and electron acceptor respectively [P.A. Liddell et al., J. Am. Chem. Soc. **119**, 1400 (1997)]. The triad undergoes photo-induced charge separation process resulting in a large dipole moment for the excited state. Density-functional theory based NRLMOL code is used to optimize the geometry and electronic structure. We find that the molecular states are somewhat localized on a given component of the triad and that excitations can lead to a huge dipole moment of about 180 Debye. The rate constants for the interesting metastable particle-hole states are determined from the Kohn-Sham orbitals. We use the calculated rate constants and excitation energies to estimate various figures of merit related to solar cells such as energy storage and maximum power. The results show that this molecule can be useful for solar-cell technologies and possibly for information storage applications.

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