

Abstract Submitted
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DFT Studies on Charge Transfer States of a Multi-chromophoric Organic Heptad Antenna LUIS BASURTO, University of Texas at El Paso —
The electronic structure of the ground and the lowest charge transfer excited state of a molecular complex containing BODIPY dye, Zn-porphyrin, bisphenyl anthracene and fullerene are studied using density functional theory. The snowflaked shaped molecule behaves like an antenna capturing photons at different frequencies and transferring the energy to the porphyrin where electron transfer occurs from the porphyrin to the fullerene. We have calculated the energy of the lowest charge transfer state with a hole on porphyrin and an electron on the fullerene using a perturbative delta-SCF method. Our calculated values are in good agreement with the experimental charge transfer energy.

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