Endohedral fullerene as acceptor: A DFT study on charge transfer

states of Sc$_3$N@C$_{80}$-porphyrin complex

FATAMEH AMERIKHEIRABADI, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — C$_{60}$ fullerene and its derivatives are the most popular acceptors which are used in molecular/polymeric complexes used in organic photovoltaics. Endohedral fullerenes are shown to produce long lived charge separated states. The Sc$_3$N@C$_{80}$, the third most abundant fullerene after C$_{60}$ and C$_{70}$, has a larger cage with a radius of 4.1 Ang. We have carried out a DFT study on the electronic structure of ground and charge transfer states of a model Sc$_3$N@C$_{80}$-Zn tetraphenyl porphyrin cofacial complex. The C$_{80}$ cage used in our calculations has icosahedral symmetry. We find that the lowest charge transfer state with a hole on the porphyrin and an electron on the Sc$_3$N@C$_{80}$ is at 2.1 eV above the ground state. The calculations show that different orientations of the Sc$_3$N unit to the porphyrin plane do not significantly alter the electronic structure. The electronic structure of the complex and its components along with the exciton binding energies will be presented.

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