Abstract Submitted
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Endohedral fullerene as acceptor: A DFT study on charge transfer states of $Sc_3N@C_{80}$-porphyrin complex[1] 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 $Sc_3N@C_{80}$, 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 $Sc_3N@C_{80}$-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 $Sc_3N@C_{80}$ is at 2.1 eV above the ground state. The calculations show that different orientations of the Sc_3N 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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