Abstract Submitted for the TSS13 Meeting of The American Physical Society

Endohedral fullerene as acceptor: A DFT study on charge transfer states of Sc3N@C80-porphyrin complex¹ FATEMEH AMERIKHEIRABADI, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, The university of Texas at El Paso — C60 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 Sc3N@C80, the third most abundant fullerene after C60 and C70, 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 Sc3N@C80-Zn tetraphenyl porphyrin cofacial complex. The C80 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 $Sc_3N@C80$ is at 2.1 eV above the ground state. The calculations show that different orientations of the Sc3N 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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