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Electronic structure and charge transfer excited states of a $Sc_3N@C_{80}$-tetraphenyl porphyrin molecular conjugate FATEMEH AMERIKHEIRABADI, TUNNA BARUAH, RAJENDRA ZOPE, University of Texas at El Paso — Organic donor-acceptor molecular conjugates are often used as the basic component in organic solar cells. The photoexcited donor molecule donates one electron to the acceptor molecule creating a charge-transfer state. Currently a large number of different molecular complexes are being tested for their efficiency in photovoltaic devices. Such molecular conjugates are often large to describe using accurate quantum chemical methods. We have used our recently developed density functional theory based method to study the charge transfer excited states of a novel $Sc_3N@C_{80}$-tetraphenyl porphyrin complex. In this complex, the porphyrin is the donor and the endohedral $Sc_3N@C_{80}$ is the acceptor molecule. This endohedral fullerene is the third most abundant fullerene. There are few studies on such molecular complexes with endohedral fullerenes as compared to the C_{60} molecule. We study the role of $Sc_3N@C_{80}$ as acceptor compared to the widely used C_{60} molecule. Our results on the electronic structure of the complex, the $Sc_3N@C_{80}$ molecule in both isolation and in the complex, and the lowest charge separated states will be presented.

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