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Electronic structure and charge transfer excitation energies of three endohedral fullerene- ZnTPP/ZnPc dyads FATEMEH AMERIKHEIRABADI, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, The University of Texas at El Paso — Organic donor-acceptor (D-A) moieties make up the main component of organic photovoltaics (OPVs). It has been proved that the open circuit voltage of these devices which is a parameter in efficiency determination, is directly related to the charge transfer excited states of the D-A pairs. Fullerenes having lots of interesting acceptor properties and porphyrins as well as phthalocyanines possessing intriguing donor characteristics, are shown to be promising nominees. In this work, we computationally analyze three donor-acceptor dyads of Zn-tetraphenyl porphyrin and Zn-phthalocyanine with novel endohedral fullerenes: $\text{Sc}_3\text{N@C}_{80}$ -ZnTPP, $\text{Y}_3\text{N@C}_{80}$ -ZnTPP and $\text{Sc}_3\text{N@C}_{80}$ -ZnPc. The $\text{Sc}_3\text{N@C}_{80}$ and $\text{Y}_3\text{N@C}_{80}$ belong to a particular class of fullerenes called trimetallic nitride endohedral fullerenes where the trimellitic nitrides form the endohedral units. Density functional theory, as implemented in NRLMOL code, is used to study the electronic structure and the related properties of these D-A complexes. The charge transfer excitation energies are calculated using the perturbative delta self-consistent field method recently developed in our group. We find that the CT excitation energies are larger for endohedral fullerene based dyads compared to similar C_{60} based dyads.

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