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Electronic structure and charge transfer excitation energies of a $Sc_3N@C_{80}$ -Zinc phthalocyanine (Znpc) complex FATEMEH AMERIKHEIRABADI, LUIS BASURTO, TUNNA BARUAH, RAJENDRA ZOPE, The University of Texas at El Paso — Organic photovoltaics (OPVs) have attracted considerable research interest due to their mechanical flexibility and low cost manufacturing. Organic donor-acceptor moieties form the main component of the organic photovoltaics. The donor molecule, which is a chromophore, absorbs a photon from sunlight and subsequently the excited electron is transferred to the acceptor molecule creating a charge transfer state in which a hole resides on the donor and a particle resides on the acceptor. The energy of the charge transfer state is important from the perspective of the organic photovoltaic device efficiency since it determines the achievable open-circuit voltage of such devices. We present the charge transfer energetics of the $Sc_3N@C_{80}$ -Zinc phthalocyanine (Znpc) complex which helps to have an insight into the CT process. We present a density functional theory study of the electronic structure of the Sc_3NC_{80}-Znpc. In this complex, the $Sc_3N@C_{80}$ plays the role of the acceptor molecule and Znpc would be the donor part. This molecular conjugate is very large to be analyzed using quantum chemical methods so in this work we use density functional theory as implemented in the NRLMOL code. We study a few charge transfer excited state energies of the mentioned molecular complex using our perturbative delta-SCF method. Our calculations are done at the all-electron generalized gradient level. We will also present the results of the analysis of the isolated donor and acceptor molecules.

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