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Charge transfer excited states of complexes of ZnTPP with dye-attached fullerenes MARINA PAGGEN, AMANDA GARNICA, RAJENDRA ZOPE, TUNNA BARUAH, Univ of Texas, El Paso — Organic photovoltaics (OPV) are prevalent in research as they exhibit high potential for flexible and cheaper solar cells. The fullerene or fullerene derivatives such as [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) are used as electron acceptors in the bulk heterojunction type solar cells. Often, functionalization of fullerenes is used to achieve optimal separation between the frontier molecular orbitals of the donor and acceptor molecules. Another purpose of such functionalization is to increase the absorption range of the active materials which can lead to higher photocurrent. Recently, one group of dye-attached fullerenes has been synthesized. We carried out a computational study on the electronic structure and charge transfer excited states of such dye-attached fullerenes in conjunction with Zn-tetraphenyl porpohyrin. Our calculations are done using density functional theory at the all-electron generalized gradient level. We study two different dye-attached fullerenes and compare their charge transfer excited states in a complex with ZnTPP.

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