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Electronic structure of dye attached fullerenes AMANDA GARNICA, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — C_{60} fullerene and its derivatives are the most popular acceptors which are used in molecular/polymeric complexes used in organic photovoltaics. Recently, Chabynic et al. have synthesized a few functionalized C60 molecules with dye molecules for use as acceptors in solar cells. The functional units are diketopyrrolo-pyrrole and TBTDT pigments. Using density functional theory and large polarized all electron Gaussian basis, we optimized the structures of the C60-DPP and C60-TBTDT molecules. The inspections of molecular orbitals of these systems indicate that the HOMO level is localized on the dye whereas the LUMO is on the C60 molecule. We have also calculated several lowest CT excited states where the charge transfer takes place from the HOMO on the dye to the LUMO on the C60 molecule. The electronic structure of the ground and the excited states will be presented.

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