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Ground and excited state properties of dye attached fullerenes AMANDA GARNICA, MARINA PAGGEN, 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. We have studies C60 molecule functionalized with two dye molecules: DPP and TBTDT. Using density functional theory and large polarized all electron Gaussian basis, we optimized the structures of the C_{60}-DPP and C_{60}-TBTDT molecules. The electronic structure of C_{60} changes upon functionalization with the dye molecules. The electron affinity of the functionalized fullerene increases. The optical spectra of the functionalized molecules will be presented. Inspection of molecular orbitals of these systems indicates that the HOMO level is localized on the dye whereas the LUMO is on the C_{60} 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 C_{60} molecule.

Amanda Garnica
University of Texas at El Paso

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