

Abstract Submitted
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Dye attached fullerene and P3HT complexes¹ AMANDA GARNICA, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — We study the electronic structure of C60 fullerenes functionalized with thiophene-diketo-pyrrolopyrrole-thiophene based chromophores using density functional theory combined with large polarized basis sets. These chromophores have electron donor character and thus the functionalization of the fullerene produces donor-acceptor (DA) systems. We examine in detail the effect of the linker and the addition site on the electronic structure of the fullerenes. We further study the charge transfer excited states of these DA complexes and also that of the complexes of these functionalized fullerenes with the poly(3-hexylthiophene-2,5-diyl) (P3HT) are studied using the perturbative Δ -SCF method. The exciton binding energies in the functionalized fullerene-P3MT complexes are found to be smaller compared to similarly prepared phenyl-C61-butyric acid methyl ester (PCBM)-P3MT complex.

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