

Abstract Submitted
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Charge transfer energies of tetraphenyl-porphyrin-fullerene dyads¹ RAJENDRA ZOPE, University of Texas at El Paso, MARCO OLGUIN, University of Texas at El Paso, TUNNA BARUAH, University of Texas at El Paso — Porphyrin-fullerene dyads are extensively studied for their photoinduced charge transfer properties. They form a donor-acceptor pair where the fullerene is the acceptor. Accurate theoretical estimate of the charge transfer energies in such systems has proven to be a challenge. In this study we examine the charge transfer energetics for such dyads using our recently developed density functional based excited state method which can yield reliable estimates of charge transfer energetics. In this study the effect of varying both the donor and acceptor components are studied by changing the tetra-phenyl-porphyrin (TPP) to Zn-TPP. Similarly the acceptor component is changed from C60 to C70. The structures were optimized using DFT-D3 theory at the all-electron level. Among the donor-acceptor pairs studied, we find that the ZnTPP-C60 has the lowest charge transfer energy (1.69 eV) and the TPP-C70 (2.13 eV) has the highest charge transfer energy.

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