

Photoinduced Electron Transfer in Donor–Acceptor Nanosystems: A Theoretical Study

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In organic photovoltaic (OPV) devices absorption of light is followed by charge separation, when electron is transferred from donor moiety to acceptor.[1] This process is called photoinduced electron transfer (PIET), which is essential in functional OPV devices.[1] Interesting class of materials used to mimic natural photosynthesis is constructed from nanosized donor-acceptor conjugates, where fullerene C₆₀ is used often as an acceptor.[2-5] Deep understanding of PIET in such nanosystems is therefore important for designing new materials for solar energy conversion.[2-5] Thus, here we report theoretical investigation of PIET in several donor-acceptor nanosystems using density functional theory (DFT) and semiempirical molecular orbital methods.

Initially we have explained experimental observations for π -stacked free and zinc porphyrin–fullerene dyads with a frozen geometry, by investigating nature of PIET and electronic excitations *via* irradiation.[6] Then we have explained nature of the charged-transfer (CT) states in benzodifuran-C₆₀ dumbbell-type triads and of other absorption bands in UV-vis spectra.[7] In the latter study, effect of system simplification from triad to benzodifuran-C₆₀ dyad has been studied computationally as well.[7]

Finally we suggested new building blocks for donor-acceptor nanosystems.[8] We have shown principal possibility of PIET in nanosystems composed from fullerene C₆₀, porphin and polycyclic aromatic hydrocarbons (PAHs) doped with interior heteroatoms, CH and SiH groups.[8] These doped PAHs can be either donors or acceptors depending on dopant and donor-acceptor properties of PIET partner.[8] Interestingly that direction of PIET depends on solvent effects for one of the systems as calculations with semiempirical unrestricted natural orbital–configuration interaction singles (UNO–CIS)[9] methods have shown.[8]

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