

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, in which an electron is transferred from the donor moiety to the acceptor.[1] This process is called photoinduced electron transfer (PIET) and is essential in functional OPV devices.[1] An interesting class of materials used to mimic natural photosynthesis is constructed from nanosized donor-acceptor conjugates, where fullerene C₆₀ is often used as an acceptor.[2] Deep understanding of PIET in such nanosystems is therefore important for designing new materials for solar energy conversion.[2] Thus, here we report theoretical investigation of PIET in several donor-acceptor nanosystems using density functional theory (DFT) and semiempirical molecular orbital methods.[3]

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