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Charge Transfer and Triplet States in High Efficiency OPV Materials and Devices[1]

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The advantage of using polymers and molecules in electronic devices, such as light-emitting diodes (LED), field-effect transistors (FET) and, more recently, solar cells (SC) is justified by the unique combination of high device performance and processing of the semiconductors used. Power conversion efficiency of nanostructured polymer SC is in the range of 10% on lab scale, making them ready for up-scaling. Efficient charge carrier generation and recombination in SC are strongly related to dissociation of the primary singlet excitons. The dissociation (or charge transfer) process should be very efficient in photovoltaics. The mechanisms governing charge carrier generation, recombination and transport in SC based on the so-called bulk-heterojunctions, i.e. blends of two or more semiconductors with different electron affinities, appear to be very complex, as they imply the presence of the intermediate excited states, neutral and charged ones [1-3]. Charge transfer states, or polaron pairs, are the intermediate states between free electrons/holes and strongly bound excitons. Interestingly, the mostly efficient OLEDs to date are based on the so-called triplet emitters, which utilize the triplet-triplet annihilation process. In SC, recent investigations indicated that on illumination of the device active layer, not only mobile charges but also triplet states were formed [4]. With respect to triplets, it is unclear how these excited states are generated, via inter-system crossing or via back transfer of the electron from acceptor to donor. Triplet formation may be considered as charge carrier loss channel; however, the fusion of two triplets may lead to a formation of singlet excitons instead. In such case, a generation of charges by utilizing of the so far unused photons will be possible. The fundamental understanding of the processes involving the charge transfer and triplet states and their relation to nanoscale morphology and/or energetics of blends is essential for the optimization of the performance of molecular photovoltaic devices. I will present the state of the art in this field and discuss the mechanisms of polaron pair generation and recombination in the novel low band gap polymer-fullerene blends as well as in high-efficiency SC.

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