

In Situ Probing of the Charge Transport Process at the Polymer/Fullerene Heterojunction Interface

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Optical spectroscopy is widely used to study the photophysical processes in organic photovoltaic (PV) material systems. In most of the spectroscopic techniques electrons and holes are generated simultaneously upon light excitation. In this work we demonstrated the use of charge modulation spectroscopy (CMS) to study localization of electrons or holes, without the interference from its counter charge, at organic donor-acceptor heterointerfaces. The CMS measurements were performed on a heterojunction field-effect transistor (FET) structure, allowing us to acquire spectra that separately represent the electronic states of electron or hole by changing the gate bias. Using this approach we studied two polymer systems, poly(N-alkyl diketopyrrolo-pyrrole dithienylthieno[3,2-b]thiophene) (PDPP-DTT), which exhibits record high hole mobility in FETs, and a thieno[3,4-b]thiophene-alt-benzodithiophene copolymer (PTB7), which yields high power conversion efficiency in a PV configuration. By comparing the frequency-dependent CMS spectra of the pure polymer, polymer/(6,6)-phenyl-C61-butyric acid methylester (PCBM) bilayer, and polymer/PCBM blend, we observe that while charge localization is greatly increased from bulk PTB7 to PTB7/PCBM interface, it remains almost unchanged for bulk PDPP-DTT and PDPP-DTT/PCBM interface. Such difference in the interface effect can be well correlated with the different spatial arrangement of PTB7 and PDPP-DTT molecules at the polymer/PCBM interface. Our study reveals a trade-off between charge transfer and charge trapping at the donor/acceptor interface in polymer bulk heterojunctions and suggests the need of creating an energy cascade at the interface to achieve a highly efficient charge separation process.