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Probing charge transfer complex states in organic solar cells using photocurrent spectroscopy DHANASHREE MOGHE, DANISH ADIL, University of Missouri-Columbia, CATHERINE KANIMOZHI, GITESH DUTTA, SATISH PATIL, Indian Institute of Science, Bangalore, India, SUCHISMITA GUHA, University of Missouri-Columbia — Diketopyrrolopyrrole (DPP) containing copolymer-fullerene blends have gained a lot of interest in organic optoelectronics with a great potential in organic photovoltaics (OPVs). The interfacial charge transfer complex (CTC) states formed in donor-acceptor blended OPVs play a major role in the overall efficiency of the device. We investigate the spectral photocurrent characteristics of five DPP based copolymers; two of them being benzothiadiazole and carbazole-based statistical copolymers of DPP. These systems provide a wide range of bandgap energies ranging from ~ 1.4 to 1.7 eV. We use Fourier transform photocurrent spectroscopy (FTPS) and monochromatic photocurrent (PC) to identify the CTC states in these DPP copolymer-fullerene blends. The stability of the CTC state is found to be dependent on the band gap energy difference between the donor copolymer and the acceptor. We support our inferences from theoretical results obtained using density-functional theory (DFT) and time-dependent DFT for two DPP based copolymers. The theoretical calculations reveal a higher contribution of the CTC states to the lowest excited state in the phenyl-based DPP monomer, which has a larger bandgap energy compared to the thiophene-based DPP system, in the presence of a fullerene molecule.

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