Public Abstract
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Title:CHARGE-TRANSFER AND OTHER EXCITONIC STATES IN CONJUGATED POLYMER: FULLERENE BLENDS-IMPLICATION IN PHOTOVOLTAICS

In 1977, A. J. Heeger, H. Shirakawa, and Alan G. MacDiarmid (Nobel Prize in Chemistry, 2000) published reports on the high conductivities in organic semiconductors (doped polyacetylene). Since then tremendous advances have been made in the field of organic electronics. Organic solar cells, fabricated with conducting organic semiconductors, have quickly taken the limelight due to the inexpensive, low-cost and flexible nature of the fabricated devices. At present, their power conversion efficiencies have reached over 10%. The steady rise in the performance has been brought about by devising new techniques to identify the origin of free charge generation, and synthesizing low-bandgap materials, to name a few.

Typically, an organic solar cell comprises of a blend of at least two organic conducting materials: a donor and an acceptor. The blend is sandwiched between two metal electrodes so that the free charges i.e. the current, can be extracted upon illumination. Unfortunately, due to the nature of the organic semiconductors, illumination does not directly result in formation of free charges. Instead, it results in the formation of bound electron-hole pair i.e. excitons. Hence, to improve the efficiency of the device, it is crucial to understand the formation and role of the excitons and excitonic states in a polymer and its blends.

In this thesis, two excitonic states: the charge-transfer (CT) and triplet excitonic states, have been probed using photocurrent (PC) and photoinduced absorption spectroscopy, respectively. To elaborate the role of CT states, a set of low-optical bandgap diketopyrrolopyrrole (DPP)-based copolymers (donor and acceptor fused in the same chain) have been utilized. The presence of donor-acceptor in the same unit gives rise to an inbuilt charge separation (intramolecular CT states). Blending the copolymer with another acceptor (such as fullerene) results in the formation of a intermolecular CT state at the copolymer/fullerene interface. Two high resolution and sensitive PC techniques: Fourier transform photocurrent spectroscopy and monochromatic PC, have been utilized to identify the intermolecular CT states in the copolymer:fullerene solar cells. It was observed that the formation of a stable intermolecular CT states results in a lower photocurrent generation of the devices. Further, theoretical calculation using density functional theory (DFT) and time dependent DFT were performed on selected DPP-based copolymers. The theoretical results help in explaining the origin of the intramolecular CT nature in DPP-based copolymers.

The triplet states have been probed using a photomodulation technique, namely, photoinduced absorption (PIA). The triplet enhanced ladder-type polymers were chosen for this study, as the triplet excitons could be accessed even at room temperature. Further, by creating quenching sights (adding PCBM as acceptor) and by tracking the quenching of the PIA signal as a function of PCBM concentration, the diffusion length and diffusivity of the triplet excitons was estimated using a 1-dimensional random walk model. A higher diffusion length and longer lifetimes of triplet exciton excitons suggests that the triplet excitons can contribute significantly to the device efficiency.