DOCTORAL THESIS

Toward better performing organic solar cells: impact of charge carrier transport and electronic interactions in bulk heterojunction blends

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ABSTRACT

Organic photovoltaic (OPV) is an exciting energy harvesting technique. Although its power conversion efficiency (PCE) now exceeds 10% in a research laboratory, the processing window of an OPV cell is still narrow. A fundamental understanding of the OPV materials is desired. This thesis presents the charge carrier transport properties and electronic interactions in the bulk heterojunction (BHJ) active layer of OPV cells. They were found to be well correlated with OPV device performances. Space-charge-limited current (SCLC) measurements and admittance spectroscopy (AS) were employed to study the charge transports, while photothermal deflection spectroscopy (PDS) was used to probe the trap densities inside the materials.

Beneficial effects of a common solvent additive, 1,8-diiodooctance (DIO), on PTB7:$PC_{71}BM$ OPV cells have been investigated**.** With DIO present in the casting solution, the resulting BHJ films have much enhanced electron mobilities, whereas the impact on the hole mobility is negligible. The origin of increased electron mobility is the reduced average electron hopping distance for those films prepared with DIO solvent additive. A balance of hole-electron mobility by tuning the DIO concentration was demonstrated to be the way to optimize the OPV device performance. In light of carrier transport measurement results, a "polymer-rich" strategy with preserved device performance was demonstrated.

After understanding the importance of balanced hole-electron mobility, the impact of donor-acceptor weight ratio on the performance of PTB7 : $PC_{71}BM$ based OPV cells was explored. Early stage electronic donor-acceptor interactions

were revealed using ultra-low dosages of fullerenes. Before electron transport pathways percolate, the unconnected fullerene domains act as traps and hinder electron transport. From PDS, the trap density observed inside BHJ films was found to be anti-correlated with the fill factor of OPV devices. The origin of low FFs is mainly due to electron traps and localized states from fullerenes. Based on the observations, it is proposed that $PC_{71}BM$ tends to intercalate with PTB7 backbone instead of forming self-aggregates before the electron pathway percolation.

Apart from investigating the fundamentals in OPV devices, a solution to improve its processing window was proposed in this thesis. Thermally stable polymer : fullerene OPV cells were fabricated by employing fluorenone-based solid additives. A charge transfer interaction between the additives and donor moiety of polymer formed a locked network which freezes the BHJ morphology under thermal stress. The most promising result retains 90% of the origin efficiency, upon thermal aging at 100 ℃ for more than 20 hours in PTB7:$PC_{71}BM$ solar cells.

Besides fullerene-based OPV, all-polymer photovoltaic solar cells (all-PSCs) were also investigated. Two new difluorobenzene-naphthalene diimide based polymer electron acceptors, one random (***P1***) and one regioregular (***P2***) structure, were compared. ***P2*** exhibited a much better molecular packing, a higher electron mobility and more balanced hole-electron mobilities in its composite film with polymer donor, PTB7-Th. An optimized PTB7-Th:***P2*** device can achieve a respectably high PCE over 5% for all-PSC devices. These all-PSCs should open a new avenue for next generation OPVs.

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