DOCTORAL THESIS

Charge injection and transport characterization of semiconducting polymers and their bulk heterojunction blends

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Charge Injection and Transport Characterization of Semiconducting Polymers and Their Bulk Heterojunction Blends

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Abstract

This thesis presents the charge injection and transport properties of organic photovoltaic (OPV) polymers and their bulk heterojunction (BHJ) blends, and their relationship to the operating mechanisms of OPV cells. Four independent techniques were employed to investigate the properties. They are time-of-flight (TOF), current-voltage (*J-V*) measurements, dark-injection space-charge-limited current (DI-SCLC) and admittance spectroscopy (AS). The OPV polymers under investigation were poly[N-9”-hepta-decanyl-2,7-carbazole-alt-5,5-(4’,7’-di-2-thienyl-2’,1’,3’-benzo thiadiazole)] (PCDTBT), poly(3-hexylthiophene) (P3HT), poly(2-methoxy-5-(3'-7'-dimethyloctyloxy)-1,4-phenylenevinylene) (MDMO-PPV), and their BHJ blends.

Three transition metal oxides (TMOs), namely, molybdenum (VI) oxide (MoO_3), vanadium (V) oxide (V_2O_5) and tungsten (VI) oxide (WO_3), were used as materials for hole injection layers (HILs) for pristine OPV polymers. For PCDTBT, both MoO_3 and V_2O_5 can form quasi-Ohmic contacts. WO_3 forms a poor contact due to a large injection barrier. Charge injection is more complex in P3HT, electron leakage and interfacial charge transfer (CT) occur during measurements. The electron leakage can be suppressed by inserting an electron blocking and trapping (EB & ET) layer between the active layer and the Au cathode. However, for the interfacial CT, it can only be prevented by a suitable choice of HIL.

For charge transport, AS can be used to study all the OPV polymers and their BHJ blends, while DI-SCLC can only be applied to the pristine polymers. For the pristine OPV polymers, the extracted hole mobilities are in good agreement among three independent techniques (TOF, DI-SCLC and AS). For the BHJ blends, the hole

mobilities of P3HT:$PC_{61}BM$ were found to be independent of the composition, while it is ratio dependent for PCDTBT:$PC_{71}BM$. We found that in the BHJ blend for P3HT:$PC_{61}BM$, the P3HT domains were well-connected. However, for the amorphous PCDTBT:$PC_{71}BM$ films, the hole transport pathways are easily blocked by the acceptors. Temperature dependent measurements were also carried out in order to obtain the energetic disorders (σ) of the polymers and BHJ blends. Since P3HT is polycrystalline film, σ is found to be the smallest. Furthermore, it is also observed that σ of both BHJ blends are independent of the composition.

Apart from charge transport and injection studies, the OPV performances of BHJ blends were also investigated. Correlations were established between the performances and the transport properties of donor materials. For the BHJ blends with larger σ, the fill factor of OPV cells is reduced due to the larger recombination rate at the tailed states of the DOS.

Finally, the effects of di(ethylene glycol) (DEG) treatment on PEDOT:PSS layer were studied. We found that the roughness of PEDOT:PSS increased after the DEG treatments. OPV cells with DED-treated PEDOT:PSS layer have enhanced short-circuit currents density and power conversion efficiency due to improved charge collection.

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