DOCTORAL THESIS

Impact of metal oxide/bulk-heterojunction interface on performance of organic solar cells

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Impact of Metal Oxide/Bulk-heterojunction Interface on Performance of Organic Solar Cells

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DECLARATION

I hereby declare that this thesis represents my own work which has been done after registration for the degree of PhD at Hong Kong Baptist University, and has not been previously included in a thesis or dissertation submitted to this or any other institution for a degree, diploma or other qualifications.

Signature:

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July 2015

Abstract

Organic photovoltaics have shown much promise as an alternative photovoltaic technology for application in low-cost, large-scale and flexible solar cells. The application of metal oxides in organic solar cells (OSCs) and the impact of the properties of metal oxide/organic hetero-interfaces on cell performance have attracted a lot of attention. The metal oxide/organic interfaces have a crucial impact on interfacial charge transfer, charge collection and the overall device performance. This thesis is aimed at clarifying the principal interfacial phenomena occurring at the metal oxide/organic hetero-interfaces as well as effective engineering of those interfacial properties in OSCs. Photo-generated electrons and holes undergo different recombination processes, e.g., bimolecular recombination and trap-assisted recombination, before being collected by the electrodes in OSCs. Light intensity-dependent current density–voltage (*J*–*V*) characteristics of OSCs were analyzed to study the effect of recombination on charge collection efficiency. Effect of metal oxide/organic hetero-interfaces on charge transfers at organic/electrode interface was analyzed using transient photocurrent (*TPC*) measurements. Light intensity-dependent *J*–*V* characteristics and *TPC* characteristics were applied to explore the charge recombination dynamics in OSCs with a metal oxide interlayer. This project concentrated on an in-depth investigation of the physics and the interface phenomena such as interfacial exciton dissociation, charge recombination processes, charge collection and interface engineering for high performing OSCs.

The fundamentals about light intensity-dependent *J*-*V* characteristics for OSCs were summarized. The relationship between the charge recombination dynamics and light intensity-dependent *J*-*V* characteristics in OSCs were developed. Light intensity-dependent J_{SC}, V_{OC} and

FF in OSCs made with different bulk-heterojunction (BHJ) systems of PTB7:$PC_{70}BM$, PTB7-Th:$PC_{70}BM$ and PNB4:$PC_{70}BM$ were investigated. It is found that bimolecular recombination is the most prominent factor limiting the performance of OSCs. For freshly made OSCs fabricated based on the commercial polymers, e.g. PTB7 & PTB7-Th, and the new polymer PNB4 synthesized in-house, the trap-assisted charge recombination process in the BHJ active layer plays a relatively small role. This suggests that reducing the bimolecular recombination in OSCs through selecting proper materials and device structures is crucial for enhancing the power conversion efficiency (PCE) of OCSs. In this work, device structures which enable reducing bimolecular recombination in OSCs were investigated.

The effect of ZnO interlayer at the interface between BHJ and Al cathode on the performance of PTB7:$PC_{71}BM$ based OSCs was studied by a combination of theoretical simulation and experimental characterization techniques, e.g., using light intensity-dependent *J*–*V* characteristic and *TPC* measurements etc. It shows that ZnO interlayer has a profound effect on the performance of the PTB7:$PC_{70}BM$-based OSCs, although it does not have a significant influence on the maximum absorptance in the active layer. The origin of the improvement in the cell performance is associated with the efficient charge collection due to the favorable exciton dissociation at the electrode/active layer interface. It is shown that the presence of the ZnO interlayer allows using a thinner active layer without moderating the absorption in the optically optimized control OSCs without the ZnO interlayer. OSCs with a ~10 nm thick ZnO interlayer are found to be favorable for the efficient charge collection, and thereby improving the cell performance. The *TPC* measurements also reveal that the dissociation of excitons at the metal/organic interface of regular OSCs hinders the electron collection. The unfavorable interfacial exciton dissociation can be removed by interposing a ZnO interlayer at the Al/organic

interface, thus bimolecular recombination at the electrode/active layer interface can be reduced for improving the charge collection efficiency. PCE of the OSCs using ZnO interlayer was 6.5%, which is about 20% higher than a control cell (5.4%), having an identical device configuration without a ZnO interlayer.

Solution-processed anode interlayer, a mixture of solution-processed MoO_X and PEDOT:PSS, was adopted for application in inverted PTB7:$PC_{71}BM$-based OSCs. The ratio of MoO_X to PEDOT:PSS in the mixed solution was optimized for achieving the best cell performance. A PCE of 7.4% was obtained for OSCs with an optimal MoO_X-PEDOT:PSS based interlayer, interposed between the BHJ active layer and Ag anode, which means 10% enhancement over the PCE of control cell made with an evaporated MoO_X interlayer. Light intensity-dependent *J–V* characteristics implied that the bimolecular recombination in OSCs with a MoO_X-PEDOT:PSS interlayer was reduced. *TPC* measurements showed that the favorable exciton dissociation occurs at the organic/MoO_X interface for the inverted OSCs. The favorable interfacial exciton dissociation generates an electrical field within a very small space near the interface, contributing significant additional photocurrent when the effective bias across the active layer in the OSCs is low, and thereby assisting in an efficient charge collection at the organic/electrode interface. In addition to the improvement in the cell performance, the solution-processed MoO_X-PEDOT:PSS interlayer does not require a post-annealing treatment, which is beneficial for application in solution-processed tandem and flexible OSCs.

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