DOCTORAL THESIS

Binary and ternary bulk heterjunction solar cells with alternative donor-to-acceptor ratios

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ABSTRACT

Bulk heterojunction (BHJ) organic photovoltaic (OPV) is one of the most promising techniques to generate electricity with advantages of flexibility, solution processing and capability for large area device fabrication. Although the power conversion efficiency (PCE) of BHJ solar cells has already achieved over 13%, there are still problems remain to be solved. This thesis presents the binary and ternary organic BHJ devices with alternative donor:acceptor (D:A) ratios, and the charge transport properties and electronic interactions in their BHJ films.

In a high performance BHJ solar cell, the commonly optimized D:A weight ratio is about 1:*x*, where *x* is commonly in excess of 1.5, when $PC_{71}BM$ is used as the acceptor. We demonstrated how to achieve high PCEs of BHJ solar cells by enriching the D:A weight ratios. The PCEs of the re-optimized cells were improved for the PTB7:$PC_{71}BM$, PCDTBT:$PC_{71}BM$, PDTSTPD:$PC_{71}BM$ devices. Current-voltage (JV) and admittance spectroscopy (AS) measurements indicate enhanced hole mobilities for the polymer-rich BHJs based on PTB7, PCDTBT, and PDTSTPD. At the same time, although the relative weight ratio of $PC_{71}BM$ is reduced, the electron mobilities are maintained due to the dispersion of fullerene domains by increased DIO concentrations.

The active layer thickness of most optimized BHJ solar cells is about 100nm. The thin active layer is unfavorable for optical absorption and film coating. We employed a ternary strategy to address this problem, and the thick-film BHJ devices can retain 90% PCEs of their optimized thin-film devices. Three model systems were studied, involving PTB7:$PC_{71}BM$,

PTB7-Th:$PC_{71}BM$ and P3HT:PCBM BHJs. Into these BHJs, a ternary component, p-DTS($fbtth_2$)$_2$ (DTS) is introduced. With DTS, the corresponding thick film devices have significantly improved PCEs. The ternary component DTS improves hole mobility and reduces sub-bandgap trap states. Both observations are well correlated with improved FFs of the ternary BHJ cells. Photothermal deflection spectroscopy (PDS) and 1H nuclear magnetic resonance (1H NMR) results indicate that DTS behaves as conducting bridges in between two neighboring polymer segments.

Most lab-based BHJ solar cells are optimized by their power conversion efficiencies (PCEs). We challenge this conventional view by showing that BHJ cells using fullerene acceptors should be optimized by their fill-factors (FFs). With the optimized-FF approach, BHJ cells tend to have higher fullerene content when compared to the BHJ cells that are optimized by PCEs. The FF-optimized BHJ cells have slightly reduced PCEs (due to smaller J_{sc}s) compared to the PCE-optimized cells. Yet, FF-optimized cells enjoy a much better thermal stability. We demonstrate that these FF-optimized BHJs possess better-balanced electron-to-hole mobility ratios due to weakly field-dependent electron mobilities. The improved mobility ratio suppresses carrier recombination. Our results suggest that BHJ cells optimized by their PCEs should be meta-stable, and other D:A ratios should be considered for practical BHJ cell development.

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