Photovoltaic Performances of Low Bandgap Conjugated Polymers with Strong Interchain Aggregations

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Polymer solar cells (PSCs) are one of the most attractive ways to use solar energy – an inexhaustible renewable clean energy. Large area roll-to-roll printing is a remarkable advantage of PSCs, which may supply 100 GW scale of electricity generation with low cost of 0.05 €/W_p.[1] For large area printing with high speed, low reliance of power conversion efficiency (PCE) of PSCs on large thickness variations of active layer should be a major concern toward good quality or yield control.[2-4] Polymer donors with PCE more than 10% for active layer thickness range from 100 to 900 nm would establish an ideal window for high speed printing.

We developed low bandgap polymer donors with high hole mobility to accelerate hole transport in thick active layer, so as to decrease recombination of holes and electrons and maintain high fill factor. A series of D-A conjugated polymers comprising oligothiophenes as the D-units and 5,6-difluorobenzothiadiazole (FBT), dithienobenzothiadiazole (DTfBT), and dithienobenzooxadiazole (DTfBO) as the A-units were synthesized. The polymers could show very strong interchain aggregation in solutions at room temperature (RT), whose absorption spectra in RT solution were almost comparable to that of corresponding thin solid film. The aggregates of the polymers in solutions could be separated upon heating, supplying enough solution-processing condition for high quality films. The strong interchain aggregation abilities of the polymers resulted in high hole mobility. For example, field-effect hole mobilities based on neat polymer films could be higher than 2 $cm^2/(V\ s)$. The polymers also displayed high space charge limited current (SCLC) hole mobilities. PSCs were fabricated with varied thickness of the active layers. Delightedly, the PSCs based on the polymer donors exhibited maximum PCEs with thick active layers of 200 nm or beyond. The PCE variations were relatively small for different thickness of active layers. For some FBT-based polymer, PSCs with 400 nm thick active layer could show PCE higher than 10%. The controls of molecular weight and aggregation extent are crucial to achieve high efficiency for polymer donors. Our results suggest that D-A conjugated polymers with strong interchain aggregation abilities would be benefit to realize high hole mobility, from which highly efficient thick-film PSCs could be achieved.

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