DOCTORAL THESIS

Stability of nonfullerene organic solar cells

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Abstract

The development of nonfullerene organic solar cells (OSCs) has attracted increasing interests because of the intrinsic advantages of nonfullerene acceptors, including their high absorption capability over the long wavelength region, tunable electronic properties, and excellent miscibility with polymer donors. Recently, power conversion efficiency (*PCE*) of >15 % for single-junction nonfullerene OSCs has been reported.

Apart from the rapid progresses made in the cell efficiency, significant improvement in the stability of nonfullerene OSCs is required if the organic photovoltaic technology is to become a viable option for commercialization. The lifetime of OSCs is closely related to the intrinsic properties of the functional photoactive materials, e.g., the acceptors with suitable energy levels, morphology of bulk heterojunction (BHJ), formation of the active layer, interlayer engineering and device configuration. However, the comprehensive study of the impacts of the morphological properties and vertical phase separation in a BHJ on charge transport, built-in potential, charge recombination processes, *PCE* as well as the lifetime of nonfullerene OSCs has not been reported yet.

This work has been focused on unraveling the stability of highly efficient OSCs using different nonfullerene acceptor/polymer blend systems, e.g., 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis (4-hexylphenyl)-dithieno[2,3-d:2’,3’-d’]-s-indaceno[1,2-b:5,6-b’]dithiophene (ITIC):poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b;4,5-b']dithiophene -2,6-diyl-alt-(4-

(2-ethylhexyl)-3-fluorothieno[3,4-b]thiophene-)-2-carboxylate-2-6-diyl)](PTB7-Th), ITIC:poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl) -benzo [1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl) benzo[1',2'-c:4', 5'-c'] dithiophene-4,8-dione)] (PBDB-T), and 3,9-bis(2-methylene-((3-(1,1-dicyanomethylene)-6,7-difluoro)-indanone))-5,5,11,11-tetrakis (4-hexylphenyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophene(IT-4F):poly[(2,6-(4,8-bis(5-(2-ethylhexyl)-4-fluorothiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione)] (PBDB-T-2F). The lifetime of the nonfullerene OSCs has been analyzed systematically using a combination of morphology, photoelectron spectroscopy, light intensity-dependent current density–voltage measurements, transient photocurrent and aging studies.

The effects of built-in potential (V_0), charge extraction, and bimolecular recombination processes on the performance and stability of nonfullerene OSCs with regular and reverse configurations were studied. The results reveal that PTB7-Th:ITIC based OSCs with a reverse configuration are more favorable for efficient operation, due to the advantages of: (1) enhancement of charge collection by avoiding the holes passing through acceptor-rich region, which would otherwise occur in an OSC with a regular configuration, and (2) suppression of bimolecular recombination enabled by a higher V_0. It shows that the PTB7-Th:ITIC based OSCs with a reverse configuration possess a slow degradation process, and >29% increase in *PCE* (8%) as compared to that of an optimized control OSC (6.1%).

We found that a gradual decrease in V_0 and hence the performance deterioration in the regular configuration PBDB-T:ITIC OSCs are caused mainly by the interfacial reaction between nonfullerene acceptor (ITIC) and poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) hole transporting layer (HTL). The reduction in V_0, due to the unavoidable interfacial reaction between ITIC and PEDOT:PSS at the BHJ/HTL interface in the OSCs, can be overcome through interfacial engineering, , e.g., introducing a thin molybdenum oxide (MoO_3) passivation layer.

The effect of the HTL on stability of PBDB-T:IT-4F based OSCs has been analyzed using different HTLs, e.g., a pristine PEDOT:PSS layer, a MoO_3-doped PEDOT:PSS layer and a pure MoO_3 layer. It shows that MoO_3-induced oxidation doping of PEDOT:PSS favors the stable and efficient operation of nonfullerene OSCs. The results suggest that a stable and high V_0 across the BHJ is a prerequisite for attaining high efficiency nonfullerene OSCs with long-term stability.

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