



Ternary blend organic solar cells with a non-fullerene acceptor as a third component to synergistically improve the efficiency



Cheng Xu*, Matthew Wright, Duanlei Ping, Haimang Yi, Xueyun Zhang, M.D. Arafat Mahmud, Kaiwen Sun, Mushfika Baishakhi Upama, Faiazul Haque, Ashraf Uddin

School of Photovoltaic and Renewable Energy Engineering, University of New South Wales, 2052, Sydney, Australia

ARTICLE INFO

Keywords:

Ternary
PDS
Energetic disorder
IDFBR

ABSTRACT

Ternary blends, where an additional component is added to a donor/acceptor blend, represent a promising route to improve upon the performance of organic solar cells. Non-fullerene acceptor materials are particularly suited for this application due to their relatively stronger absorption coefficients and tuneable molecular energy levels. This paper demonstrates a ternary blend solar cell by incorporating a promising non-fullerene acceptor, IDFBR, into a PffBT4T-2OD:PC₇₁BM blend. The addition of IDFBR to this blend leads to the formation of a cascading energy band structure in the device, which is required for the operation of an efficient ternary system. Ternary blend solar cells with an IDFBR concentration of 5 wt% demonstrated improved photovoltaic performance, when compared to the host binary blends. This improved performance was attributed to a reduction in energetic disorder and improved charge carrier transport in the ternary blend.

1. Introduction

Bulk heterojunction (BHJ) organic solar cells (OSCs) have attracted significant attention, due to low fabrication cost, high flexibility and large throughput via facile solution-processing [1–5]. Intense research has been devoted to elevating the performance of OSCs via synthesis of new materials and device structure engineering, resulting in an impressive enhancement of power conversion efficiency (PCE) for binary OSCs from 5% in 2005 [6] to the current record at 14% [7]. Despite the successful improvement achieved, there are still some limitations in binary OSCs. Fullerene derivatives as acceptors in binary OSCs play a crucial role in determining OSC performance, however, they have disadvantages, such as insufficient absorption in the visible region, energy loss due to mismatch of energy levels, and inefficient charge dissociation, which impedes further enhancement in PCE in binary OSCs [8–12]. Recently, non-fullerene derivative acceptor materials have been considered as a breakthrough to this limitation, thanks largely to the simultaneous advantages of stronger light absorbing ability, improved thermal stability, tuneable molecular energy level, simple synthesis process and potentially cheap fabrication cost [11,13–15]. 5,5'-[(6,12-dihydro-6,6,12,12-tetraoctylindeno[1,2-*b*]fluorene-2,8-diyl)bis(2,1,3-benzothiadiazole-7,4-diylmethylidene)]bis[3-ethyl-2-thioxo-4-thiazolidinone (IDFBR) is one of newly developed non-fullerene derivative acceptors, having a maximum absorption peak located at around

540 nm with the highest occupied molecular orbital/the lowest unoccupied molecular orbital (HOMO/LUMO) levels of $-5.75/-3.70$ eV [16]. When paired with the widely studied donor material P3HT, a power conversion efficiency of 6.4% has been demonstrated [17].

The ternary strategy is emerging as a promising solution for achieving high performance binary OSCs without complex fabrication process [18–21]. Furthermore, several studies exhibited that ternary OSCs have a better stability than binary OSCs [22,23]. Compared with the binary structure, ternary blends consist of three components, with either an extra donor, or an extra acceptor. The third component is carefully selected to increase the light absorbing ability, aiming to increase the short circuit current density (J_{sc}) of the device. The material must have a cascading energy level between the highest occupied molecular orbital (HOMO) level of the primary donor and the lowest unoccupied molecular orbital (LUMO) level of the primary acceptor to promote charge transfer [24,25]. Based on this concept, several reports introduced fullerene materials of PC₇₁BM and Bis-PC₇₁BM as a third component into different non-fullerene binary systems to achieve efficient ternary OSCs [26,27]. Incorporation of this third component can effectively increase the PCE of binary OSCs, in which fullerene derivatives are frequently employed as third components or acceptors. Hence, the ternary strategy can combine the advantages of high electron mobility in fullerene material [28] and strong light absorption in non-fullerene materials in achieving high efficiency OSCs. However,

* Corresponding author.

E-mail addresses: z5084835@student.unsw.edu.au (C. Xu), a.uddin@unsw.edu.au (A. Uddin).

<https://doi.org/10.1016/j.orgel.2018.08.029>

Received 25 June 2018; Received in revised form 12 August 2018; Accepted 12 August 2018

Available online 13 August 2018

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some details behind the working mechanisms of non-fullerene acceptor in the such complex ternary system are still unclear and needed to be explored. For instance, third component may play a role as recombination centre or morphological trap rather than sensitizer to extend the absorption spectrum, since unfavourable interactions between primary blend and the third component are undesired [29].

In this work, a novel ternary organic solar cell was fabricated by incorporating a non-fullerene material, IDFBR, as the third component into the host Poly[(5,6-difluoro-2,1,3-benzothiadiazol-4,7-diyl)-alt-(3,3''-di(2-octyldodecyl)-2,2';5',2'';5'',2'''-quaterthiophen-5,5'''-diy)] PffBT4T-2OD donor and the fullerene derivative [6,6]-Phenyl C₇₁ butyric acid methyl ester PC₇₁BM binary system. IDFBR demonstrates a complementary absorption spectrum and a well-matched HOMO/LUMO level forming cascaded energy alignment with host donor material of PffBT4T-2OD and electron accepting material of PC₇₁BM. The ternary OSC demonstrated a PCE of 8.51%, which is a relative increase of 15% compared to PffBT4T-2OD based binary OSCs. To deeply investigate the origins of the performance enhancement in ternary OSCs, sub-bandgap absorption was probed using photothermal deflection spectroscopy (PDS). This showed that adding 5 wt% IDFBR in the blend leads to a reduction in disorder in the active layer film, which correlates with improved charge transport and increased efficiency.

2. Experimental

PffBT4T-2OD, PC₇₁BM, and IDFBR were purchased from Solarmer and used without further purification. Zinc acetate dihydrate (purity > 99.0%), 2-methoxyethanol, aluminium nitrate nonahydrate (purity 99.8%) and ethanolamine (purity > 98.0%) were purchased from Sigma-Aldrich. Chlorobenzene (purity 99.8%), 1,2-dichlorobenzene (purity 99.0%), and 1,8-diiodooctane (purity 98.0%) were purchased from Sigma-Aldrich.

Fig. 1b displays the inverted device used in this work with the following structure glass/ITO/ZnO/Active layer/MoO₃/Ag. The patterned ITO/glass was cleaned sequentially with Hellmanex III, DI water, acetone and isopropanol, using a sonicator for 15 min at each step. A ZnO precursor solution was prepared in air by dissolving a total of 108 mg of zinc acetate dihydrate in 1 mL of 2-methoxyethanol with 32 μL of ethanolamine as additive. For the active layer, the solution

(15 mg/ml of PffBT4T-2OD and 18 mg/ml PC₇₁BM; 1:1.2 ratio) was prepared in chlorobenzene/dichlorobenzene (CB/DCB) solvents at 1:1 vol ratios with 3 wt% of 1,8-Diiodooctane (DIO). With fixed donor and acceptor ratio, the investigated fractions of IDFBR, with respect to the total acceptor weight fraction, were 0, 3, 5, 10 and 100. The active layer solution was dissolved on a hotplate at 110 °C for at least 4 h. Before spin coating, both the active layer solution and ITO substrate were preheated on a hot plate at a temperature of 110 °C for 10 min. The active layer solution was then immediately spin coated on the preheated ITO substrate at 900 rpm, leading to an average layer thickness of ~310 nm. Next, the coated ITO substrate was transferred to the glovebox antechamber to vacuum dry for 2 h and was then annealed at 85 °C for 6 min inside a N₂ glovebox. A thermal evaporation process was conducted to deposit a 11 nm MoO₃ hole transport layer and 100 nm Ag electrode at a vacuum level of 3 × 10⁻⁶ Torr. The device area for each cell was 0.12 cm².

3. Device characterization

The current density-voltage (J-V) measurements were obtained from a calibrated Keithley 2400 Source Meter under 100 mW cm⁻² (AM 1.5G) solar spectra illumination. The hole mobilities were measured by using a Keithley 2400 Source Meter under dark conditions, the hole-only devices with structure of ITO/PEDOT:PSS/Active layer/MoO₃/Ag were prepared for mobilities using space charge limited current (SCLC) method. Impedance measurements were conducted on an Autolab PGSTAT-30 impedance analyser. All samples were measured via a frequency analyser module with a frequency range from 1 MHz to 1 Hz at different DC biasing voltages. The transmittance and absorbance characteristics of the devices were recorded using a UV-Vis-NIR spectrometer (Perkin Elmer lambda 950). Photoluminescence (PL) spectra were taken using a 1/4 m monochromator (Cornerstone TM260) equipped with a silicon charge coupled device camera. The surface morphologies were investigated using atomic force microscopy (AFM) and scanning electron microscopy (SEM). AFM images were taken by tapping mode using a Bruker dimension icon SPM and SEM images were taken using a NanoSEM 230 system. Photothermal deflection spectroscopy (PDS) measurements were made on an in house-built system, containing a monochromator (Cornerstone TM130) equipped

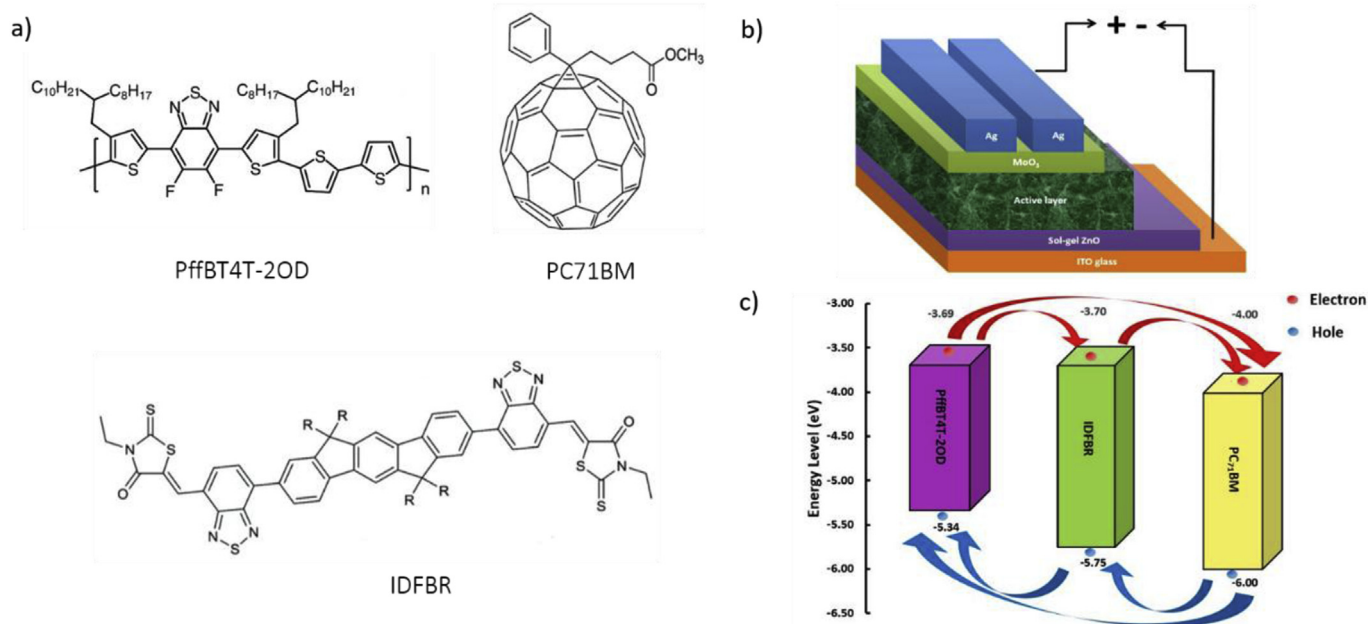


Fig. 1. a) Chemical structures of PffBT4T-2OD, PC₇₁BM and IDFBR; b) Schematic diagram of inverted device structure; c) Energy levels of materials used in the organic solar cell.

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