

Full paper

Regulating the vertical phase distribution by fullerene-derivative in high performance ternary organic solar cells



Pengqing Bi^a, Tong Xiao^b, Xiaoyu Yang^a, Mengsi Niu^a, Zhenchuan Wen^a, Kangning Zhang^a, Wei Qin^a, Shu Kong So^c, Guanghao Lu^{b,*}, Xiaotao Hao^{a,d,*}, Hong Liu^a

^a School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan, Shandong 250100, China

^b Frontier Institute of Science and Technology, Xi'an Jiaotong University, Xi'an 710054, China

^c Department of Physics and Institute of Advanced Materials, Hong Kong Baptist University, Kowloon Tong, Hong Kong, China

^d ARC Centre of Excellence in Exciton Science, School of Chemistry, The University of Melbourne, Parkville, Victoria 3010, Australia

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ABSTRACT

The vertical phase distribution of components in bulk heterojunction is diversified in organic solar cells (OSCs). The electron donors (acceptors) can be accumulated (depleted) at the interface of active layer and charge extraction layer. The variation of vertical phase distribution significantly influences device performance because of its impact on the charge transport and charge recombination. In order to achieve favorable vertical phase distribution in OSCs based on poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene))-co-(1,3-di(5-thiophene-2-yl)-5,7-bis(2-ethylhexyl) benzo[1,2-c:4,5-c']dithiophene-4,8-dione)] (PBDB-T):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), phenyl-C71-butyric-acid-methyl ester (PC₇₁BM) was incorporated into the binary system to fabricate ternary OSCs. In the ternary blend, PC₇₁BM can effectively regulate the phase distribution of PBDB-T and ITIC in vertical direction, which provides favorable vertical phase distribution for charge transport. Moreover, the addition of PC₇₁BM can also effectively increase the π - π stacking coherence length of both donor and acceptor, which facilitates charge transport and reduces the bimolecular recombination. The addition of an appropriate quantity of PC₇₁BM can obviously improve both fill factor and short-circuit current density of the OSC based on PBDB-T:ITIC while open-circuit voltage reduces only about 0.01 V, which indicates a rational low energy loss. Consequently, the ternary OSC exhibits a best PCE of 11.0% compared to the 9.6% PCE of the binary counterpart.

1. Introduction

Organic solar cells (OSCs) have attracted considerable attention because of their advantages of light-weight, low-cost, flexibility, semi-transparency, simple preparation and roll-to-roll production [1–10]. The state-of-art power conversion efficiency (PCE) has exceeded 11% for many types of OSCs, especially more than 13% for the non-fullerene OSCs due to the major efforts developing new organic materials, optimizing the device structures and nanomorphology etc. [11–15]. Further improvement in performance is still in progress for OSC to be commercialized. However, the absorption spectrum of a blend film with a single donor and acceptor or even the non-fullerene acceptor cannot provide full coverage of the solar spectrum in visible region due to the narrow intrinsic absorption window of organic materials, which limits the photon absorption and thus restricts the enhancement of PCE [16–18]. The concept of ternary OSCs, typically consisting of two

donors with complementary absorption spectral and one acceptor (or one donor and two acceptors) in a single active layer, is proposed as an effective strategy to overcome the limitation of the narrow absorption spectra of binary OSCs [19,20]. More importantly, the ternary OSCs are fabricated by using the simple craftsmanship adopted in binary OSCs, which can be scaled up with roll-to-roll printing technique [21–23]. Obvious improvements in short circuit current (J_{SC}) and fill factor (FF) and therefore the improved PCE have been obtained because of the introduction of the third components into binary OSCs [19,21,24]. However, the open-circuit voltage (V_{OC}) and FF are reduced by the third components in some ternary systems, although they can increase the J_{SC} in many ternary OSCs. In detail, the third components may disturb the molecule packing and decrease the coherence length of the host donor or acceptor and increase the trap states density resulting in increased charge recombination and high energy loss [17,25,26].

Recently, fullerene derivatives such as phenyl-C71-butyric-acid-

* Corresponding authors.

E-mail addresses: guanghao.lu@mail.xjtu.edu.cn (G. Lu), haoxt@sdu.edu.cn (X. Hao).

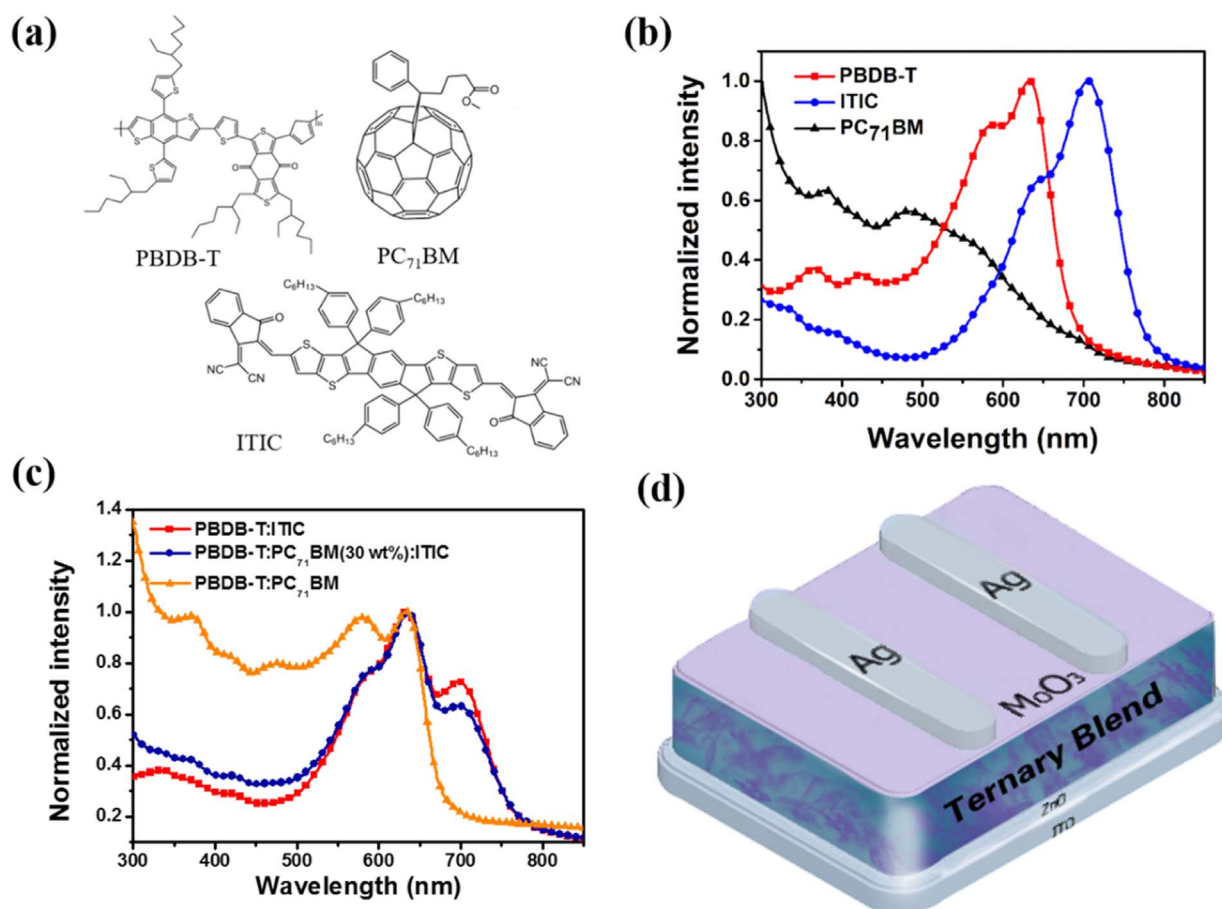


Fig. 1. (a) Molecular structures of PBDB-T, PC₇₁BM and ITIC. (b) UV-vis absorption spectra of PBDB-T, PC₇₁BM and ITIC. (c) UV-vis absorption spectra of binary references and ternary blend film. (d) Diagram of the device structure used in this study.

methyl ester (PC₇₁BM), bisadduct of phenyl-C71-butyric acid methyl ester (bis-PC₇₁BM) and indene-C60 bisadduct (ICBA) as the third components have been introduced into non-fullerene binary systems to achieve higher performance ternary OSCs [27–29]. It is proved that both advantages of high charge mobility in fullerene based acceptors and the advantage of high light absorption intensity in non-fullerene acceptors can be utilized simultaneously in this type of ternary OSCs. Moreover, the additional PC₇₁BM can optimize the nanomorphology and increase the absorption intensity of the active layer in short wavelength region. However, to the best of our knowledge, few reports revealed the role of the fullerene-derivatives on vertical phase distribution in fullerene-derivatives based two-acceptor ternary system.

In this study, we demonstrate a ternary OSC with poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene)-co-(1,3-di(5-thiophene-2-yl)-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)-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) as the host donor and acceptor, and PC₇₁BM as the third component. It is proved that PC₇₁BM can effectively optimize the vertical phase distribution and energy band distribution to facilitate the charge transport and reduce the energy loss.

2. Experimental section

2.1. Materials

PBDB-T and ITIC were purchased from Solarmer Materials, Inc. PC₇₁BM were purchased from Nano-C materials, Inc. All of the materials were used as received without further purification.

2.2. Materials characterization

The conventional absorption spectra (in Fig. 1) were obtained by ultraviolet-visible (UV-vis) dual beam spectrophotometer (TU-1900, PG Instruments, Ltd.). Steady-state Photoluminescence (PL) spectra were collected by a spectrometer (DU420A-OE, ANDOR), the excitation wavelength was 500 nm. Atomic force microscopy (AFM) with tapping mode (Solver P47 PRO, NTMDT Co.) was used to study the nanomorphology of the films. Fluorescence lifetime imaging microscopy (FLIM) (Nanofinder FLEX2, Tokyo Instruments, Inc.) attached with TCSPC module (Becker & Hickl, SPC-150) was performed to study the two-dimensional (2D) fluorescence lifetime distribution. Grazing-incidence wide-angle X-ray scattering (GIWAXS) and Grazing-incidence small-angle X-ray scattering (GISAXS) were performed at BL16B1 beamline of Shanghai Synchrotron Radiation Facility. During the measurements of GIWAXS, the wavelength of incident X-ray was 0.124 nm and sample-to-detector distance was 200 mm. The incidence light angle was 0.12° and mar165CCD was used to collect the scattering signal. For the GISAXS measurements, sample-to-detector distance was 2000 mm and the wavelength of incident X-ray was also 0.124 nm. The incidence angle of X ray was 0.3°. The data was also collected by a mar165 CCD. All of the samples used for GIWAXS and GISAXS measurements were prepared by spin-coating the blend solutions onto Si wafers. The pump beam used in Transient absorption spectroscopy (TAS) was generated by an optical parametric amplifier (OPA, ORPHEUS, Light Conversion, 400 nm, 190 fs). The beam was chopped at 9 kHz and the laser spot size on sample was 2 mm in diameter. The excitation density of the laser was kept as low as 10 μJ cm⁻² in order to avoid the exciton-exciton and exciton-charge annihilation effects [30]. The probe light was a supercontinuum white light. Depth resolved absorption spectra was recorded by oxygen

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