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Improved mobility and lifetime of carrier for highly efficient ternary polymer solar cells based on TIPS-pentacene in PTB7: $PC_{71}BM$

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ABSTRACT

Highly efficient ternary polymer solar cells (T-PSCs) realized by the improved mobility and lifetime of carrier in PTB7: $PC_{71}BM$: TIPS-pentacene blends were fabricated. By adjusting the weight ratios of third component TIPS-pentacene in the binary PTB7: $PC_{71}BM$ blends, we found that the short circuit current and fill factor (FF) were simultaneously enhanced, resulting in a maximum power conversion efficiency (PCE) of 8.09% with 21.3% improvement. The improved photovoltaic performance of T-PSC was mainly due to the enhanced light absorption, energy level cascading, optimized blend morphology, and increased hole mobility. It was also found that the incorporation of TIPS-pentacene increased the average hole lifetime, ensuring efficient hole transport and collection with suppressed bimolecular recombination, contributing to the photocurrent. Additionally, the low thickness dependent row-off of FF indicates TIPS-pentacene is a promising third component for the realization of thick film T-PSC. The improved PCEs were obtained as well for other ternary donor: acceptor: TIPS-pentacene systems, demonstrating that the incorporation of TIPS-pentacene is a wide practicable methodology for the development of highly efficient T-PSCs.

1. Introduction

Polymer solar cell (PSC) consisting of semiconducting polymer and C_{60} derivative as donor and acceptor, respectively, is an emerging device that has the advantages of lightweight, large-area, mechanical flexibility, low-cost and easy fabrication [1–5]. Research efforts during the last decade have significantly improved the photovoltaic performance of PSCs. Although the power conversion efficiencies (PCEs) reaching 10% have recently been achieved for both single junction and multiple junction PSCs [6,7], further performance improvement remains a formidable challenge. The major bottlenecks that hamper the PCE improvement of PSCs are generally attributed to narrow light absorption, unsatisfied exciton migration and dissociation, limited charge transport and collection [8].

Ternary PSCs (T-PSCs) featuring multiple donor materials and one fullerene acceptor in the active layer have emerged as a promising strategy to improve the photovoltaic performance while maintaining the simplicity of the processing conditions used for binary PSCs [9]. Recently, the third component with complementary absorption spectrum was added into the high performance low-bandgap copolymer systems to extend the absorption spectrum and increase the short circuit current (J_{SC}). For example, Yu et al. added a wide-bandgap polymer into PTB7: $PC_{71}BM$ blends to enhance the absorption at middle wavelength, leading to a 12% enhancement in J_{SC} [10]. Yang et al. used two compatible donor polymers with same backbone to form the T-PSCs with fullerene that achieved an increased J_{SC} of 18.7 mA/cm^2, accounting for 23.8% improvement [11].

However, it's still difficult to simultaneously enhance the J_{SC} and fill factor (FF) in ternary systems. In some cases, the performance of T-PSCs is further reduced by the third component acting as recombination center in the ternary blends [12]. One limitation of low-bandgap polymers based T-PSCs is the short hole lifetime causing by low hole mobility. Short hole lifetime typically leads to a serious charge carrier recombination, which prohibit the further improvement of device performance [13]. In addition, charge carrier recombination has negative effect on fabricating thick active layer devices. The photovoltaic performance of thick PSCs is strongly dependent on the competition between charge carrier

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recombination and collection. The effective collection length (L_D) of charge carrier can be expressed as Eq. (1)

$$L_D = \mu\tau E \quad (1)$$

where μ is the carrier mobility, τ is the average carrier lifetime and E is the electric field in the device [14]. Thus, increasing the mobility and lifetime of carrier is beneficial to form high performance T-PSCs with thick active layers.

A reasonable approach to overcome this limitation is to introduce a third component with high mobility into the active layer, where the incorporated third component provides well-matched energy alignment [15], enhances photoconductivity of the active layer [16], mediates the charge transport [17], and suppresses the bimolecular recombination [18], resulting in the overall enhancement of J_{SC}, FF and PCE in T-PSCs. Considering some recently reported high mobility small molecules applied in organic field-effect transistor exhibiting carrier mobilities several orders of magnitude higher than those of PSCs [19], the addition of high mobility small molecule with combined benefits of good absorption in the visible region and suitable band structure in a low-bandgap copolymer system would be a promising strategy for simultaneous enhancement of J_{SC} and FF.

In this work, a high hole mobility (>1 $cm^2V^{-1}s^{-1}$) pentacene derivative of TIPS-pentacene [20], with good absorption in the visible region and cascade energy alignment [21], was adopted to construct Poly({4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b′] dithiophene-2,6-diyl}{3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno [3,4-b]thiophenediyl}) (PTB7) [6,6]:-phenyl C71-butyric acid methyl ester ($PC_{71}BM$): TIPS-pentacene T-PSCs. By controlling the TIPS-pentacene weight ratio in PTB7, the enhanced PCE from 6.67 to 8.09% was obtained due to the increased J_{SC} and FF. The mechanism of TIPS-pentacene based T-PSCs was elucidated by characterizing both the blend morphology of ternary active layers by atomic force microscopy (AFM) and the charge carrier mobility by theoretic simulation using space-charge-limited current (SCLC). Also, the average lifetime and extraction time of hole were also deduced from the impedance spectra. Furthermore, the thick film T-PSCs based on PTB7: $PC_{71}BM$: TIPS-pentacene blends were fabricated to demonstrate the feasibility of printable manufacture with high PCE. Additionally, other kinds of TIPS-pentacene based T-PSCs were studied to exhibit the wide practicability of this strategy for constructing highly efficient T-PSCs.

2. Experimental section

The chemical structures of PTB7, $PC_{71}BM$ and TIPS-pentacene are shown in Fig. 1a, and the structure of T-PSCs is indium tin oxide (ITO)/ZnO (30 nm)/PTB7: $PC_{71}BM$: TIPS-pentacene (100 nm)/MoO_X (15 nm)/Ag (100 nm) as depicted in Fig. 1b. The ITO-coated glass substrates were cleaned according to a routine cleaning procedure [22]. A thin layer of sol–gel ZnO (30 nm) was spin-coated on the top of pre-cleaned ITO-coated glass substrates, and baked at 200 °C for 60 min in ambient. Then, the substrates were transferred to a high-purity N_2 filled glove box. The PTB7, $PC_{71}BM$ and TIPS-pentacene were purchased from Lumtec, Solarmer and Sigma, respectively, and were used as received. The PTB7 was blended with $PC_{71}BM$ at a weight ratio of 1: 1.5 and dissolved in chlorobenzene (CB) with the addition of a small amount of 1,8-diiodooctane (DIO, Sigma, 99.9%) (CB: DIO = 97: 3, vol/vol), with a total concentration of 20 mg/ml. TIPS-pentacene (Sigma, 99.9%) solution was separately prepared in CB at a concentration of 2 mg/mL and then mixed with the blend solutions of PTB7: $PC_{71}BM$. The TIPS-pentacene ratios were increased from 0.25, 0.50, 0.75, to 1.00 wt%, and the PTB7: $PC_{71}BM$: TIPS-pentacene ternary blend solutions were stirred at 50 °C overnight. Then, the solutions were spin-coated on ZnO thin layer. Finally, MoO_X (99.98%, Aldrich) layer was deposited onto the top of active layer at a rate of 1 Å/s at a vacuum pressure of 3.0×10^{-3} Pa, followed by the deposition of Ag anode at a rate of 10 Å/s in the same vacuum chamber. The typical area of T-PSCs was 0.02 cm^2.

Ultraviolet–visible (UV–vis) absorption spectra were recorded by a Shimazu UV1700 system. The current density–voltage (J–V) characteristics of T-PSCs were measured with a simulated light source (CHF-XM35, Beijing Trusttech) with an illumination power of 100 mW/cm^2. Electrical data were recorded using a Keithley 4200 source-measure unit. External quantum efficiency (EQE) spectra were measured under the lump light passing through a monochromator, which was calibrated by a standard Si solar cell. The blend morphology was characterized by AFM (Agilent, AFM 5500). The hole-only devices were fabricated with the structure of ITO/MoO_X (15 nm)/PTB7: $PC_{71}BM$: TIPS-pentacene (100 nm)/MoO_X (15 nm)/Ag (100 nm), and the electron-only devices were fabricated with the structure of ITO/ZnO (30 nm)/PTB7: $PC_{71}BM$: TIPS-pentacene (100 nm)/bathophenanthroline (Bphen) (5 nm)/Ag (100 nm). The impedance spectra were measured by Agilent precision impedance analyzer 4294A. All measurements were carried out under ambient condition without encapsulation.

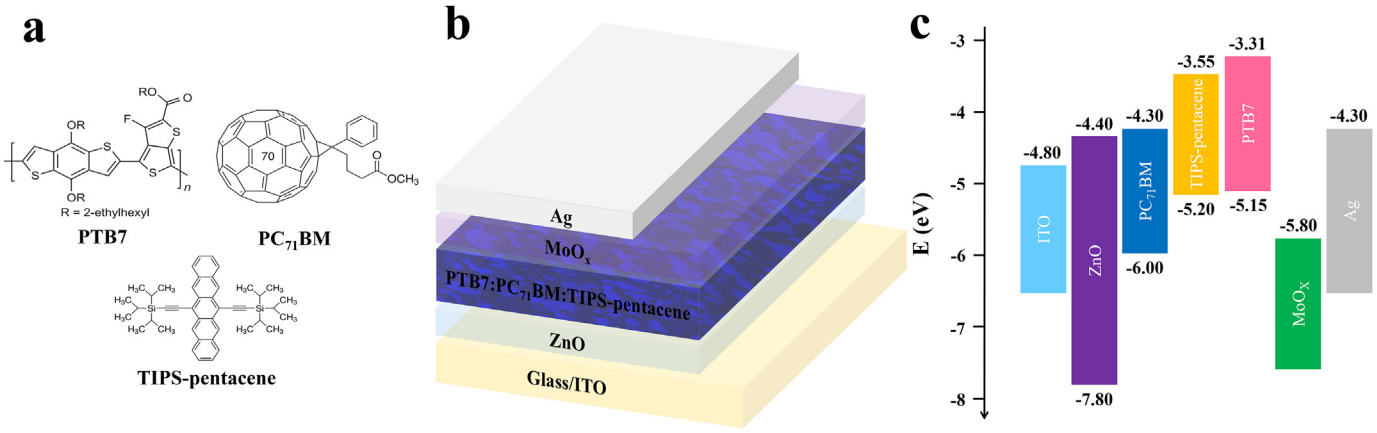

Fig. 1. (a) Chemical structures of components in active layer. (b) Device structure of T-PSCs. (c) Energy band diagram of materials used in T-PSCs.