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Simultaneous enhancement of short-circuit current density, open circuit voltage and fill factor in ternary organic solar cells based on PTB7-Th:IT-M:$PC_{71}BM$

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ABSTRACT

Recently, studies on ternary organic solar cells (OSCs) have revealed their potentials for achieving the improved device performances. However, owing to the trade-off between the short-circuit current density (J_{SC}) and open circuit voltage (V_{OC}), the mismatch of the energy levels between donors and acceptors leads to a large energy loss and then leads to a lower V_{OC} in most ternary systems. In this study, we incorporated 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)− 5-methylindanone)− 5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2′,3′-d′]-s-indaceno[1,2-b:5,6-b']-dithiophene (IT-M) into a PTB7-Th:$PC_{71}BM$ host system as the third component, which has a higher energy level of the lowest unoccupied molecular orbital (LUMO) than that of $PC_{71}BM$. The introduction of IT-M adjusts the energy-level cascade, enhances the absorption intensity and modulates the film morphology, which facilitate the charge generation, enhance the charge transport, and suppress the charge recombination, as manifested by the significantly enhanced V_{OC}, J_{SC}, and fill factor (FF). Therefore, the results indicate that a simultaneous enhancement of V_{OC}, J_{SC}, and FF can be achieved by incorporation of IT-M in ternary OSCs, providing a higher efficiency.

1. Introduction

In recent years, bulk-heterojunction (BHJ) solar cells consisting of conjugated polymer donor and fullerene derivative acceptor have attracted a significant attention owing to their advantage of low cost, lightweight, ease of fabrication [1], and compatibility with flexible substrates [2–7]. Furthermore, they are advantageous owing to their low temperature solution processability and mechanical flexibility [8–11] which enable us to fabricate BHJ solar cells using the roll-to-roll printing technology [10] and realize the aim of grid parity. At present, the application of organic solar cells (OSCs) is limited by their insufficient stability and relatively low power conversion efficiency (PCE) [12]. Various approaches have been employed to improve the PCE of OSCs, which involve active materials design [13,14], nanoscale morphology optimization [15] and interface engineering [16]. Furthermore, two main strategies of tandem [17] and ternary solar cells [18] have been rapidly developed to broaden the absorption and improve the open circuit viltage (V_{OC}), which can facilitate the exciton dissociation and enhance the carrier transport, thus providing a higher PCE. However, there are various challenges in fabricating sophisticated configurations of tandem OSCs, including the processing of the intermediate layer, the strict-control of the film thickness and high production cost, which reduce their potentials for practical applications [17,19].

Compared with tandem systems, ternary OSCs containing two donors and one acceptor (or one donor and two acceptors) provide a potentially effective route to overcome the above challenges, achieving a high short circuit current (J_{SC}), and thus a high efficiency, owing to the simple active layer fabrication with only one processing step and high reproducibility [19,20]. In addition to the broadened and enhanced absorption, ternary OSCs have various other unique advantages. The introduced third components can not only improve the film morphology, alter the local environment at the donor-acceptor (D-A) interface, and adjust the charge carrier mobility, but also it can optimize the cascade energy levels [21,22]. Owing to the above potentials, ternary PSCs have been extensively investigated. Various third components have been reported, such as donor polymers, fullerene [23] and fullerene-free [24] derivative acceptors, etc. Certainly, some performance of ternary OSCs is worse than that of binary OSCs [25].

The PCE of solar cells is proportional with the product of V_{OC}, J_{SC},

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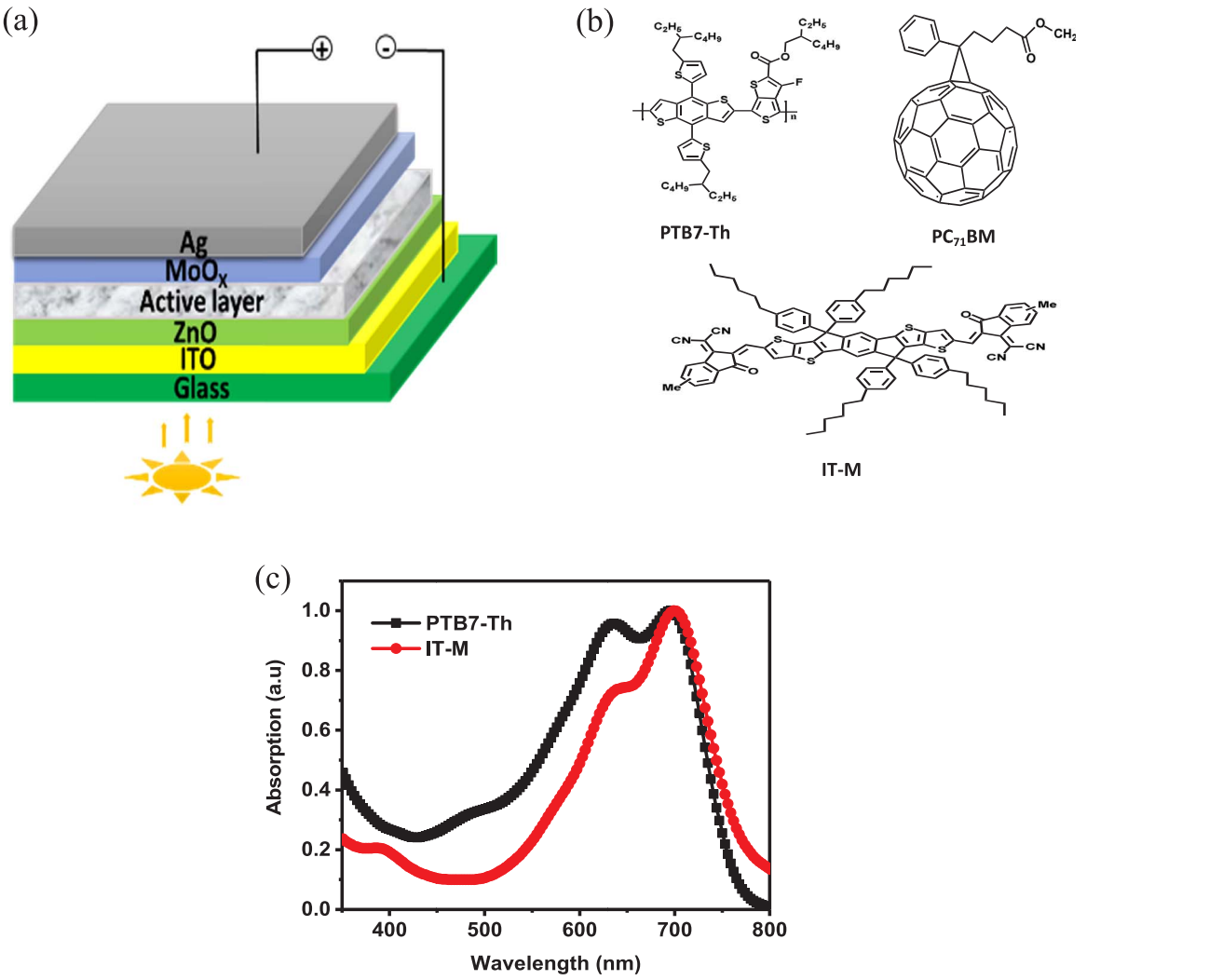

Fig. 1. (a) Device diagrammatic sketch. (b) PTB7-Th, $PC_{71}BM$ and IT-M molecular structures. (c) Absorption spectra of PTB7-Th and IT-M.

and fill factor (FF). However, owing to the trade-off between J_{SC} and V_{OC} [26], the PCE can be enhanced only if a decrease of V_{OC} can be avoided. Many ternary systems can simultaneously improve usually only one or two key parameters of the OSCs. For example, BDT-3T-CNCOO was added into a blend of PBDTTPD-HT: $PC_{71}BM$, which yielded a PCE of 8.40% with increased J_{SC} and FF but decreased V_{OC} [27]. Similarly, a ternary OSCs with a PCE of 10.35% was achieved through incorporating $PC_{71}BM$ into a binary system based on PPBDTBT:ITIC [24]. The mismatch in energy levels between acceptors and polymer donors cannot be eliminated in some ternary systems, which causes a large energy loss, and consequently a low V_{OC} [28–30]. Nevertheless, Thompson et al. demonstrated that V_{OC} of ternary OSCs is composition-dependent and tunable over the full range of the corresponding limited number of binary blends in 2011 [31]. In the following, they observed that even the smallest amount of the third component in the ternary blend had a large effect on V_{OC}, which evolved linearly with composition across the ternary blend regime [32]. Recently,Yu et al. incorporated a polymer donor PID2 into a blend active layer of PTB7-Th and $PC_{71}BM$, and obtained a simultaneous improvement of J_{SC}, V_{OC}, and FF, leading to a PCE of 9.2% of the ternary polymer solar cells (PSCs) [33]. In 2016, IFBR was mixed with a blend film of PBTA-BO and $PC_{61}BM$, which yieded a PCE of 8.11% with the enhanced J_{SC}, V_{OC}, and FF [22]. In the same year, Hou et al. synthesized IT-M and introduced Bis[70]PCBM into a binary system based on PBDB-T:IT-M, which yielded a PCE of 12.2%. In addition to the enhanced J_{SC} and FF, V_{OC} changed linearly with the content of the third acceptor Bis[70]PCBM in the BHJ blend of PBDB-T:IT-M reported by Hou et al. in 2016 [18]. These results indicate that the improved V_{OC}, J_{SC}, and FF in ternary OSCs can be obtained only if an appropriate donor/acceptor can be introduced as the third component [34]. It is worth noting that the third component should have tunable highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, which would provide a low energy loss and large V_{OC} [35]. Similar phenomena have been reported in several other systems as well, indicating the versatility of this approach [36,37].

In this study, a series of ternary inverted OSCs were fabricated by introducing nonfullerene acceptor into a host binary blend of conjugated polymer poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-*co*-3-fluorothieno[3,4-b]thiophene-2-carboxylate] (PTB7-Th):fullerene [6,6]-phenyl-C_{71}-butyric acid methyl ester ($PC_{71}BM$) system. IT-M was selected as the third component owing to a higher LUMO energy of − 3.91 eV, compared with the value of − 4.3 eV of $PC_{71}BM$, which can provide a larger driving force for an efficient charge separation. Furthermore, the two acceptors are miscible with PTB7-Th in chlorobenzene (CB). IT-M exhibited cascaded HOMO and LUMO energy levels, in those of PTB7-Th and $PC_{71}BM$, which energetically favor the charge transfer at the interfaces between the three components. The main absorption of IT-M is similar to that of PTB7-Th, as showed in Fig. 1(c). The absorption intensity of the ternary blend films increases with the doping amount in the range of 600–750 nm.