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Novel brominated compounds using in binary additives based organic solar cells to achieve high efficiency over 10.3%

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ABSTRACT

Solvent additives have been considered as a simple and efficient method to increase the performance of bulk-heterojunction (BHJ) organic solar cells, in which, the morphology of the active layer could obtain further improvements by using the binary solvent additives. In this paper, a series of brominated compounds, 1-Bromo-4-butylbenzene (Brbb), 1-Bromo-4-*n*-hexylbenzene (Brbh) and 1-Bromo-4-*n*-octylbenzene (Brbo), have been respectively incorporated with 1, 8-diiodooctane (DIO) and regarded as binary solvent additives to fabricate highly efficient bulk heterojunction (BHJ) organic solar cells (OSCs). Compared with the BHJ film based on single additive, the binary additives contained BHJ film shows increased optical absorption, efficient charge transport and better active layer morphology, leading to an enhancement of short-circuit current (J_{SC}) together with a higher achieved fill factor (FF). The conventional BHJ device using PTB7: $PC_{71}BM$ or PTB7-th: $PC_{71}BM$ with the binary solvent additives exhibit enhanced PCE of 8.13% and 10.31%, respectively, which is much higher than that of single additive based devices (7.04% for PTB7 and 8.73% for PTB7-th). The optimized performance of BHJ devices indicates that these brominated compounds are promising additives to improve device efficiency.

1. Introduction

The bulk-heterojunction (BHJ) organic solar cells (OSCs) based on the blends of polymer and fullerene derivative have obtained considerable improvements in recent years due to their unprecedented features of mechanical flexibility, light weight, low-cost, and easy fabrication [1–3]. The OSCs have been expected to become promising candidates for the technology to reach a commercially viable state with new materials and techniques, which allows for devices with power conversion efficiency (PCE) exceeding 10% [4–6]. There are also many challenges to improve the BHJ devices PCE, liking the light absorption, charge generation and the morphology of the interpenetrating networks of donor and acceptor materials, which could limit the PCE [7,8]. Among them, the morphology of the active layer plays an important role in the BHJ solar cells for the performance of the OSCs. To achieve high PCE, the active layer should have suitable phase-separated domains and a bi-continuous interpenetrating network, which provides not only the interfaces for charge separation of the photo-generated excitons, but also serves as percolation pathways for the separated charge carriers [9,10].

The BHJ OSCs efficiencies have been optimized by processing conditions, such as solvent annealing [11], thermal annealing [12] and the application of solvent additives [13]. These methods can affect the surface morphologies of BHJ films, the phase separation, charge generation and transport as well as light absorption [14,15]. Among various processing methods, the solvent additives have been considered as a simplest and efficient approach to optimize performance of the devices [16,17]. According to the reported works, solvent additives, 1, 8-diiodooctane (DIO) [18,19], 1,8-octanedithiol (ODT) [20,21] and 1-chloronaphthalene (CN) [22] have been selected to prevent oversized phase separation and improve the morphology of OSCs based on different BHJ systems. The most representative processing additive is DIO that has been used to select solubility of $PC_{71}BM$ resulting in reducing phase separation and improvement of the BHJ morphology [23,24]. Although it is an attractive method to improve device performance

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by introducing additives, most reported work on a single additive principally influences one aspect, making detailed control of the morphology difficult [25]. To address this, binary additives strategies have been utilized in OSCs to balance these crucial aspects. However, few reports are focused on binary additives up to now, especially brominated additives, and the working mechanism is not to study systematically. The introducing of binary additives in bulk-heterojunction OSCs systems can be attributed to the modification of the surface morphology and the improvement of phase separation in active layers [26,27].

In this work, three novel brominated additives, 1-Bromo-4-butylbenzene (Brbb), 1-Bromo-4-*n*-hexylbenzene (Brbh) and 1-Bromo-4-*n*-octylbenzene (Brbo) that differ only in the length of alkyl side-chains were firstly used and studied in additive system. The use of alkyl side-chains is able to achieve optimal phase separation and tunable light absorption [28,29]. They have simple and stable structure, and they are normally stored under nitrogen atmosphere. Their boiling point are 242 °C, 145 °C and 200 °C respectively comparing to 131 °C of the solvent chlorobenzene (CB). Herein, we provide a systematic investigation on the blend of 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) or poly[[2,6′-4,8-di(5-ethylhexylthienyl)benzo [1,2-b,3,3-*b*]dithiophene][3-fluoro-2[(2ethylhexyl)carbonyl]thieno [3,4-*b*]thio-phenediyl]] (PTB7-Th): [6,6]-phenyl-C71-butyric acid methyl ester ($PC_{71}BM$), using mixture solvent additive to improve the absorption and modify the morphology of the blend. We have demonstrated enhancing PCE of the polymer solar cell fabricated by insertion of binary processing additive of Brbb/DIO, Brbh/DIO and Brbo/DIO in CB with an optimized ratio. The best device performance is increased from 8.73% to 10.31% with the V_{OC} of 0.78 V, J_{SC} of 19.23 mA/cm^2 and FF of 69.1% using the conventional device. We also investigate the applicability of mixed additives in PTB7:$PC_{71}BM$ blend system, enhancing PCE from 7.04% to 8.13%. The results indicate that the novel brominated additives are promising candidates to increase the light-absorption and improve the size of phase separation. Our researches also enriched the choice of auxiliary additives and demonstrate a new approach to realize high performance OSCs.

2. Experimental section

The molecular structures of low band-gap polymer, the donor, PTB7 and PTB7-Th, the acceptor, $PC_{71}BM$, and all additives (DIO, 1-Bromo-4-butylbenzene (Brbb), 1-Bromo-4-*n*-hexylbenzene (Brbh) and 1-Bromo-4-*n*-octylbenzene (Brbo)) are shown in Fig. 1a. All the devices were fabricated on conventional structure of glass/indium tin oxide (ITO)/ZnO/active layer/MoO_3/Ag as depicted in Fig. 1b. Fig. 1c illustrates the highest occupied molecular orbital (HOMO), lowest occupied molecular orbital (LUMO) energy levels. The pre-coated ITO glass substrate was cleaned sequentially with detergent, deionized water, acetone, alcohol followed by drying and ultraviolet-ozone treatment for 30 min. About 30 nm ZnO layer was spin-coated onto the ITO glass. After annealing at 200 °C for 60 min, the substrates were transferred into a nitrogen-filled glove box. The PTB7:$PC_{71}BM$ and PTB7-Th: $PC_{71}BM$ were dissolved in chlorobenzene (CB) solvent (1:1.5, 25 mg/ml in total) with stirring and heating overnight. Then, this mixture solution was spin-coated onto the ZnO layer from (a) CB with 3% DIO solution (CB = 97 vol% and DIO = 3 vol%); (b) CB with 3% DIO and 3% Brbb solution (CB = 94 vol%, DIO = 3 vol% and Brbo = 3 vol%); (c) CB with 3% DIO and 3% Brbh solution (CB = 94 vol%, DIO = 3 vol% and Brbb = 3 vol%); (d) CB with 3% DIO and 3% Brbo solution (CB = 94 vol%, DIO = 3 vol% and Brbh = 3 vol%). Active layer

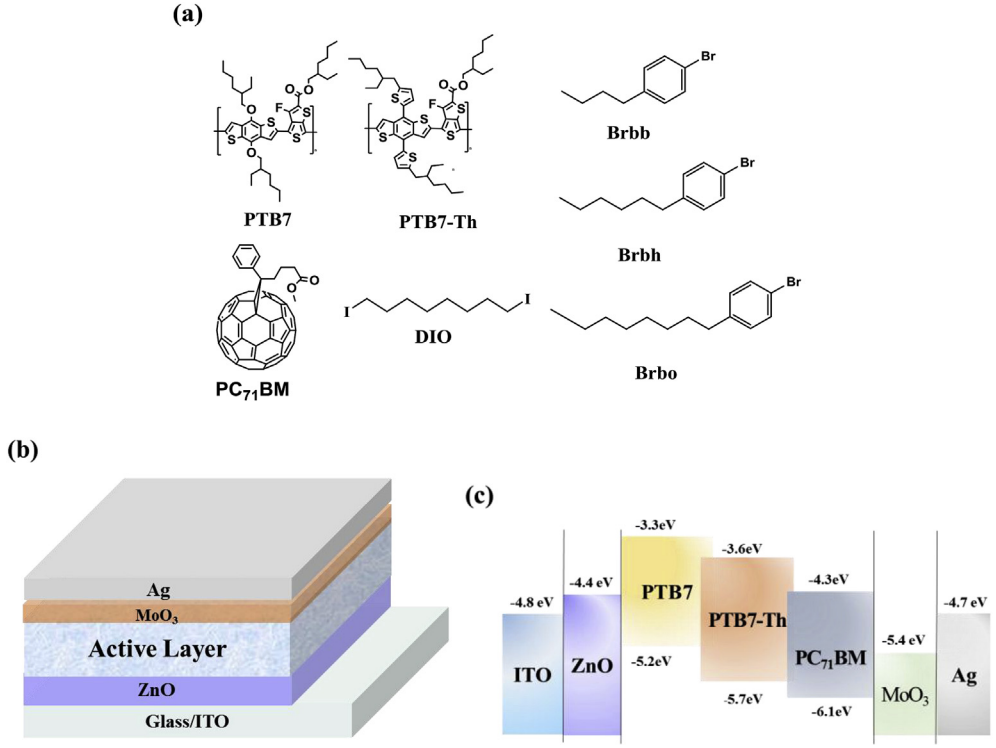

Fig. 1. (a) Chemical structure of the acceptor, the donor and the additives used in this study. (b) Device structure of the BHJ solar cells. (c) Band diagram levels of the proposed device structure.