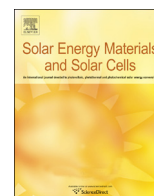




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journal homepage: www.elsevier.com/locate/solmatEffect of solvent additive and ethanol treatment on the performance of PIDTDTQx:PC₇₁BM polymer solar cellsXixiang Zhu^a, Fujun Zhang^{a,*}, Qiaoshi An^a, Hui Huang^b, Qianqian Sun^a, Lingliang Li^a, Feng Teng^{a,*}, Weihua Tang^c^a Key Laboratory of Luminescence and Optical Information, Ministry of Education, Beijing Jiaotong University, Beijing 100044, PR China^b School of Electrical Engineering, Beijing Jiaotong University, Beijing 100044, PR China^c Key Laboratory of Soft Chemistry and Functional Materials, Ministry of Education, Nanjing University of Science and Technology, Nanjing 210094, PR China

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ABSTRACT

Solvent additive 1,8-diiodooctane (DIO) is not almighty for improving the performance of polymer solar cells (PSCs). In this paper, the effect of solvent additive DIO and ethanol treatment on the performance of polymer solar cells (PSCs) with poly{[4,9-dihydro-4,4,9,9-tetra(4-hexylbenzyl)-s-indaceno[1,2-b:5,6-b']-dithiophene-2,7-diyl]-alt-[2,3-bis(3-(octyloxy)phenyl)-2,3-dihydro-quinoxaline-2,2'-diyl]} (PIDTDTQx) and [6,6]-phenyl-C71-butyric acid methyl ester (PC₇₁BM) as the active layer was investigated. The power conversion efficiency (PCE) was decreased from 4.57% to 1.96% by adding 4 vol% DIO solvent additive for the active layer processed with 1,2-dichlorobenzene (DCB) as solvent. The negative effect of DIO on PCE from 1.94% to 1.18% of PSCs processed with chlorobenzene (CB) as solvent was further demonstrated. The PCE values of PSCs with DIO additive can be effectively increased from 1.96% to 3.71% for DCB as solvent and from 1.18% to 1.89% for CB as solvent by ethanol treatment on the active layer. The crystalline and morphology of active layers play the key role in determining the performance of PSCs.

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1. Introduction

Polymer solar cells (PSCs) have attracted extensive attention for their potential to be clean and sustainable energy sources with several advantages, including low processing cost, light weight and flexible fabrication [1–4]. The manufacture and installation of a solar park based on PSCs following a concept has been realized by Krebs et al., a series of iconic research results have been achieved based on large scale PSCs [5–8], which strongly promote the basic research on performance improvement of PSCs. Since the discovery of the photo-induced electron transfer from conjugated polymer to fullerene derivatives, the bulk-heterojunction structure has been extensively applied for better exciton dissociation due to bi-continuous interpenetrating network structure of electron donor and acceptor [9]. The molecular arrangement of electron donor/acceptor materials plays an important role in exciton dissociation and charge carriers transport, which strongly impacts on the performance of PSCs [10,11]. Many strategies have been successfully developed and employed to optimize the morphology of active layers, such as solution treatment, solvent additives, and thermal

annealing treatments [12–16]. Among them, adopting solvent additives has been demonstrated to be an effective and simple method to adjust morphology of active layers. The common used solvent additives, such as 1-chloronaphthalene (CN), 1,8-diiodooctane (DIO) and diphenylether (DPE), have selective dissolution of fullerene derivatives and relative high boiling points [17–19]. The high boiling point (BP) solvent additives have played an important role in controlling electron donor or acceptor domain sizes, which would effect of the balance between exciton dissociation and charge carrier transport. In fact, DIO as a high BP solvent additive has been proved to be the most successful additive for performance improvement of PSCs [20–22]. Liang et al. reported that the PCE of PSCs with PTB7: [6,6]-phenyl-C71-butyric acid methyl ester (PC₇₁BM) as active layer was increased to 7.40% from 3.92% upon mixing of 3 vol% DIO to the host solvent chlorobenzene (CB) [23]. Klein et al. also reported that the PCE of PSCs with PCDTBPt:PC₇₁BM as active layer was increased from 2.5% to 4.6% by adding 3 vol% solvent additive DIO to the host solvent 1,2-dichlorobenzene (DCB) [24]. Recently, Gedefaw et al. reported that the PCE of PSCs with PBDFQ-T:PC₆₁BM as active layer was increased from 2.18% to 5.30% by adding 3 vol% solvent additive DIO, the PCE improvement should be attributed to the finer adjustment on nanostructure of active layer for the better balance between charge transport properties and light absorption [25]. Up to now, there are few researches about the negative effect

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of DIO additive on performance of PSCs. Kyaw et al. reported that the PCE of small-molecule solar cells with p-DTS(FBTTh₂)₂:PC₇₁BM as active layer was decreased to 3.32% from 8.03% by an excess amount of DIO (from 0.4 vol% to 0.8 vol%), resulting in the over-aggregation of the donor phase [26]. Do et al. reported that the PCE of PSCs based on 3T-BO20:PC₆₁BM reduced from 1.92% to 1.76% by addition of 1 vol% DIO additive [27]. Therefore, the underlying reason of DIO additive function on performance of PSCs should be further needed to be clarified in the different polymers system.

Another effective strategy for PCE improvement of PSCs is using low boiling point polar solvent treatment on pristine active layer, which can wash out used solvent and solvent additive from active layer before deposition of metal electrodes. Many research results exhibited that polar solvent, such as ethanol and methanol, have positive effect on the device performance for optimization of the phase separation in the active layer, the increase of built-in potential due to the passivation of surface traps [28,29]. Guo et al. successfully synthesized a novel band gap polymer poly{[4,9-dihydro-4,4,9,9-tetra(4-hexylbenzyl)-s-indaceno[1,2-b:5,6-b']-dithiophene-2,7-diyl]-alt-[2,3-bis(3-(octyloxy)phenyl)-2,3-dihydro-quinoxaline-2,2'-diyl]} (PIDTDTQx) and obtained a high PCE of 7.11% with optimized PIDTDTQx:PC₇₁BM doping weight ratio as 1:4 [30]. In this paper, we investigated the effect of solvent additive DIO on performance of PSCs based on the blend of PIDTDTQx/PC₇₁BM with DCB or CB as solvent, respectively. It is apparent that PCE values of PSCs with DIO decreased from 4.57% to 1.96% for DCB as solvent and decreased to 1.18% from 1.94% for CB as solvent. The PCE values of PSCs with DIO additive were a large extent restored from 1.96% to 3.71% and from 1.18% to 1.89% by ethanol treatment on the active layers.

2. Experimental details

The indium tin oxide (ITO) glass substrates with sheet resistance 15 Ω/sq were cleaned continuously in the ultrasonic baths containing acetone, detergent, de-ionized water, and ethanol. Then, the cleaned ITO substrates were blow-dried by high pure nitrogen gas and then treated by UV ozone for 10 min. PEDOT:PSS (Clevios P VPAI 4083,

purchased from H.C. Starck co. Ltd.) films were fabricated onto the cleaned ITO substrate by the spin coating method at 5000 rpm for 40 s and then annealed at 120 °C for 10 min in room conditions. The polymer material PIDTDTQx (Product no: OT51501, purchased from Organtec Materials Inc.), and PC₇₁BM (Product no: LT-S923, purchased from Luminescence Technology Corp) with a weight ratio of 1:4 were dissolved in DCB or CB at a concentration of 50 mg/ml, respectively. The 1,8-diiodooctane (DIO) (Product no: A10867, purchased from Alfa Aesar Chemical Co., Ltd.) additive was added into the solutions before the spin-coating process. The blend solutions were stirred with a magnetic stirrer at 70 °C for 12 h. Then the active layers were fabricated by the spin-coating method at 2500 rpm for 40 s in a high-purity nitrogen-filled glove box. And then 10 min for drying the active layer, ethanol solvent was spin-coated on top of the active layers for further optimizing the morphology of active layer. The LiF/Al (0.9 nm/100 nm) combined cathode was deposited by thermal evaporation under 10⁻⁴ Pa conditions. The thickness was monitored by a quartz crystal microbalance. The vertical overlap of the ITO anode and Al cathode is defined as the active area about 3.8 mm².

The current density voltage (*J*-*V*) characteristics of the devices were measured using a Keithley 4200 source measurement unit. The absorption spectra of the films were obtained using a Shimadzu UV-3101 PC spectrometer. The external quantum efficiency (EQE) spectra of the ternary PSCs were measured by a Zolix Solar Cell Scan 100. The X-ray diffraction (XRD) spectra of the PIDTDTQx:PC₇₁BM films drop-cast onto PEDOT:PSS/ITO substrate were obtained by using a Bruker D8 Advance X-Ray diffractometer (XRD). The morphology and phase images of blend films were investigated with atomic force microscopy (AFM) using a multi-mode Nanoscope IIIa operated in tapping mode. The chemical structures and energy levels of the used materials as well as the schematic diagram of PSCs are shown in Fig. 1.

3. Results and discussion

Solvent additive DIO has been widely applied in improving performance of PSCs by adjusting the donor/acceptor phase separation,

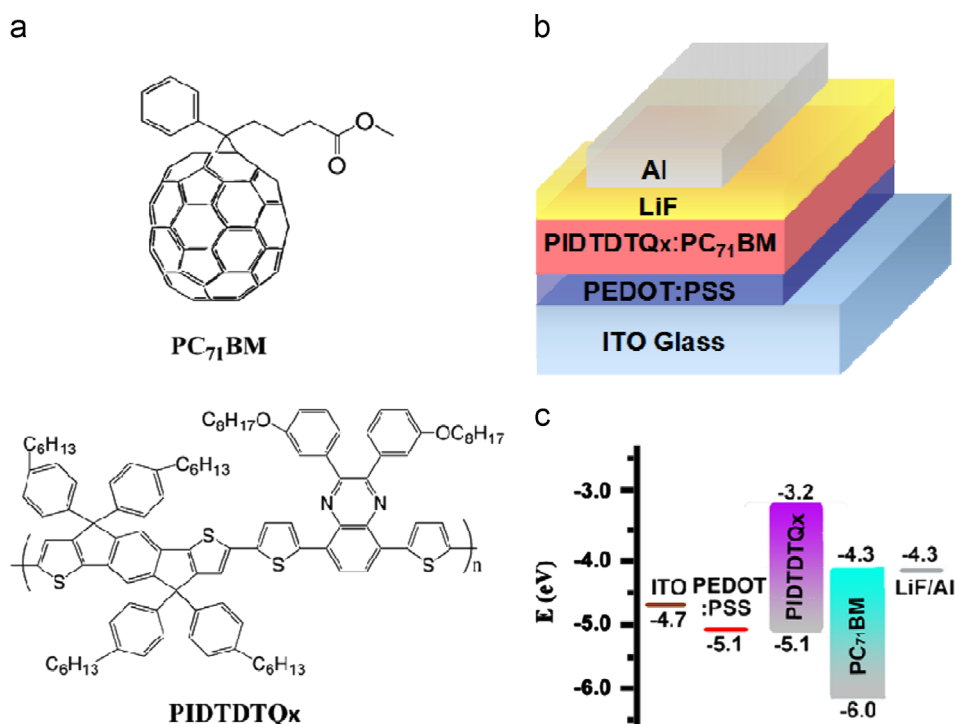


Fig. 1. (a) Chemical structures of PIDTDTQx and PC₇₁BM. (b) Schematic configuration of the PSCs. (c) Energy levels of the used materials.

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