



Additive assisted morphological optimization of photoactive layer in polymer solar cells



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ABSTRACT

Herein, we clearly demonstrate that the inclusion of the organic solid additive (2,3-dihydropyridine, DOH) into the poly(diketopyrrolopyrrole-terthiophene) (PDPP3T) and phenyl-C₆₁-butyric acid methyl ester (PCBM) (PDPP3T:PCBM) photoactive blend system alters the nanoscale morphology and enhances the photovoltaic (PV) performance of the inverted bulk heterojunction (BHJ) based polymer solar cells (PSCs). The influence of DOH additive casted PDPP3T:PCBM thin films on the optical, morphology and structural features is evaluated and correlated with PV characteristics. Topography images through atomic force microscopy reveal that the incorporation of DOH into PDPP3T:PCBM induces a finer nanoscale phase segregation between polymer and fullerene domains with fibrillar morphology. The PV performance of the DOH processed PDPP3T:PCBM devices is evaluated by current-voltage (*J-V*) characteristics and compared with pristine and 1, 8-diiodooctane (DIO) modified PDPP3T:PCBM devices. Interestingly, the incorporation of DOH (0.5 wt%) into PDPP3T:PCBM device witnessed the best PCE of 6.36%, which is significantly higher (69.1%) than that of the reference (3.76%). This significant enhancement in the performance of the device is mainly attributed to a dramatic increase in the short-circuit current density and fill-factor due to the improved bicontinuous interpenetrated phase separation and balanced charge transport. In addition, the measurements on photo-induced charge carrier extraction by linearly increasing voltage reveal that DOH incorporated devices exhibit higher mobility and charge carrier density as compared to those of pristine modified BHJ PSCs. The presence of vicinal functional groups in DOH contributes to the possible molecular level interactions with the blend components and accounts for the morphology and device performance enhancements.

1. Introduction

Bulk heterojunction polymer solar cells (BHJ PSCs) based on donor/acceptor (D/A) bicontinuous interpenetrating networks receive much promise due to their ease of fabrication, light weight, flexibility, large area processability, low cost and environment friendliness [1]. The development of various performance improvement strategies such as designing an efficient photoactive donors [2,3], altering the nanoscale morphology of active layer [4–7], incorporation of buffer/interfacial

layers [8–12] and engineering and designing new device architectures [13] resulted in a power conversion efficiency (PCE) of the single junction BHJ PSCs to exceed over ~10% [14–17]. Besides, the intrinsic properties of photoactive layer materials such as band gaps, energy level alignment with buffer layer and textural properties of D/A blends which include crystallinity of polymers, conformations, domain size/purity, material miscibility and hierarchical structures, play important roles in influencing the performance of PSCs [18]. Many efforts have been devoted to understand the relation between the morphology and

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the performance of PSCs [19,20]. For example, the morphology of the active layer has been controlled by adopting several techniques including the choice of host solvent [21,22], utilizing mixed solvents or co-solvents [23,24], varying the blending ratio of polymer and fullerene [6], chemical modification [25,26], thermal annealing or heat treatment [27], solvent treatment [28,29], solvent-vapor treatment [30] and inclusion of a liquid/solid additive as a processing additive [31]. Two independent or synergistic factors, namely, self assembly via π - π^* stacking and segregation of blend components through chemical and non-chemical interactions were primarily identified to influence the morphology of the active layer.

Among the various strategies to modulate the morphology of active layer blend, the utilities of processing additives have been reported to be simple for obtaining enhanced PCE in BHJ PSCs. It must be noted that several aspects need to be considered on the selection of additive for modifying the D/A blend characteristics. Few guidelines are deduced in choosing the parent or host solvent and the processing additives [32–34]. Based on the literature, the roles of processing additives in BHJ PSCs are identified based on any of the three requirements: (i) non-reactive with the polymer or fullerene derivative, (ii) selective solubility towards one of the blend components (typically fullerenes) and (iii) higher boiling point than the host solvent. The mechanism of PCE enhancement depends on the nature of the processing additive which satisfies any of the above-mentioned requirements. Functional additives are known to manipulate the morphology of the active layer components and prevent the use of post-annealing steps [35]. Few of the high boiling point additives such as 1,8-diodooctane (DIO) [36], nitrobenzene [37], 1-chloronaphthalene (CN), N-methyl pyrrolidine (NMP) [38], methylthiophene, hexylthiophene [39], several alkanedithiols [40], butanedithiol [41], diphenyl ether [42], etc. have been utilized to enhance the PCE of PSCs. Generally, DIO is used in BHJ PSCs as a solvent additive having a boiling point higher than the host solvent. DIO hinders the solidification of polymers and augments the blend film to develop desirable nanomorphology without PCBM aggregation. Upon introduction of an additive (liquid/solid) into photoactive layer with the parent solvent, it is found that the film formation kinetics changes dramatically to result in optimal morphology. The readers are strongly encouraged to refer relevant articles outlining the beneficial use of various additives for morphology optimization to achieve high-efficiency BHJ solar cells [33,43–45]. In all cases, the molecular structures of the additive and its interactibility with the blend components play vital roles in influencing the morphology and PCE of the fabricated devices.

The PCE of BHJ PSCs is defined as the ratio between the open-circuit voltage (V_{OC}), the output current at short-circuit conditions (J_{SC}) and fill-factor (FF) to the incident light intensity. It is imperative that maximum PCE is achievable through increasing V_{OC} , J_{SC} and FF. The high value for J_{SC} can be achieved by selecting efficient photoactive materials with absorption spectra overlapping the photon flux density or incident solar spectrum. Recently, the use of low band gap (E_g) polymers ($E_g < 1.80$ eV) shows great promise in improving PCE of BHJ PSCs [46]. The most successful approach to developing low E_g photoactive donor polymer involves the introduction of electron rich and deficient moieties along with the conjugated chains and produce push-pull or donor-acceptor conjugated polymer chains. Based on the modular approach a variety of conjugated polymers have been developed.

Diketopyrrolopyrrole (DPP) based conjugated polymers have emerged as the promising low E_g donors having alternating electron rich moieties and conjugated chains [47,48]. DPP-based conjugated polymers exhibit strong electron withdrawing nature, tunable optical properties (up to 1000 nm), and high mobilities for holes and electrons, which can result in high photocurrents and good fill factors in BHJ PSCs [49]. Specifically, poly(diketopyrrolopyrrole-terthiophene) (PDPP3T) having alternate DPP and terthiophene units possess a high hole mobility ($\mu_h \sim 0.04$ cm²/V s) compared to standard p-type conjugated polymers, P3HT ($\mu_h \sim 10^{-3}$ cm²/V s) and almost balanced electron and

hole mobility [50]. Interestingly, solution processed pristine PDPP3T has also been proven to be an efficient hole transport layer in perovskite solar cells based on our previous report [51]. The literatures on BHJ PSCs with PDPP3T as the donor polymer confirm that the enhancement of the PCE can be achieved using solid additives. Studies have been reported to optimize the morphology of PDPP3T:[phenyl-C61-butyric acid methyl ester] (PCBM) blend film using ternary solvents including 1,2-dichlorobenzene (DCB), chloroform and DIO [23]. The effect of DIO on the performance enhancement of PDPP3T based BHJ PSCs has been investigated by us and few other researchers [23,36,52,53]. It should be noted that the aggregation behaviour depends on the multiple variables such as chemical structures of the blend components [54], the molecular weight of the donor polymer [55], the concentration of processing solvent, and annealing temperatures [56], etc. However, major challenges exist in predicting the morphology of the photoactive blend with multiple influencing factors such as intermolecular interactions, self-assembly, and segregation of the polymer and fullerene domains. Reports on the use of a functional solid additive which can have both chemical and non-chemical interactions with either PDPP3T or PCBM in BHJ PSCs are scarce.

In our previous work, we demonstrated the effect of at least two widely used different solvent additives (DIO and ODT) concerning their functional groups, on the morphology, structural, and charge carrier dynamics in solution processed inverted type PDPP3T:PCBM blend system and correlated their PV performances [52,53]. Previous reports suggested that hydrogen bonding has also been utilized to stabilize the active layer by manipulating the distribution of polymer and fullerene aggregates in the active layer [18,25,29,57]. We also demonstrated through another study that treatment of isopropyl alcohol atop the active layer poly(3-hexylthiophene)(P3HT) (P3HT:PCBM) induces hydrophilic and polar/hydrogen bonding interactions with the active layer components significantly enhanced the device performance [29]. Further, we reported that the device fabricated with the inclusion of the multifunctional additive, 2,3-dihydroxypyridine (DOH) in the PEDOT:PSS layer exhibited an enhanced PSC performance and thermal/air stability [58]. The addition of DOH into PEDOT:PSS influences the conformational transformation of PEDOT and PSS chains via the formation of intermolecular hydrogen bonding between the hydrogen atoms of the hydroxyl groups in the DOH molecule and the sulfonate or sulfonic acid groups of PSS [58].

In our previous work, we reported that the incorporation of optimal quantity of DOH (1.0 wt%) into the PEDOT:PSS (PEDOT:PSS@DOH) buffer layer clearly outperformed the photovoltaic performance (PCE = 3.49%) of pristine PEDOT:PSS based BHJ PSC (PCE = 2.92%) accounting a PCE enhancement of 20%. Interestingly, the inclusion of DOH into the PEDOT:PSS not only enhances the PV performance but also resulted in better thermal/air-stability suggesting the suitability for use in thermoelectric applications. In this work, we evaluated the influence of DOH on the performance of BHJ PSC by introducing DOH in the active layer comprising of PDPP3T and PCBM for the first time. We demonstrated a remarkable increase in PCE for DOH casted PDPP3T:PCBM (PCE = 6.36%) as compared to that of pristine (PCE = 3.76%) and DIO incorporated PDPP3T:PCBM PSC (PCE = 4.75%) signifying a 69.1% improvements in the device performance over the pristine device. The results revealed that inclusion of DOH provided much superior performance over the inclusion of DOH in the buffer layer (PEDOT:PSS). We have systematically studied the beneficial roles of DOH modified PDPP3T:PCBM BHJ PSC through various photo-physical characterizations. Our results revealed the roles of DOH and demonstrated that the inclusion of DOH concurrently modify the morphology of the blend film, improve the optoelectronic properties and PV performances of the PDPP3T:PCBM BHJ PSC due to the functional characteristics of DOH.

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