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Review

Highly efficient regular polymer solar cells based on Li-TFSI doping ZnO as electron-transporting interlayers

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ABSTRACT

Zinc oxide is an attractive material applied for electron-transporting interlayers of polymer solar cells. Some factors limited the efficiency and performance of the ZnO-based PSCs, such as the poor conductivity and the traps existing on ZnO film. Here, we introduce a novel approach to optimize the property of ZnO electron-transporting interlayers for the further improvement of device performance by doping bis (trifluoromethane)-sulfonimide lithium salt (Li-TFSI) in ZnO film. It is found that this way not only increased electrical conductivity and charge extraction ability of the electron-transporting interlayers but also reduced charge recombination occurred at interface that was very important for fill factor improvement. Therefore, an optimized power conversion efficiency (PCE) of 9.94% was achieved, which was observed with 13.2% enhancement (9.94% vs 8.78%) compared to that of pure ZnO-based ones. This indicates that doping Li-TFSI in ZnO film is a promising strategy to optimize the ZnO film and enhance the performance of regular polymer solar cells.

1. Introduction

Polymer solar cells (PSCs) have attracted great attention due to their ease of low-cost fabrication, simple solution processability, light-weight, mechanical flexibility, and potential capability for large-area and high-throughput roll-to-roll manufacturing production (He et al., 2011; Lee et al., 2014; Nam et al., 2015). Currently, great progress has been made in this field by developing new photoactive materials, interfacial layers and alternative device architectures. Interfacial layers, located between the active layer and electrodes, play a critical role in determining the performance of PSCs devices (Manders et al., 2013; Xie et al., 2013). Such interfacial layers can be multifunctional materials that serve as selective charge injection layers or modify electrodes so that they can block charges from recombination at the active layer-electrode interfaces. However, the lack of understanding of interface engineering and impact of surface properties limits their further specification and development. Therefore, the requirement to introduce new approaches of optimizing interfacial layers is urgent for enhancing PSCs performance (Po et al., 2011; Yip et al., 2012; Dibb et al., 2011; Lange et al., 2013).

Zinc oxide (ZnO) is an attractive material applied for electron-transporting interlayers (ETLs) for polymer solar cells (PSCs) due to its appealing properties such as suitable energy levels, excellent visible transparency, high electron mobility, and easy to synthesize and process with low cost techniques (Lee et al., 2013a; Li et al., 2014; Yang et al., 2010). However, some factors have been limiting the efficiency and performance of the ZnO-based PSCs, such as the poor conductivity and the traps existing on ZnO film. A number of approaches have been adopted to engineer ZnO film to improve the property of that, for example, self-assembly monolayers, cross-linked layers, surface modification of ZnO ETLs, and doping in ZnO ETLs, etc (Cheng et al., 2012, 2013; Kim et al., 2013; Shao et al., 2013; Lee et al., 2013b; Yip et al., 2008; Yin et al., 2016). Brown group has reported that coating ZnO nanoparticle films with DNA nanolayers could improve the electron extracting properties and performance of polymer solar cells (Dagar et al., 2017). Fang group has reported that ZnO doping with Al can serve as an efficient electron extracting layer in inverted OSCs with the model blend system of PTB7-Th:$PC_{71}BM$ (Liu et al., 2017.). Zheng group has reported that inverted PSCs based on Zn_1-xMgxO (ZMO) as cathode buffer layer could significantly improve the performance compare with eh devices with pure ZnO (Yin et al., 2014). Among these approaches, doping is an efficient way to enhance the conductivity and decrease the defects of ZnO film.

In the present work, we introduce a novel approach to enhance the

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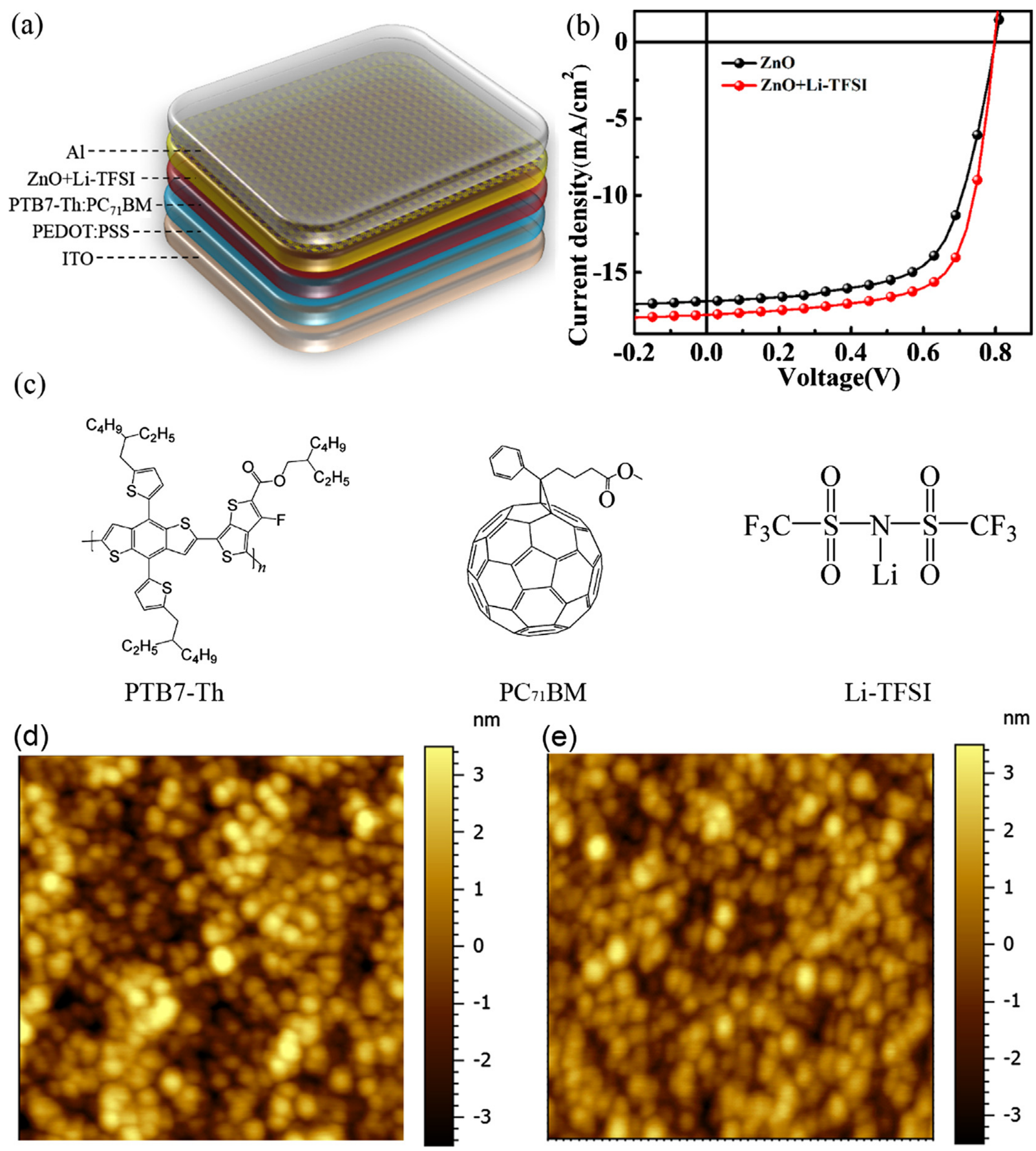

Fig. 1. (a) The device architecture. (b) Illuminated *J-V* characteristics. (c) Chemical structures of the materials used for device fabrication. AFM (500 nm × 500 nm) topographical images using tapping mode: (d) ITO/PEDOT/PTB7-Th/ZnO (e) ITO/PEDOT/PTB7-Th/ZnO + Li-TFSI used in the device fabrication.

Table 1
Parameters of optimized devices based on different electron transport layers.

ETL	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)	
				Best	Average
ZnO	0.799	16.88	65.1	8.78	8.53
ZnO + Li-TFSI	0.797	17.75	70.3	9.94	9.62

conductivity property of ZnO ETLs for the further improvement of PSCs by doping Li-TFSI in ZnO. The way resulted in the improved performance of PSCs with the power conversion efficiency (PCE) increased from 8.78% to 9.94%. It is found that this way not only increased the conductivity of ZnO ETLs by increasing electrical conductivity and charge extraction ability in the ZnO ETLs but also reduced charge recombination occurred at interface which was very important for the improvement of fill factor (FF). To find out the effects of doping Li-TFSI on PSCs devices, the morphology and optoelectronic properties such as surface morphology, photoluminescence properties, electron mobility, current–voltage model for a single heterojunction solar cell, and electrochemical impedance spectroscopy have been investigated in details. The active materials in polymer solar cell that we used comprises poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b‘]dithiophene-alt-3-fluorothieno[3,4-b]thiophene-2-carboxylate] (PTB7-Th) and [6,6]-phenyl-C71-butyric acid methyl ester ($PC_{71}BM$).

2. Experimental details

The details of material and characterizations, device fabrications, measurements, and synthesis are provided in the Supplementary material.

3. Results and discussion

The regular device architecture is presented in Fig. 1(a). The current density–voltage (*J-V*) characteristics obtained under AM 1.5G irradiation (100 mW cm^{-2}) are depicted in Fig. 1(b) and the chemical structures of materials used for the fabrication of the device are shown in Fig. 1(c). To figure out the impact of doping Li-TFSI on the performance of the polymer solar cells, current density–voltage (*J-V*) characteristics