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Efficient ternary polymer solar cells with dihydronaphthyl-based C60 bisadduct as an third component material

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ABSTRACT

A dihydronaphthyl-based C60 bisadduct (NCBA) acceptor is introduce as a third component to typical PTB7:$PC_{71}BM$ binary polymer solar cells (PSCs). NCBA play bridging role between the lowest unoccupied molecular orbital (LUMO) of PTB7 and $PC_{71}BM$ and provides more routes for charge carrier transfer at the interface between PTB7 and $PC_{71}BM$, a higher open-circuit voltage (V_{OC}) realize upon addition of NCBA can be achieve relative to the neat $PC_{71}BM$ as an electron acceptor. The strong visible light absorption in the range from 350 to 700 nm of NCBA molecule compared with $PC_{71}BM$ molecule, it has the effect of apparently complementary visible light absorption compare with the binary PTB7:$PC_{71}BM$ thin films. The current density–voltage (*J-V*) characteristics dependent on incident light intensity were employed and to analyze the effect of NCBA concentration on the charge carrier recombination process of ternary PSCs. The crystallinity and surface morphology of the ternary PTB7:NCBA:$PC_{71}BM$ thin films with NCBA concentration is 15% of blend acceptor is similar to that of the binary PTB7:$PC_{71}BM$ thin films, which guarantees suitable efficient exciton dissociation and charge carrier transport. The transient photovoltage (TPV) and transient photocurrent (TPC) were measured, and the results illustrate the effect of NCBA as the third component materials in terms of higher charge carrier density and long charge carrier lifetime and weaken charge carrier recombination.

1. Introduction

The last decade has witnessed rapid progress in the development of polymer solar cells (PSCs), and now power-conversion efficiencies (*PCE*) exceeding 13% have been realized in different types of PSCs (Cui et al., 2017; Arı et al., 2016). The performance of PSCs is strongly correlated with the excitonic nature of photoactive materials. However, despite the enormous strides achieved in past years, insufficient partial absorption in solar irradiation is still an inevitable issue restraining the photovoltaic performance of PSCs (Chen et al., 2017; Armin et al., 2015). Therefore, to overcome the absorption and open-circuit voltage (V_{OC}) limitations of PSCs, various strategies at different levels of maturity are currently in the exploration phase, e.g., the addition of some appropriate complementary absorbers and the shallower energy-level electron-acceptor materials into the binary PSCs, realizing so-called ternary PSCs (An et al., 2016b; Lu et al., 2015). A ternary strategy with two donors and one acceptor or two acceptors and one donor has been demonstrated as an effective method to improve the photovoltaic performance of PSCs by enhancing photogenerated charge carrier generation and collection efficiency (An et al., 2016b, 2016c). Ternary PSCs present some advantages: the simplicity of single-step processing for photoactive layers rather than the more complex tandem cells compared with tandem PSCs and higher V_{OC} and J_{SC} compared with binary PSCs.

Nowadays, the most representative single-layer PSCs are those with a blend thin films of PTB7 and $PC_{71}BM$ as the photoactive layer, and the corresponding best power-conversion efficiency (*PCE*) has exceeded 10% under AM 1.5G illumination at an illumination intensity of 100 mW cm^{-2} (He et al., 2015; Lin et al., 2015). For most PSCs devices, the photoactive layer consists of a blend thin films of conjugated polymer donor and fullerene acceptor materials. The ideal polymer donor materials should have the advantage of a broad and strong absorption band in the visible and near-infrared regions, which can match well the solar spectrum (Brabec et al., 2002; Peet et al., 2007). The ideal acceptor materials should have the advantages of shallower lowest unoccupied molecular orbital (LUMO) energy level, electron mobility and electron affinity, which can ensure the acquisition of high V_{OC} in real devices. The [6,6]-phenyl-C71-butyric acid methyl ester ($PC_{71}BM$)

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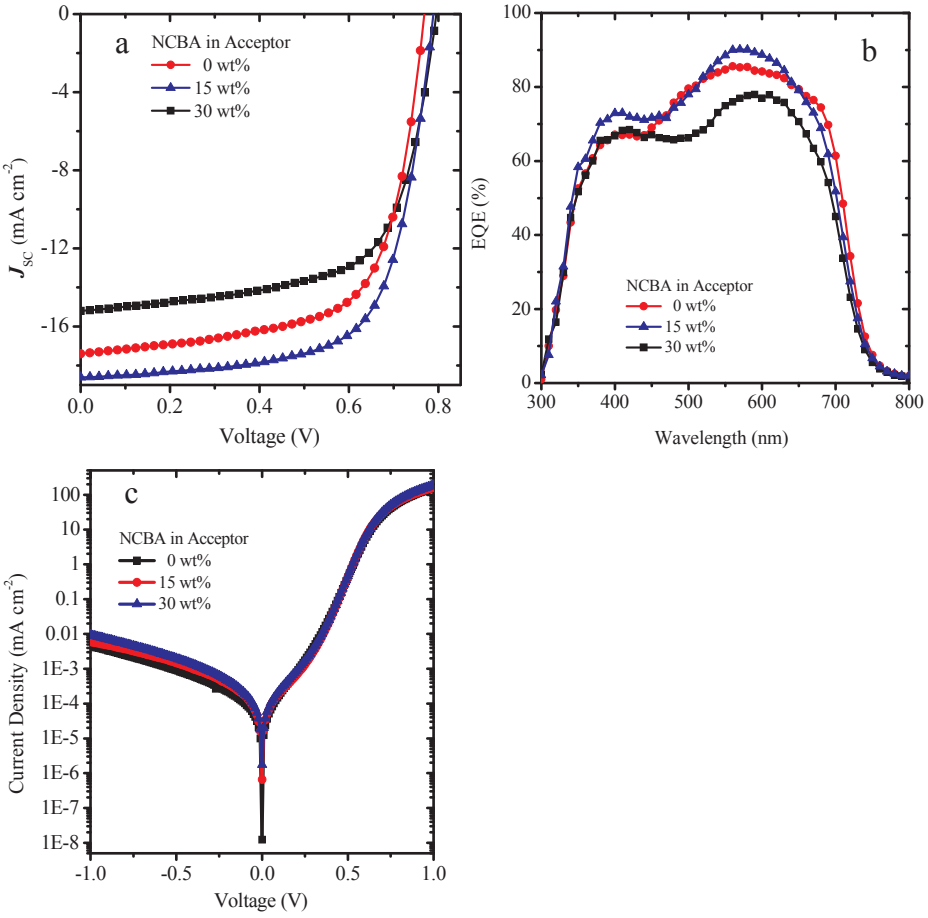

Fig. 1. (a) *J-V* curves of inverted structure "ITO/ZnO/PTB7:NCBA:$PC_{71}BM$/MoO_3/Ag" with different weight ratios of NCBA as an acceptor under illumination of an AM 1.5G solar simulator at an illumination intensity of 100 mW cm^{-2}. (b) EQE spectra of devices with the same specifications as (a). (c) *J–V* curves under dark conditions of (a).

comprises typical electron acceptor materials and matches the LUMO of most low-bandgap conjugated polymers for most PSC devices (Foertig et al., 2014; Liu et al., 2014). Chunru's group has synthesized fullerene derivatives of the dihydronaphthyl-based C60 bisadduct (NCBA) as an electron acceptor (Meng et al., 2012, 2014). NCBA has the advantages of improved absorption in the 400–500 nm region and a shallower LUMO energy level, which leads to a high V_{OC} and *PCE* [0.82 V and 5.85% and the similar photovoltaic parameter compared with indene-C60 bisadduct (ICBA) as an electron acceptor, respectively] based on poly(3-hexylthiophene) (P3HT) as donor materials (Meng and Zhang, 2012). NCBA, then, has a higher thermally driven crystallization, over 280 °C, which illustrates better thermal stability compared to PCBM and $PC_{71}BM$ (Meng et al., 2012, 2014).

The PSCs with P3HT:NCBA and PTB7:$PC_{71}BM$ as photoactive layers exhibit better photovoltaic performance, and the best value exceeds 6% and 10%, respectively (Ganesamoorthy et al., 2017). Unfortunately, binary PSCs based on PTB7 as the donor material and NCBA as acceptors yielded lower *PCE* relative to the common low-bandgap PTB7:$PC_{71}BM$ system, which is attributed to two main reasons: low charge carrier generation efficiency for the PTB7:NCBA interface and a correspondingly small short-circuit current density (J_{SC}), and poor charge carrier collection efficiency compared with the PTB7:$PC_{71}BM$ thin films as a photoactive layer and a corresponding decrease of J_{SC} and fill factor (FF) Zhang et al., 2017a. Compared with PTB7/$PC_{71}BM$ thin films, the PTB7/NCBA interface exhibits a lower free-energy driving force and energy-level difference, which cannot guarantee efficient photogenerated charge carrier generation and exciton dissociation (Foertig et al., 2014; Hawks et al., 2013). Charge carrier transport and collection is related to the morphology and crystallization of the photoactive layer (Chang et al., 2013; Kim et al., 2012). Owing to the nature of the weaker crystallinity of PTB7, fine intermixing of PTB7:NCBA thin films poses a difficulty for the elimination of disrupted molecular ordering and blocked charge carrier transport pathways, which can reduce charge carrier collection efficiency and photovoltaic performance (Lu et al., 2013; Cheng et al., 2014). However, the ternary PSCs may provide an alternative approach to achieve high performance by mixing the second fullerene derivative acceptor (Ferenczi et al., 2011; Li et al., 2011).

In this work, NCBA is employed as an third component material in PTB7:$PC_{71}BM$ photoactive layer and a partial replacement of $PC_{71}BM$. Owing to the shallower LUMO energy level of NCBA compared to $PC_{71}BM$, and to the fact that NCBA plays a bridging role between PTB7 and $PC_{71}BM$, substantial improvement in V_{OC} and efficient exciton dissociation at the PTB7/acceptor interface with the addition of NCBA are realized. Analysis of the effect of NCBA concentration on photogenerated charge carrier generation and on collection efficiency and photovoltaic performance are carried out in detail.

2. Experimental details

The fabrication method and parameters are provided in the Supplementary Materials. The PSC devices were fabricated with the following inverted structure: ITO/ZnO/PTB7:NCBA:$PC_{71}BM$/MoO_3/Ag. The charge carrier mobility was measured by the space charge limited current (SCLC) method. Hole-only and electron-only diodes were fabricated using the architectures "ITO/PEDOT:PSS/PTB7:NCBA:$PC_{71}BM$/Au" and "Al/PTB7:NCBA:$PC_{71}BM$/Al," respectively. The chemical structures of PTB7, NCBA, and $PC_{71}BM$ and the energy-level diagram of the device are shown in Fig. S1. The average photovoltaic parameters were obtained from five PSCs fabricated in parallel.