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# A comprehensively theoretical and experimental study of carrier generation and transport for achieving high performance ternary blend organic solar cells

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## ABSTRACT

Ternary blend organic solar cells (OSCs) composed of three components in the active layer shows the potential to achieve higher power conversion efficiency (PCE) as compared to the binary counterpart due to the wider absorption spectrum, higher generation rate, and better morphology. However, the physical understanding of carrier generation and transport processes in the ternary blend OSCs has been limited explored. In the work, together with experimental studies of the two donors, one acceptor ternary blend OSCs with PCE > 12%, we will theoretically and experimentally describe the roles of the carrier generation (including exciton transfer, delocalization and dissociation), and carrier transport (particularly the hole transport) on the performance of ternary blend OSCs. Through theoretical and experimental investigations, critical design rules for improving the device performance are concluded: (1) improving the exciton delocalization ratio via donor ratio optimization with physical understanding, (2) selecting the donors with well overlap of emission and absorption spectra to promote a beneficial exciton transfer, (3) engineering the energy level of donors to form the blocking barrier for reducing hole transfer into the donor with high recombination loss. The work unveils the device physics which is fundamentally important for designing and optimizing high-performance ternary blend OSCs.

## 1. Introduction

According to detailed balance theory [1,2], the dominant efficiency loss of a solar cell lies at the spectrum loss. Only photons with energy larger than the band gap of active semiconductor materials will be sufficiently absorbed and converted to electron-hole pair. Thus, fully exploiting sun spectrum in a broadband range is essential to elevate the power conversion efficiency (PCE) of a solar cell system. Recently, ternary blend active layer structure has been intensively investigated in bulk-heterojunction (BHJ) organic solar cells (OSCs) for utilizing the wide spectrally distributed solar irradiation [3–11]. Different from the optimization designs for traditional binary donor: acceptor system, ternary blend OSCs contain the third component in the active layer, and the third component with the complementary absorption spectrum to the binary one, which can be a polymer or small molecule [3,9], offer better matching to the solar spectrum and improve the total absorption. Furthermore, by careful material selection and device fabrication, the incorporation of the third component can improve the morphology of the active layer, so that higher carrier mobility and more efficient

carrier generation can be achieved [10]. By taking such advantages, ternary blend OSCs have reached the state-of-the-art PCE of about 14% [12,13], highlighting their great potentials in the field.

The working mechanism of ternary blend OSCs has attracted a lot of interest from both the theoretical and experimental researchers. Several alternative working principles of the ternary OSCs have been proposed, based on different assumptions including the alloy model, parallel-linkage model or sensitizer model [10,14–16]. All of these models qualitatively explain some of the properties of ternary blend OSCs. However, there are still issues that cannot be clearly and quantitatively described, such as the exciton generation, dissociation, and transfer, as well as the carrier transport and transfer, which are critically important in understanding and optimizing the ternary blend OSCs.

The ternary blend OSCs can be simply divided into two categories: two donors/one acceptor (D<sub>1</sub>/D<sub>2</sub>/A) and two acceptors/one donor (A<sub>1</sub>/A<sub>2</sub>/D) [10]. In D<sub>1</sub>/D<sub>2</sub>/A system, solar energy can be absorbed by the three components simultaneously, and excitons will be generated in the active layer. Then, the generated excitons will dissociate into the free carriers at the interfaces of D<sub>1</sub>/A or D<sub>2</sub>/A subsystems. During the

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process, two important excitonic physics concepts of exciton delocalization and exciton transfer are involved, which govern the unique carrier generation mechanism in the ternary blend OSCs.

The first exciton physics is exciton delocalization [17–19]. The exciton behaviors after the photon absorption should be divided into two parts: 1) the ultrafast exciton generation will occur in a very short time regime ( $< 100$  fs) at the interfaces between the donor and acceptor [19,20], and the excited exciton has a very large spatial delocalization, and thus behaves like Wannier exciton, with a large initial exciton radius. The large initial exciton radius indicates the weak Coulomb interaction between the electron and hole, and thus the high dissociation probability. However, the experimental results [18–20] showed that a part of the delocalized excitonic states will collapse to the localized excitonic states at the same time, which behaves like Frankel exciton. 2) The localized excitons will continue to diffuse towards the donor/acceptor interface, forming the charge-transfer (CT) state, and finally dissociate into free carriers. The ratio of the delocalized excitonic states to the total excitonic states plays a very important role in achieving the high performance OSCs [17], while it is intrinsically determined by donor-acceptor material and morphology [20,21]. However, the study of delocalization mechanism in ternary blend OSCs is very limited, and the role of delocalization mechanism in the efficiency improvement of ternary blend OSCs is still unclear.

The exciton transfer physics for the diffusion of localized excitons to the interfaces is considered as the second important excitonic physics. Between the p-type components in ternary blend (i.e.  $D_1$ ,  $D_2$  in  $D_1/D_2/A$  system), the Förster energy-transfer can occur through non-radiative process that are confirmed from the photoluminescence (PL) and absorption spectra [22]. The exciton transfer may change the total exciton dissociation probability afterward determined by the probabilities at  $D_1/A$  and  $D_2/A$  interfaces. In addition, after the exciton dissociation, the carrier (i.e. hole) transfer may also exist between  $D_1$  and  $D_2$ , and can further influence the performance of the ternary blend OSCs. It is because two conducting channels of  $D_1/A$  and  $D_2/A$  subsystems have different carrier transport properties including mobility, recombination and injection/extraction barriers. Therefore, the carrier transfer between the  $D_1/A$  and  $D_2/A$  subsystems will influence the total recombination loss and thus the device performance. However, the effects of both exciton and carrier transfer in the ternary blend OSCs have not yet been explored.

In this work, through both experimental and theoretical studies, the carrier generation mechanism includes the exciton delocalization, dissociation and transfer, as well as the charge transfer during the carrier transport process in ternary OSCs, which are very limited studied, will be discussed. The efficiency changes in the physical processes of carrier generation, exciton transfer and hole transfer will be quantified. Our result indicates that the main loss of ternary blend OSCs is the inefficient localized exciton dissociation. In addition, the carrier loss introduced by the detrimental exciton transfer (i.e. exciton transfer from the donor with more efficient exciton dissociation  $D/A$  interfaces to the one with less efficient exciton dissociation  $D/A$  interfaces) will reduce short-circuit current density ( $J_{SC}$ ), while the extra recombination loss caused by the disadvantageous hole transfer into the donor with low mobility and high carrier recombination will reduce the open-circuit voltage ( $V_{OC}$ ) and fill factor (FF). Based on the experimental and modeling results, we outline the systematic design rules i.e. increase the exciton delocalization by optimizing the donor component ratio, select the donor materials with proper overlap of the emission and absorption spectrum to allow beneficial exciton transfer, and engineer the energy level of donor materials to form blocking barrier for inhibiting disadvantageous hole transfer. This work enables to gain the insight of device physics for developing high-performance ternary blend OSCs, which will contribute to promote green energy application.

## 2. Experimental section

### 2.1. Device fabrication

The non-fullerene acceptor has the advantages including the tunability of light absorption and energy level, diversity of donor-to-acceptor combination, and large-scale production of acceptor materials, which is the hot topic of ternary blend OSCs. To gain the insights of device physics, here we have fabricated a new type of non-fullerene ternary blend OSCs, which comprises a wide-bandgap non-fullerene acceptor [23] (SFBCRN), a medium bandgap polymer donor (PBDB-T: poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene))-*alt*-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione))]), and a low bandgap polymer donor (PTB7-Th). Details of device fabrication are described in this section.

#### 2.1.1. Materials

PTB7-Th was purchased from 1-Material, PBDB-T and SFBCRN were synthesized according to previously reported procedures. [23,24] All other chemicals were purchased as reagent grade and used without further purification.

#### 2.1.2. Devices

The device structure is ITO/ZnO/PBDB-T<sub>1-x</sub>:PTB7-Th<sub>x</sub>:SFBCRN/MoO<sub>3</sub>/Ag. Pre-patterned ITO substrates (sheet resistance =  $15 \Omega \text{ sq}^{-1}$ ) were sequentially ultrasonicated in detergent, deionized water, acetone, and isopropanol, and then UV-cleaned in a UV-Ozone chamber for 20 min. The ZnO solution (2 M in toluene, diluted by tetrahydrofuran) was spin-coated onto the surface of the ITO substrates at a rate of 5000 rpm for 30 s in the 20 L min<sup>-1</sup> dry airflow, and then baked on a hot plate at 100 °C for 10 min to form a thin layer of about 30 nm. Ternary blend films with the fixed D: A ratio of 1:0.8 and the total concentration of 18 mg mL<sup>-1</sup> in chlorobenzene (adding 0.75 v/v% of 1,8-Diodooctane, DIO) were prepared by spin-coating at 2000 rpm for 60 s. The thickness of the ternary blend films is about 110 nm. A molybdenum trioxide interlayer (MoO<sub>3</sub>, 10 nm) and a silver anode (Ag 100 nm) were finally deposited onto the surface of the active layer in an evaporation chamber under high vacuum ( $\leq 10^{-6}$  mbar). The fabrication details of hole-only and electron-only devices can be found in the Supporting Information.

#### 2.1.3. Device measurement

The thickness of the each layer was screened by using a Dektak 6 M surface profilometer. The device area was fixed at 4.0 mm<sup>2</sup>. The *J-V* characterization of the devices was carried out on a computer-controlled Keithley 2400 source meter with an Air Mass 1.5 Global (AM 1.5G) solar simulator (XES-70S1, SAN EI Co., Ltd.) as the light source with an irradiation intensity of 100 mW cm<sup>-2</sup>, which was calibrated by using a standard silicon solar cell. The EQE values were tested with a Newport Model 77890 (Newport Co. Ltd.) during the illumination with a monochromatic light from a xenon lamp. The refractive indices (*n*, *k*) of perovskite were performed under a dark ambient environment by using spectroscopic ellipsometry (Woollam). All fabrication and characterization processes, except for the refractive indices and EQE measurements, were conducted in a glove box filled with argon atmosphere ( $< 0.1$  ppm O<sub>2</sub> and H<sub>2</sub>O).

### 2.2. Device modeling

Since a systematic device model to describe carrier generation and transport processes in the ternary blend OSCs has not been explored in details, we will develop a new model together with the series of experiment for studying the carrier and exciton dynamics of ternary blend OSCs. Different to the existing works like the alloy or cascade model [10,14–16], a more realistic assumption is applied to this parallel-like

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