

Insight into correlation between molecular length and exciton dissociation, charge transport and recombination in Polymer: Oligomer based solar cells

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ABSTRACT

Four fluorene-alt-di-2-thienyl-benzothiadiazole (FTBT) based oligomers with different number of repeated units are selected as electron acceptors in P3HT:oligomer solar cells. The effect of oligomer length on the phase separation behavior has been studied in detail. It is disclosed that the oligomer length strongly affects the film morphology and hence the exciton dissociation probability, charge transport as well as recombination characteristics. The short oligomer FITBT1 is prone to aggregate and form large-scale phase separation which impedes exciton dissociation in the blend films. With increasing the acceptor length, large-scale aggregations are gradually suppressed due to the weakened migration ability of long FTBT oligomers in polymer matrix. Meanwhile, electron mobilities are enhanced with extending the oligomer length, which is favorable to suppress charge recombination in the blends. Finally, optimal photovoltaic performances with a PCE of 4.19% are achieved in P3HT:F3TBT3 based solar cell that compromises well between efficient exciton dissociation and balanced charge transport, which is almost three times higher than the FITBT1 based device. This work highlights that tailoring the oligomer length can be used as an effective strategy to control phase separation and to enhance the photovoltaic performance in non-fullerene based polymer solar cells.

1. Introduction

Over the past decades, bulk-heterojunction polymer solar cells (PSCs) have been intensively studied due to their evident superiorities such as low cost, light weight, solution processing and suitability for large scale fabrication [1–7]. Power conversion efficiencies (PCEs) up to 12% have been achieved for the single-junction PSCs [8–10]. The fullerenes and their derivatives as electron acceptors have made a great success in PSCs due to their high electron mobility, the tunable phase separation in the blend films as well as the efficient and ultrafast electron transfer from polymer donors to fullerene derivatives [11–16]. However, the widely used fullerenes and their derivative acceptors always show weak light-harvesting properties in visible and near-infrared region and limited tunability of energy levels, and thus impede further enhancement of photovoltaic performance in the fullerene-based PSCs. The drawbacks of fullerene derivatives motivate researcher to explore novel non-fullerene acceptors. A lot of promising molecules and conjugated polymers have been developed serve as electron acceptors, including perylene diimide (PDI) derivatives [17–22], naphthalene

diimide (NDI) derivatives [23–26], polymers based on double B←N bridged bipyridine (BNBP) units [27–30], and fused ring electron acceptors (FREAs) [5,8,31–39]. Outstanding progress has been achieved with the PCEs of the non-fullerene based PSCs surpassing their fullerene-based counterparts due to enhanced solar absorption and reduced energy loss [35–39].

In addition to the active materials, the film morphology also plays an important role in determining the photovoltaic properties of bulk-heterojunction PSCs which require a trade-off between exciton dissociation and charge collection [40–42]. High exciton dissociation efficiency needs sufficiently intimate mixing between donors and acceptors to provide high interfacial areas. Meanwhile, efficient charge extraction requires a certain degree of phase separation to transport free holes and electrons individually with low recombination probability. Therefore, a bicontinuous interpenetrating donor/acceptor network with domain size of 10–20 nm is usually preferred for efficient photovoltaic conversion. Getting benefit from the totally different geometrical structures between linear polymer donors and spherical fullerene acceptors, the nanoscale phase separation in

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polymer:fullerene derivative blend can be well constructed in virtue of post-thermal annealing, solvent annealing or addition of high-boiling point solvents [43–46]. However, the morphology issue in polymer donor:non-fullerene acceptor blends, especially in the polymer:polymer blends, is more complicated due to analogous geometrical structures. This always leads to severe charge recombination and low charge extraction efficiency, hindering the potential of such kind of polymer/polymer blend solar cells. With taking the polymer blend of typical poly(3-hexylthiophene) (P3HT) donor and fluorene-alt-benzothiadiazole-based polymer (PFTBT) acceptor as an example, it has a potential to realize an open-circuit voltage (V_{OC}) over 1.2 V, but the external quantum efficiency (EQE) of the resultant polymer blend PSCs is as low as 20% due to possible polymer entanglement and poor P3HT:PFTBT phase separation [47]. Recent research disclosed that an oligomer acceptor can favour to avoid polymer entanglement and improve phase separation, and finally enhances distinctly the photovoltaic performance in the case of P3HT:PFTBT blend [47]. This demonstrates that it is promising to optimize phase separation by using oligomer to replace polymer acceptor. However, a fundamental understanding on how the oligomers affect the polymer:oligomer blend phase separation and photovoltaic performance is still lacking.

Herein, a series of fluorene-alt-di-2-thienyl-benzothiadiazole (FTBT) based oligomers with increased molecular contour length are employed as electron acceptors in combination with poly(3-hexylthiophene) (P3HT) as donor in the non-fullerene solar cells. The effects of acceptor length on phase separation and photovoltaic performance in solar cells based on P3HT: oligomer blends have been systematically investigated. A clear correlation between the oligomer acceptor contour length and the donor: acceptor phase separation, exciton dissociation and charge recombination is well demonstrated. This work may be helpful to design suitable oligomer acceptors toward constructing ideal phase separation in the non-fullerene based polymer solar cells.

2. Experimental section

2.1. Materials

The FTBT-based oligomers with different number of repeated units of fluorene-alt-di-2-thienyl-benzothiadiazole (1, 2, 3 and 4) are synthesized in Geng's Lab. P3HT is purchased from Rieke Metals with a weight-average molecular weight (Mw) of 50–70 kDa (PDI = 1.8) and a regioregularity of 91%–94%. Poly(ethylenedioxythiophene): poly(styrene sulfonate) (PEDOT:PSS) (Baytron P AI 4083) is obtained from H. C. Starck. All of these materials are used as received.

2.2. Film characterization

The absorption and photoluminescence (PL) spectra are recorded on a Perkin-Elmer 35 UV-visible spectrophotometer and a PG2000

spectrometer, respectively. Time-resolved PL spectra are measured by a fluorescence up-conversion system (FOG100, CDP) with excitation at 400 nm. Transmission electron microscopy (TEM) images are recorded with a JEOL JEM-1011 transmission electron microscope at an acceleration voltage of 100 kV and atomic force microscopy (AFM) measurement is performed on SPA-300 instrument (Seiko) in a tapping mode. The film samples for morphological studies are prepared under the same condition with device fabrication.

2.3. Device fabrication and measurement

The PSCs with a configuration of ITO/PEDOT:PSS (30 nm)/active layer (105 nm)/Ca (20 nm)/Al (100 nm) are fabricated as follows. The ITO glass substrates are subjected to ultrasonic cleaning in de-ionized water, acetone, and isopropyl alcohol sequentially. After drying at 120 °C in an oven for 30 min, the ITO substrates are subjected to UV-ozone treatment for 25 min. A PEDOT:PSS layer is then spin-coated on ITO substrates at 5000 rpm for 1 min, following by thermal annealing at 150 °C for 10 min. The blends of P3HT donor and FTBT oligomer acceptor are dissolved in *o*-dichlorobenzene (*o*DCB) with a weight ratio of 1:1 (w/w) and are stirred overnight. 1,8-Diiodooctane (DIO, 3% in volume) is employed as processing additive. The active layers are obtained by spin-coating the blend solutions atop of the PEDOT:PSS in a N₂-filled glovebox and thermal annealing at 50 °C for 30 min. A cathode of Ca (20 nm)/Al (100 nm) is deposited in a vacuum chamber under a pressure of 10⁻⁶ Torr. The active area of the devices is about 0.08 cm² which is defined by the overlapping area of the ITO and Al electrodes. The current density-voltage (*J*-*V*) characteristics of the photovoltaic cells is traced by a Keithley 2400 source meter with the devices under simulated solar light illumination (AM 1.5G, 100 mW cm⁻²) in a glove box. A calibrated silicon diode with KG-5 visible colour filter is used to determine the light intensity. In order to test the solar cells under various light intensities, a series of two neutral density filter wheels of five filters apiece is employed to modulate the intensity from 100 to 1 mW cm⁻². The incident photon-to-electron conversion efficiency (IPCE) is measured by the QE-R 3011 equipment (Enli Tech) in ambient air.

3. Results and discussion

3.1. Molecular structures, electrochemical and optical properties

The chemical structures of FTBT-based oligomers consisting of different number of fluorene-alt-di-2-thienyl-benzothiadiazole units are shown in Fig. 1, which can also be seen as monomer, dimer, trimer and tetramer, respectively. The monomer is made up from a fluorene (F) as electron-rich moiety and a di-thienyl-benzothiadiazole (TBT) as electron-deficient moiety. Because of low molecular weight and good planarity of the backbones, the contour length of even F4TBT4 is still much

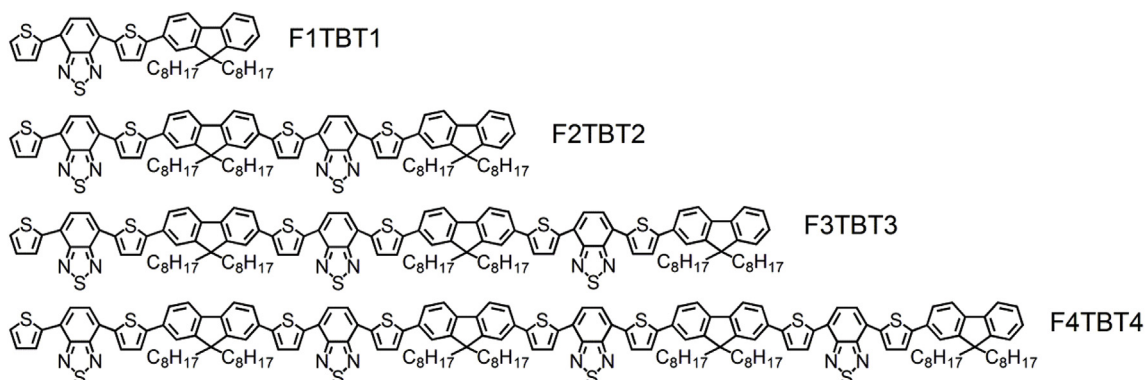


Fig. 1. The chemical structures of FTBT-based oligomers F1TBT1, F2TBT2, F3TBT3 and F4TBT4, respectively.

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