



# Tuning the fused aromatic rings to enhance photovoltaic performance in wide band-gap polymer solar cells



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## ABSTRACT

Two novel wide band-gap polymers of PFT1 and PFT2 were designed as the alternative to P3HT in organic electronics, in which the fused aromatic rings were utilized and altered to tune their molecular co-planarity and photovoltaic performance in solar cells. As observed, although PFT1 exhibited strong inter-molecular interaction, slightly twisted molecular structure was observed, thus leading to an inferior PCE value of 1.95% in BHJ solar cells and holes mobility of  $2.04 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  in OFETs in contrast to its isomeric polymer PBTFT. On the other hand, when the fused thiophene rings was tuned to construct PFT2, much planar polymer backbone was achieved, finally leading to the maximum PCE value of 3.34% in polymer solar cells and much enhanced holes mobility up to  $3.93 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  in OFETs. Our results here further indicated that tuning the fused aromatic rings in polymer backbone could improve their charge transfer properties and enhance their photovoltaic performance in solar cells significantly.

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## 1. Introduction

Bulk-heterojunction polymer solar cells (BHJ-PSCs) [1] have been investigated intensively over the past few decades for their advantages of light weight, low cost and easy fabrication for large-area devices [2–5]. Among these reported BHJ-PSCs, tremendous efforts were devoted to the narrowed band-gap (NBG) polymers [6–10], but their wide band-gap (WBG) counterparts are seldom investigated [11–16]. However, it's worth noting that the seriously overlooked WBG polymers are still of importance for their potential application in the multi-junction devices [17–19], such as tandem solar cells. Also, WBG polymers exhibited great potentials in the non-fullerene solar cells (NF-PSCs) and highly efficient NF-PSCs was

reported by Zhan et al. using these polymers as the electron-donors [20–23]. Nowadays, building the D-A type polymers is one well-known approach to obtain the high performance WBG polymers [24–30], in which the appropriate electron-rich moiety (D) and electron-deficient moiety (A) were introduced in molecular backbone simultaneously. For instance, Sun et al. reported serious novel wide band-gap polymers with a D-A framework and obtained the impressive power conversion efficiency (PCE) values up to 9% [31]. However, owing to the existing of effective intra-molecular charge transfer (ICT) [32], it's much difficult to obtain the large optical band-gap (>2 eV) for the reported WBG polymers in D-A architecture. In this case, just employing the electron-rich building blocks in polymer backbone is the most straightforward method

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[33–35]. Among these, poly(3-hexylthiophene) (P3HT) has been demonstrated as one of the most studied systems [36]. On the other hand, to further enrich the tool-box of WBG polymers with large optical band-gap (>2 eV) and enhance their photovoltaic performance in solar cells, fused aromatic rings [37], such as benzo[1,2-*b*:4,5-*b'*] dithiophene (BDT) [38], are incorporated in backbone for their much planar molecular structures and effective conjugation length [39]. Recently, our group synthesized the fused aromatic dibenzosixthiophene (DBST, Fig. S1, Supporting information) units to construct polymer PBTF with a large optical band-gap of 2.02 eV, finally leading to the efficient PSCs with a moderate PCE value of 3.0% and organic field-effect transistors (OFETs) with holes mobility up to  $0.028 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  owing to its highly planar molecular structures [40]. Furthermore, it should also be mentioned that the intra-molecular and inter-molecular interaction can be tuned effectively in the fused aromatic polymers to further enhance the performance of solar cells or OFETs [41]. Therefore, based on the above consideration, WBG polymer with fused aromatic rings could be one promising alternative to P3HT in organic electronics, such as PSCs and OFETs.

In this work, an isomeric building blocks (*i*-DBST, Fig. S1, Supporting information) with strong inter-molecular interaction to the fused aromatic DBST building block in PBTF [40] was designed to construct novel wide band-gap polymer PFT1. Meanwhile, to further enhance the molecular planarity and improve the performance in OSCs and OFETs, WBG polymer of PFT2 with large and much planar DBTT skeleton (Fig. S1, Supporting information) was also synthesized. As displayed, both PFT1 and PFT2 exhibited a broad UV–Vis absorption spectra in the region from 400 nm to 620 nm, leading to a large optical band-gap of 2.05 eV. Also the suitable highest occupied molecular orbital (HOMO) energy levels and lowest unoccupied molecular orbital (LUMO) energy levels were observed for PFT1 and PFT2. To further investigate the photovoltaic properties and charge transfer properties, PFT1 and PFT2-based BHJ-PSCs and OFETs were also fabricated here. As indicated, compared with that of PBTF, an inferior PCE value of 1.95% was observed in PFT1-based PSCs with holes mobility of  $0.02 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  in OFETs. However, when PFT2 was employed by tuning the fused aromatic rings in polymer backbone, all these key parameters in solar cells, including the short-circuit current ( $J_{sc}$ ), open circuit voltage ( $V_{oc}$ ) and fill factor ( $FF$ ), were improved simultaneously in contrast to that of PFT1, finally leading to the maximum PCE values of 3.34%. It's worth noting that increased charge carrier mobility up to  $0.039 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  were also achieved in its corresponding OFETs. Therefore, our results here indicated that tuning the fused aromatic rings in polymer backbone could be an effective method to construct WBG polymers and enhance their performance in the corresponding PSCs and OFETs devices.

## 2. Experimental section

### 2.1. Materials

All reagents and chemicals were purchased from commercial sources (Aldrich, Acros, TCI) and used without further purification unless stated otherwise. Poly(3,4-ethylenedioxy-thiophene)-poly(styrenesulfonate) (PEDOT:PSS) (Clevious P VP Al 4083) was purchased from H. C. Stark with the viscosity value in the range of 5–12 mPa and the resistivity value in the range of 500–5000  $\Omega\text{cm}$ . The indium tin oxide (ITO) used here is purchased from CSG HOLDING CO., LTD with the  $R_s$  value of 10  $\Omega/\text{sq}$ . Compound 3-dodecyl-5-(4-dodecyl-5-(trimethylstannyl)thiophen-2-yl)-2-(trimethylstannyl)thiophene (M1) was purchased from Solarmer Materials Inc. Compound M2 and M3 as well as wide band-gap polymer PFT1 and PFT2 were prepared and synthesized according

to the corresponding literature [40,42].

### 2.2. Characterization and measurement

All  $^1\text{H}$  NMR spectra were recorded on a Bruker Advance 400 MHz using  $\text{CDCl}_3$  as the solvent. MALDI-TOF mass spectrometric measurements were performed on Bruker Biflex III MALDI TOF. IR spectra were recorded on a JASCO FT/IR-4100 spectrometer. Average molecular weight and poly-dispersity index (PDI) were determined by a Waters 1515 gel permeation chromatography using polystyrene as a standard. Thermogravimetric analyses (TGA) were performed on a Netzsch TG 209 analyzer and differential scanning calorimeter (DSC) was measured on a TA Q200 instrument under nitrogen atmosphere at a heating rate of  $20 \text{ }^\circ\text{C}/\text{min}$ . UV–Vis spectra were measured on a Shimadzu UV-2250 spectrophotometer. The thin films for the UV measurement is prepared by the Spin-Coater instrument (Sile) with a concentration of 10 mg/mL in *o*-DCB solution. Cyclic voltammograms (CV) were performed with a three electrode electrochemical cell in a 0.1 M tetra(*n*-butyl) ammonium hexa-fluorophosphate ( $\text{TBAPF}_6$ ) solution with a scan  $100 \text{ mV s}^{-1}$  at room temperature under argon atmosphere. A platinum wire and Ag/AgCl (0.1 M) as were used as counter electrode and reference electrode. The thin films on the Pt disk, formed by drop-casting the molecule solution in chloroform (analytical reagent, 10 mg/mL), was used as the working electrode. The theoretical study was performed by using the density functional theory (DFT) by the PBE function. Surface morphologies were recorded by atomic force microscopy (AFM) on a Veeco-DI Multimode NS-3D apparatus in a trapping mode under normal air condition at room temperature.

### 2.3. Fabrication and characterization of organic solar cells

The photovoltaic cells were constructed with a traditional sandwich structure through the following steps. Firstly, the ITO-coated glass substrates were cleaned by a series of ultrasonic treatments in acetone, following by deionized water, then 2-propanol each for 10 min. The substrates were dried under a stream of nitrogen and subjected to the treatment of Ar/ $\text{O}_2$  plasma for 5 min. Secondly, a filtered aqueous solution of PEDOT:PSS was spun-cast onto the ITO surface at 4000 rpm for 30 s and then baked at  $150 \text{ }^\circ\text{C}$  for 30 min to form a PEDOT:PSS thin film with a thickness of 30 nm. Thirdly, a blend solution of polymers and [6,6]-phenyl-C-71-butyric acid methyl ester ( $\text{PC}_{71}\text{BM}$ ) in *o*-dichlorobenzene (*o*-DCB), filtered through a  $0.45 \mu\text{m}$  poly(tetrafluoroethylene) filter, spun cast at 3000 rpm for 30s onto the PEDOT:PSS layer. The substrates were dried under  $\text{N}_2$  at room temperature and then annealed at  $150 \text{ }^\circ\text{C}$  for 15 min in a nitrogen-filled glove-box. The devices were completed after thermal deposition of a 10 nm calcium and a 100 nm aluminum film as the cathode at a pressure of  $6 \times 10^{-4} \text{ Pa}$ . There are five solar cells on each ITO substrate with the active area was  $0.1 \text{ cm}^2$  for each device. The thicknesses of the spun-cast films were recorded by a profilometer (Alpha-Step 200; Tencor Instruments).

Device characterization was characterized under an AM 1.5 G irradiation with an intensity of  $100 \text{ mW cm}^{-2}$  (Oriol 91160, 300 W). Current density-voltage ( $J$ - $V$ ) characteristics were measured by a computer-controlled Keithley 2602 source measurement unit in the dark. PCE was detected under a monochromatic illumination (Oriol Cornerstone 260 1/4 m monochromator equipped with Oriol 70613NS QTH lamp) and the calibration of the incident light was performed with a mono-crystalline silicon diode. The external quantum efficiency (EQE) was measured by a source meter, silicon photodiode and a computer-controlled light source-monochromator-lock-in system. All device fabrication

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