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Molecular design of a wide-band-gap conjugated polymer for efficient fullerene-free polymer solar cells[†]

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Two p-type conjugated polymers with disparate optical and electronic properties, PB3T and PB2T, were developed and applied in fullerenefree polymer solar cells (PSCs). The photovoltaic performance of the PB3T-based PSC device processed by anisole achieved a high power conversion efficiency of 11.9% with a J_{sc} of 18.8 mA cm⁻² and V_{oc} of 1.00 V.

In recent years, considerable developments have been made in fullerene-free polymer solar cells (PSCs),¹⁻¹¹ in which the active layer consists of a p-type conjugated polymer as the electron donor and a non-fullerene (NF) N-type organic compound as the electron acceptor; the power conversion efficiency (PCE) of the state-of-the-art fullerene-free PSCs has surpassed 11%,^{12,13} which is comparable to that of fullerene-based PSCs. However, most polymer donors used in fullerene-free PSCs are typical low-band-gap (LBG) or medium-band-gap (MBG) materials with optical band gaps (E_g^{opt}) smaller than 1.8 eV and optical absorption spectra that greatly overlap with those of LBG NF-acceptors such as ITIC,¹⁴ IEIC,¹⁵ and IT-M.¹² Moreover, these fullerene-free devices always exhibit relatively poor EQE at low wavelengths, which limits the short-circuit current density (I_{sc}) of the devices.^{16–20} Thus, for further optimization of fullerene-free PSCs, the development of efficient wide-bandgap (WBG) polymer donors is urgent and important.

Recently, the design of WBG polymer donors has attracted extensive research interest. For example, several polymer donors have been designed and applied in fullerene-free PSCs with ITIC as the acceptor.¹⁴ Yan *et al.* synthesized the polymer PffT2-FTAZ-2DT with an E_g^{opt} of 1.91 eV and obtained a PCE of 7.2%.²¹ Li *et al.* developed the polymer donor J61 with an E_g^{opt} of 1.93 eV,

Broader context

Polymer solar cells (PSCs) have emerged as a promising renewable energy source because of their ease of fabrication, promising flexibility, and capability for use on a large-scale. In this work, two wide band gap (WBG) polymers, namely PB2T and PB3T, were designed and synthesized based on benzodithiophene (BDT) and oligothiophene units as efficient photovoltaic donor materials for fullerene-free polymer solar cells (PSCs). PB3T is considered to be a suitable candidate as a polymer donor in fullerene-free PSCs due to its WBG optical absorption, suitable frontier orbital level, and strong π - π stacking effect in a solid film. Using an IT-M small molecule acceptor, the PSC based on the PB3T:IT-M active layer exhibited a remarkably high power conversion efficiency (PCE) of 11.7%. Moreover, PB3T could be processed by the environment-friendly solvent anisole without any other solvent additive or post-treatments, achieving a PCE of 11.9%. These results demonstrate that PB3T is a promising polymer donor for high-performance fullerene-free PSCs.

which demonstrated a high PCE of 9.5%.²² Our group also reported a few WBG polymers that yielded good efficiencies of ~8% when blended with ITIC.^{23,24} According to these previous reports, polymers with low-lying highest occupied molecular orbital (HOMO) levels are needed to reduce energy loss (E_{loss}) and achieve high V_{oc} (> 0.9 V).^{25,26} However, even though these polymers have optical absorption bands complementary to ITIC, the overall PCEs of the corresponding devices remain lower than 10%. Therefore, room remains for further improvement in the photovoltaic performance of PSCs using a WBG polymer donor.

Design strategies for WBG polymer donors in fullerene-free PSCs have not been well established, but previous reports provide hints. First, the HOMO level of WBG polymer donors should be fine-tuned to ensure sufficient exciton dissociation and to avoid substantial E_{loss} to simultaneously achieve a high J_{sc} and a high V_{oc} in the device.^{27–29} Second, nanoscale bicontinuous phase separation is necessary in the bulk heterojunction active layers. Although many researchers have demonstrated that crystalline polymer donors with strong aggregation effects in solution often exhibit better photovoltaic properties than amorphous polymers, the relationship between the molecular conformation of the polymer donor and the amorphous acceptor in

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Fig. 1 (a) Molecular structures of PB2T, PB3T and IT-M. (b) Synthetic routes for M1, M2, PB2T and PB3T: (i) CH₃COOH, Br₂, THF, 0 °C, 2 h; (ii) DMAP, DCC, CH₂Cl₂, R.T., 24 h; (iii) LDA, ether, -78 °C, 1 h, then CuCl₂, R.T., overnight; (iv) LDA, THF, 78 °C, 1 h, then CBr₄, R.T., overnight; (v) DMAP, DCC, CH₂Cl₂, R.T., 24 h; (vi) Pd(PPh₃)₄, toluene, 110 °C, 24 h; (vii) NBS, CHCl₃, R.T., 24 h; and (viii) Pd(PPh₃)₄, toluene, 110 °C, 24 h.

achieving appropriate phase separation (a few tens of nanometers) is unknown. Therefore, designing an ideal WBG polymer donor with superior photovoltaic properties in fullerene-free PSCs remains a formidable challenge.

In this work, we designed and synthesized two new WBG conjugated polymers, PB2T and PB3T, as shown in Fig. 1, and discussed the molecular design of these two polymers. From the results of various characterization techniques, we predicted that PB3T should be a more suitable candidate than PB2T for the polymer donor in fullerene-free PSCs because of its WBG optical absorption, suitable HOMO level, and strong π - π stacking effect in solid films. We then fabricated fullerene-free PSCs using PB2T or PB3T as the donor by blending them with the small molecule N-type material IT-M as the acceptor. The performance of the PB3T:IT-M-based PSC was substantially better than that of the PB2T:IT-M-based device: 11.9% vs. 0.01%. The Eloss in the PB3T: IT-M device was only 0.60 eV, which is an outstanding result for a PSC. The PB3T:IT-M blend also demonstrated broad light absorption, covering the entire visible range from 400 to 800 nm, and the device exhibited an EQE better than 75% from 400 to 700 nm, leading to a high J_{sc} of 19 mA cm⁻². Moreover, we also fabricated a highly efficient device based on PB3T:IT-M by adopting nonhalogenated anisole as the processing solvent. Therefore, PB3T is a promising WBG polymer donor in fullerene-free PSCs for practical applications because of its high efficiency and environmentally friendly processing.

The chemical structures of PB2T and PB3T are shown in Fig. 1a. Both polymers contain benzodithiophene (BDT) units. As reported in previous studies,^{30,31} the polymers based on BDT and thiophene or α -linked bi-alkylthiophene exhibit optical absorption edges at wavelengths shorter than 650 nm, corresponding to $E_{\rm gopt}^{\rm opt} > 1.9$ eV, and their absorption spectra are complementary to that of IT-M, a new derivative of ITIC.

However, the HOMO levels of these polymers are too high to achieve a high V_{oc} in PSCs.^{12,15} Therefore, strong electron withdrawing carboxylate groups were introduced to the β -position of the α -linked bithiophene to reduce the HOMO level of the polymer. However, the two carboxylate groups at the adjacent β -positions of the α -linked bithiophene may cause strong steric hindrance, which breaks chain planarity. To reduce the steric hindrance, an unsubstituted thiophene was inserted between the two carboxylated thiophenes to obtain α -linked terthiophene (see M2 in Fig. 1b). Then, using two bromide monomers and one BDT monomer, we synthesized two conjugated polymers, PB2T and PB3T.

The polycondensation was carried out through the Stille coupling reaction using Pd(PPh₃)₄ as the catalyst, which resulted in good yields (60–70%). The chemical structures of the two polymers were confirmed by ¹H NMR and elemental analyses. The molecular weights of these two polymers were determined using high-temperature gel permeation chromatography (GPC) at 145 °C using *o*-dichlorobenzene (*o*-DCB) as the eluent. The number-average molecular weight (M_n) was 30.4 kDa for PB2T (PDI = 1.97) and 35.7 kDa for PB3T (PDI = 3.01). These two polymers were well dissolved in chlorobenzene (CB) and chloroform. As shown in Fig. S1 (see the ESI†), the thermogravimetric analysis (TGA) profiles reveal that the decomposition temperature (T_d) at 5% weight loss for the two polymers is greater than 340 °C, indicating that these materials are compatible with PSC fabrication processes.

Theoretical calculations by density functional theory (DFT) at the B3LYP/6-31G(d,p) level were carried out to determine the optimal geometries and molecular energy levels of the two polymers. As shown in Fig. 2, the optimal geometries of the two polymers differ substantially. PB2T has a highly twisted backbone conformation, and the dihedral angle between the two adjacent thiophene units is 78°; by contrast, the backbone of PB3T exhibits a planar geometry. Therefore, we predicted that PB3T can form stronger π - π stacking in solid thin films than PB2T.

Temperature-dependent absorbance (TD-Abs) measurements were carried out to investigate the aggregation behaviors of the



Fig. 2 Molecular backbone conformations and frontier molecular orbitals of copolymers based on two repeat units determined using DFT at the B3LYP/6-31g(d,p) level.

two polymers in CB solution. As shown in Fig. 2(a), at a high temperature of 120 °C, PB2T shows a broad absorption band with three transition peaks in the wavelength of 350, 410 and 445 nm. After decreasing the solution temperature to -30 °C, the absorption profile remains similar to that at 120 °C with a slightly red-shifted absorption edge from 540 to 558 nm, implying that PB2T does not aggregate extensively in solution. For PB3T, obvious changes of absorption spectra (Fig. 2(b)) in solution were observed during the cooling process. The absorbance peak at 470 nm decreased continuously and finally disappeared as the temperature decreased. It was also observed that a new main peak at 534 nm emerged at 40 $^\circ$ C and the absorption edge of PB3T was largely red-shifted from 575 to 638 nm. The results indicate that the strong aggregation of PB3T chains formed in the room temperature solution can be disaggregated at a higher temperature. The TD-Abs results are consistent with the theoretical calculation results; i.e., the optimal backbone geometry of PB3T is planar, thus interchain π - π interactions in PB3T should be very strong, whereas PB2T has a highly twisted backbone, which leads to a weak aggregation effect. Fig. 3(c) displays the absorption spectra of PB2T, PB3T and IT-M non-fullerene acceptors (for comparison) in solid films. On the basis of the absorption onsets of the films, the E_{g}^{opt} values were calculated to be 2.24 eV for PB2T and 1.96 eV for PB3T. In addition, the absorption spectra of both PB2T and PB3T are complementary to IT-M.

The cyclic voltammograms are plotted in Fig. S3 (see the ESI†), and the relevant data are summarized in Table 1. On the basis of the onset oxidation potentials, the HOMO levels of PB2T, PB3T and IT-M were estimated to be -5.63, -5.39 and -5.58 eV, respectively, and the LUMO levels were -3.63 eV for PB2T, -3.37 eV for PB3T and -3.96 eV for IT-M, according to their reduction potentials. The frontier orbital energy level alignments of the two blends, PB2T:IT-M and PB3T:IT-M, are presented in Fig. 2(d). As is well known, a higher HOMO level of the electron donor relative to that of the electron acceptor is imperative to achieve sufficient driving force for exciton dissociation and to



Fig. 3 Temperature-dependent UV-vis absorption spectra of (a) PB2T and (b) PB3T solutions (1 mg ml⁻¹ in CB); (c) UV-vis absorption spectra of PB2T, PB3T and IT-M films; (d) energy-level diagram.

avoid charge recombination. Therefore, because the HOMO level of PB2T is lower than that of IT-M, the driving force is reversed to hole transfer from IT-M to PB2T; this reversal will lead to inefficient exciton dissociation and substantial charge recombination in the device. By contrast, the HOMO level of PB3T is higher than that of IT-M, which favors efficient photovoltaic performance.

Afterwards, to investigate charge transfer in the blends of PB2T:IT-M and PB3T:IT-M, we collected the photoluminescence (PL) spectra of the two neat polymer films, the IT-M film and the two blends. As shown in Fig. 4(a) and (b), the PL spectra of the three neat films showed emission maxima at 615 nm, 648 nm and 754 nm for PB2T, PB3T and IT-M, respectively. In the PB2T:IT-M blend, the PL emission (under excitation at 500 nm) of PB2T was partially quenched by IT-M; however, the PL emission of IT-M (under excitation at 700 nm) could not be quenched by PB2T, implying that the photoexcited electron could be transferred from PB2T to IT-M, whereas the hole could not be transferred from IT-M to PB2T. This observation in the PL spectra is consistent with the CV results, where the mismatch in HOMO levels between PB2T and IT-M inhibits hole transfer from IT-M to PB2T, whereas both the PL of PB3T and IT-M can be completely quenched by each other in the PB3T:IT-M blend, indicating that exciton dissociation in this blend is highly efficient. Therefore, the PB3T:IT-M blend is expected to exhibit better photovoltaic performance than the PB2T:IT-M blend.

PSCs were fabricated with a conventional device structure of ITO/PEDOT:PSS/polymer:IT-M/PFN-Br^{32,33}/Al. The processing conditions for the active layer, such as the donor/acceptor (D/A) ratio and the thermal annealing temperature and time, were optimized to achieve the optimal photovoltaic performance (see Tables S2 and S3, ESI⁺). The current density-voltage (J-V) curves of the devices are displayed in Fig. 5(a), and the corresponding photovoltaic parameters are summarized in Table 2. Notably, the photovoltaic performance of the PB3Tbased PSCs was insensitive to the D/A ratio of the active layer; the PCE values of the PB3T-based devices remained at approximately 11% when the D/A ratios were varied from 7:3 to 4:6. Moreover, the PB3T:IT-M blend films were prepared without any solvent additive, and the thickness of the films was controlled to approximately 100 nm by tuning the spinning rate during the spin-coating process.³⁴ The best PB3T-based PSC device exhibited a remarkably high PCE of 11.7% with a $V_{\rm oc}$ of 1.00 V, a J_{sc} of 19.2 mA cm⁻², and a fill factor (FF) of 0.61. The device performances exhibited good reproducibility considering that a PCE of 11.6% was realized for the device fabricated after an interval of twenty days. By contrast, the PB2T:IT-M device exhibited a very low PCE of 0.01%. Furthermore, PSCs based on PB3T:IT-M with 1.00 cm² areas were prepared and a PCE of 9.60% was realized with a $V_{\rm oc}$ of 0.99 V, a $J_{\rm sc}$ of 16.7 mA cm^{-2} and a FF of 0.58. To further assess the photovoltaic performance of both polymers, PSCs have been fabricated using PC₆₁BM and PC₇₁BM as acceptors, respectively. The best PB3T:PC₆₁BM-based device exhibited a PCE of 7.24% with a V_{oc} of 0.98 V, a $J_{\rm sc}$ of 10.4 mA cm⁻², and a FF of 0.71. The PB3T:PC₇₁BM device gave a $V_{\rm oc}$ of 0.98 V, a $J_{\rm sc}$ of 9.73 mA cm⁻², and a FF of

Table 1 Optical parameters, frontier energy levels and hole mobilities of the polymers

Polymer	Soln λ_{\max} (nm)	Film λ_{\max} (nm)	Film λ_{edge} (nm)	$rac{\epsilon (10^4)}{\mathrm{M}^{-1} \mathrm{~cm}^{-1}}$	$E_{ m g}^{ m opt}$ (eV)	HOMO ^a (eV)	LUMO ^a (eV)	M _n (kDa)	PDI	T_{d}^{b} (°C)	${{{{{}^{\mu_{{\rm{h}}}}}^c}}\atop{\left({{{ m{cm}}^2}\;{{ m{V}}^{ - 1}\;{ m{s}}^{ - 1}} ight)}}}$
PB3T PB2T	534 413	540 416	633 554	5.57 3.62	1.96 2.24	$-5.39 \\ -5.63$	$-3.37 \\ -3.63$	35.7 30.4	3.01 1.97	344 368	$\begin{array}{c} 9.4 \times 10^{-5} \\ 2.8 \times 10^{-6} \end{array}$

^{*a*} Energy levels evaluated by CV. ^{*b*} 5% weight loss temperature. ^{*c*} $\mu_{\rm h}$ measured by using the SCLC model.



Fig. 4 PL spectra of (a) PB2T, IT-M and the PB2T:IT-M blend and (b) PB3T, IT-M and the PB3T:IT-M blend; the samples were excited at 500 nm and 700 nm.



Fig. 5 (a) J-V curves of PB2T:IT-M and PB3T:IT-M solar cells under AM 1.5G illumination. (b) EQE spectra of the corresponding devices.

0.68, yielding a PCE of 6.52%. However, the PB2T:PC₆₁BM and PB2T:PC₇₁BM devices gave a PCE of 0.03% and 0.07%, respectively. The corresponding device performance is summarized in Table S4 (see the ESI†). Energy loss ($E_{\rm loss}$) is considered an important parameter in evaluating the photovoltaic performance of devices. $E_{\rm loss}$ can be estimated by the equation $E_{\rm loss} = E_{\rm g}^{\rm opt} - eV_{\rm oc}$, where $E_{\rm g}^{\rm opt}$ is the smallest optical band gap of the donor and acceptor. Considering that the smallest $E_{\rm g}^{\rm opt}$ is 1.60 eV for IT-M and $eV_{\rm oc} = 1.00$ eV in the PB3T-based PSC device, the $E_{\rm loss}$ is calculated to be 0.60 eV. The $E_{\rm loss}$ values reported in the literature typically range from 0.7 to 1.0 eV;²² thus, the $E_{\rm loss}$ of 0.60 V in the PB3T-based device is smaller than that of most PSCs and has achieved the empirically low threshold of 0.60 eV. Such a small $E_{\rm loss}$ is critical to achieve a high PCE in PB3T-based PSCs.

Fig. 5(b) shows the EQE spectra of the devices. The PB3T:IT-M device displayed a broad EQE response from 300 to 800 nm, and the EQE in the range from 400 to 700 nm reached over 75%, indicating that both PB3T and IT-M contribute greatly to light harvesting. By contrast, the EQE of the PB2T:IT-M device was very low over the entire wavelength range. The calculated $J_{\rm sc}$ from the EQE curve of the PB3T:IT-M device is 18.6 mA cm⁻², which is consistent with the *J*-*V* measurement results and is outstanding among PSCs with similar response ranges. Notably, both the EQE of the PB3T:IT-M device in the wavelength range from 350 to 450 nm and the overall $J_{\rm sc}$ are clear improvements over those of fullerene-free PSCs with similar band gaps, and these improvements are attributed to the contribution of the WBG polymer PB3T.

The hole and electron mobilities ($\mu_{\rm h}$ and $\mu_{\rm e}$) of the pristine polymer films and blends were measured using the spacecharge-limited current (SCLC) method (see Fig. S5, ESI[†]). The $\mu_{\rm h}$ of the neat PB3T film (9.4 \times 10⁻⁵ cm² V⁻¹ s⁻¹) is higher than that of PB2T (2.8×10^{-6} cm² V⁻¹ s⁻¹). In the case of the blends, the PB3T:IT-M film exhibited a $\mu_{\rm h}$ (1.1 \times 10⁻⁴ cm² V⁻¹ s⁻¹) similar to that of the pristine PB3T film, indicating that hole transport in PB3T was not disrupted by blending with IT-M; however, the PB2T:IT-M film showed a very low μ_h of $6.4 \times 10^{-8} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, which is approximately two orders of magnitude lower than that of the neat PB2T film. These results imply that blending with IT-M does not disrupt the crystallinity or interchain packing of PB3T but substantially distorts that of PB2T. The μ_e values of the PB3T:IT-M and PB2T:IT-M blend films were 6.5 \times 10^{-5} cm 2 V $^{-1}$ s $^{-1}$ and 7.0 \times 10^{-7} cm 2 V $^{-1}$ s $^{-1}$ respectively. The balanced $\mu_{\rm b}$ and $\mu_{\rm c}$ in the PB3T:IT-M blend $(\mu_{\rm b}/\mu_{\rm e} = 1.7)$ facilitates charge transport and extraction.

Fig. 6 presents the two-dimensional (2D) grazing incident wide-angle X-ray scattering (GIWAXS) patterns of neat polymers and blend films with the corresponding out-of-plane (OOP) and in-plane (IP) line-cut profiles. No clear X-ray diffraction peaks were observed in the neat PB2T film or in the PB2T:IT-M blend, indicating the amorphous nature of the PB2T. The absence of ordered packing in PB2T is ascribed to its distorted chain

Table 2	Photovoltaic parameters	of PB2T:IT-M and PE	3T:IT-M devices with	n different D/A ratios und	der AM 1.5G illumination	, 100 mW cm ⁻²
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Active layer	D/A ratio [wt/wt]	Processing solvent	$V_{\rm oc} \left[V \right]$	$J_{\rm sc}(J_{\rm calc.}^{c})$ [mA cm ⁻²]	FF	PCE _{max} /PCE _{ave} [%]
PB3T:IT-M	70:30	CB^a	1.00	18.7(17.2)	0.57	$10.6/10.2\pm0.26$
	60:40	CB^a	1.00	19.2(18.6)	0.61	$11.7/11.4 \pm 0.20$
	50:50	CB^a	1.00	18.0(17.3)	0.63	$11.3/11.0\pm0.22$
	40:60	CB^a	0.99	17.9(16.7)	0.62	$11.1/10.6\pm0.35$
	60:40	Anisole ^b	1.00	18.9(18.2)	0.63	$11.9/11.4 \pm 0.23$
PB2T	50:50	CB^{a}	0.56	0.08(0.06)	0.26	0.01/0.01

^{*a*} With thermal annealing at 150 °C for 10 min. ^{*b*} As-cast film. ^{*c*} The J_{sc} calculated from the EQE spectrum. The average PCE values are calculated from 10 independent cells.



Fig. 6 (a) Two-dimensional GIWAXS images of neat polymers and polymer:IT-M blend films. (b) The corresponding out-of-plane and in-plane line-cut reflection profiles.

conformation, which prevents interchain π - π stacking of the PB2T polymers. In the case of PB3T, a strong lamellar (100) diffraction peak was observed in the neat polymer film in the IP direction, indicating a preferential face-on orientation. The interlamellar distance of PB3T was calculated to be 25.1 Å. Furthermore, the PB3T film exhibited a strong π - π stacking (010) peak in the OOP direction with a *d*-spacing of \sim 3.8 Å, revealing its high crystallinity with tight cofacial face-on packing. The strong π - π stacking (010) diffraction peak suggested that the coplanar polymer backbone of PB3T is favorable for ordered molecular packing, which is beneficial for intermolecular charge transport in the vertical direction and is correlated with the higher hole mobility of the PB3T film. For the PB3T:IT-M blend, a diffraction pattern similar to that of the neat polymer film was obtained, indicating that PB3T has a stacking similar to that in the pristine polymer film. Moreover, the lamellar (300) diffraction peaks of IT-M at $q_{xy} = 0.85$ Å⁻¹ were also observed in the polymer:IT-M blends in the IP direction, consistent with previously reported observations.¹² The high crystallinity, ordered molecular packing and predominant faceon orientation favor higher charge mobility, resulting in improved photovoltaic properties in the PB3T:IT-M blend.

The surface morphologies of the polymer:IT-M blend films were investigated using atomic force microscopy (AFM) and



Fig. 7 Tapping-mode AFM (a and d) topography and (b and e) phase images and (c and f) TEM images of (a, b, and c) PB3T:IT-M and (d-f) PB2T:IT-M blend films (1.5:1 processed by CB).

transmission electron microscopy (TEM). As shown in Fig. 7(a) and (d), the PB2T:IT-M and PB3T:IT-M blend films exhibited a root-mean-square surface roughness (R_q) of 0.31 nm and 0.78 nm, respectively. The AFM phase image of the PB3T:IT-M blend film showed more pronounced phase separation than the PB2T:IT-M film. Moreover, as displayed in Fig. 7(c) and (f), the TEM image of the PB3T:IT-M blend exhibited stronger and more finely dispersed phase separation relative to the PB2T:IT-M blend, which is consistent with the morphologies observed by AFM. The nanoscale bicontinuous phase separation in the PB3T: IT-M blend is beneficial for exciton dissociation and charge transport in fullerene-free PSCs.

In addition to its outstanding PCE in PSCs, the PB3T:IT-M blend also offers several advantages for potential practical applications. First, with respect to mass production, the development of PSCs processed by environmentally friendly solvents is important for satisfying environmental protection and safety requirements. Thus, the environmentally friendly solvent anisole was used to prepare the PB3T:IT-M active layer in this work, and the device achieved a high PCE of 11.9% (see Fig. 3 and Table 2). Second, the high performance of the anisole-processed device was achieved without using any solvent additives or post-treatments, which can greatly simplify device fabrication.

Conclusions

In summary, two new WBG polymers (PB2T and PB3T) were synthesized based on BDT and oligothiophene units. The theoretical calculation results reveal that PB3T exhibits a planar geometry, whereas PB2T has a highly twisted backbone conformation. Due to the WBG optical absorption, suitable HOMO level and strong π - π stacking of PB3T, the PSC device based on the PB3T:IT-M active layer achieved an outstanding PCE of 11.7%. Moreover, PB3T could be processed by the environmentally friendly solvent anisole without using any solvent additive or post-treatments, affording a PCE of 11.9%. These results suggest that PB3T is a promising polymer donor for practical application because of its high PCE, D/A blend ratio tolerance and environmentally friendly fabrication. Although the photovoltaic performance of the PB3T-based PSC is outstanding among the current PSCs, opportunities exist for improving the FF of the device, which would further enhance the PCE of the PSC. Therefore, in future work, we will continue to optimize the molecular structure of this type of WBG polymer and improve the FF of the corresponding PSC devices.

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