Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

New polymer donor for efficient polymer solar cells: simultaneously realizing high short-circuit current density and transparency

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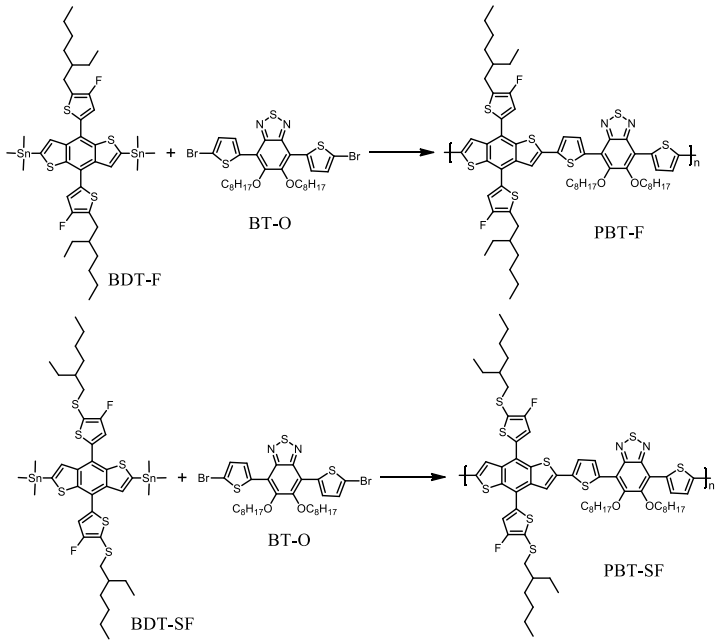
Experimental Section



Scheme S1 Synthetic routes of **PBT-F** and **PBT-SF**.

Synthesis of ***PBT-F*** (or ***PBT-SF***): In a 25 mL flask, monomers BDT-F[1] (0.282 mg, 0.3 mmol) (or 0.301 mg BDT-SF[2]) and BT-O[3] (0.214 mg, 0.3 mmol) were dissolved in 10 mL toluene, and the flask was flushed with argon for 10 min. Then 20 mg of $Pd(PPh_3)_4$ was added into the solution, and the mixture was flushed with argon for another 15 min. The solution was heated to reflux for 16 h under argon protection. After cooling to ambient temperature, the polymer was precipitated in 200 mL of methanol, filtered through a Soxhlet thimble. The precipitate was then subjected to Soxhlet extraction with methanol, hexane, and chloroform. The polymer was precipitated from 100 mL of methanol. The precipitates were collected and dried under vacuum overnight to get polymer as solid.

PBT-F: M_n = 14.7 kDa, PDI = 1.83. T_d = 314 °C.

PBT-SF: M_n = 12.5 kDa, PDI = 3.02. T_d = 308 °C.

Materials Characterization: Cyclic voltammetry was performend on a Zahner IM6e electrochemical workstation with a three-electrode system in a solution of 0.1 M $[Bu_4N]PF_6$ acetonitrile solution at a scan rate of 100 mV s^{-1}. Glassy carbon dis coated with polymer film was used as the working electrode. A Pt wire was used the counter electrode and Ag/Ag^+ was used as the reference electrode. Ferrocene/ferrocenium redox couple was used as the external standard and its redox potential is 0.06 V versus Ag/Ag^+. The HOMO and LUMO energy levels were calculated from the onset of the oxidation and reduction potential of polymer using the following equations: HOMO = $-e(\varphi_{ox} + 4.74)$ (eV); LUMO = $-e(\varphi_{red} + 4.74)$ (eV), respectively.

Device Fabrication and Characterization: The devices with a conventional architecture of glass/ITO/PDEOT:PSS/**PBT-F** (or **PBT-SF**):IT-4F/PFN-Br/Al were fabricated and characterized in an N_2-filled glove box. PFN-Br was used as cathode interlayer. 100 nm Al layer were subsequently evaporated though a shadow mask to define the active area (2 × 2 mm^2) of the devices and form a top anode. The current density-voltage (*J*-*V*) measurement of the PSCs were measured under a illumination of AM 1.5G (100 mW cm^{-2}) using a SS-F5-3A solar simulator (AAA grade, 50 × 50 mm^2 photobeam size) of Enli Technology CO., Ltd.. The EQE was measured by using a Solar Cell Spectral Response

Measurement System QE-R3011 (Enli Technology Co., Ltd.). The light intensity at each wavelength was calibrated by a standard single-crystal Si solar cell.

Mobility Measurement: The hole and electron mobilities were calculated by using the space-charge-limited current (SCLC) method.[4, 5]

$$J \cong (9/8)\varepsilon\varepsilon_0\mu_0 V^2 \exp(0.89\sqrt{V/E_0 L})/L^3$$

where ε is the dielectric constant of the polymers, ε_0 is the permittivity of the vacuum, μ_0 is the zero-field mobility, E_0 is the characteristic field, J is the current density, and L is the thickness of the film.

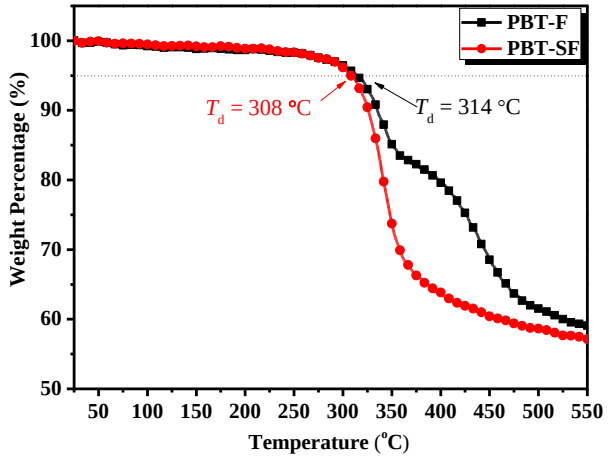


Fig. S1 TGA plots of **PBT-F** and **PBT-SF** with a heating rate of 10 °C min^{-1} under a N_2 atmosphere.

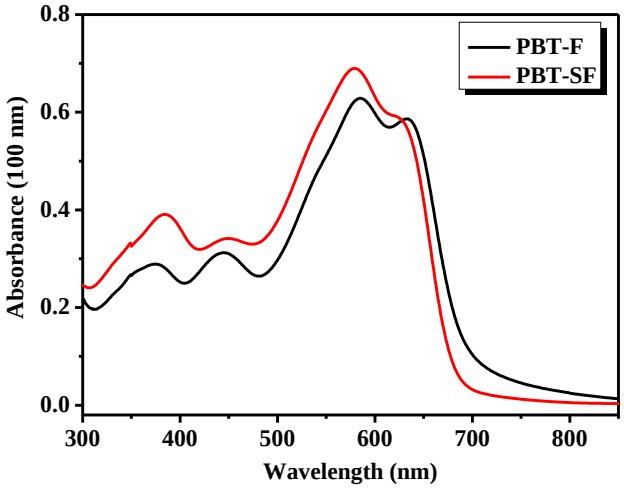


Fig. S2 The absorbance features of neat **PBT-F** and **PBT-SF** films at 100 nm thickness.

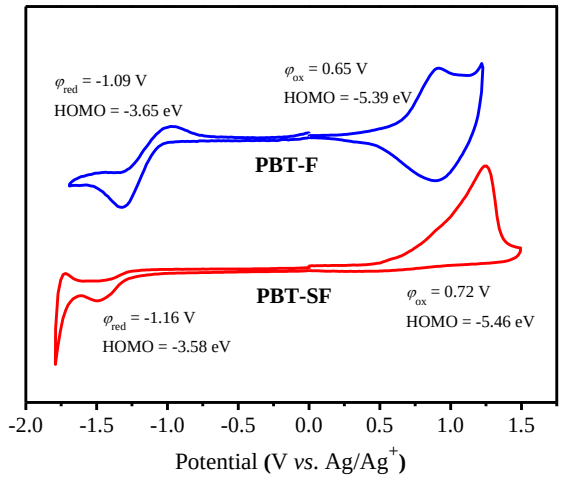


Fig. S3 Cyclic voltammograms of **PBT-F** and **PBT-SF** films on a glassy carbon electrode in 0.1 mol L^{-1} Bu_4NPF_6 acetonitrile solution at a scan rate of 100 mV s^{-1}.

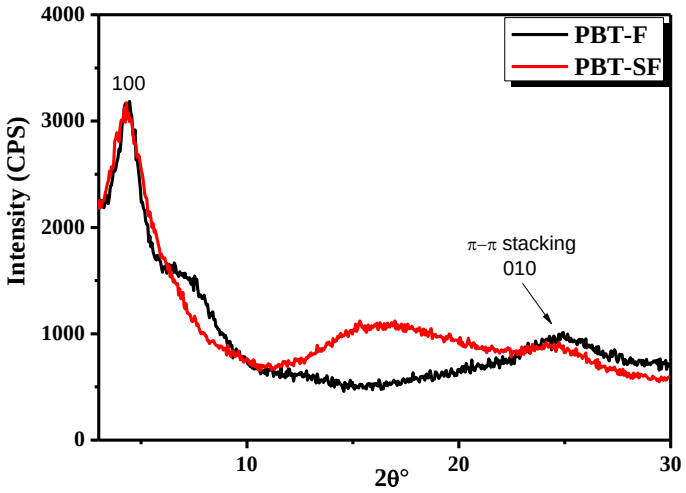


Fig. S4 XRD patterns of neat **PBT-F** and **PBT-SF** films.

Table S1 Photovoltaic performance of the PSCs based on **PBT-F**:IT-4F and **PBT-SF**:IT-4F with different D/A ratio under the illumination of AM 1.5 G at 100 mW cm^{-2}.

Active layer	D/A ratio	V_{oc} [V]	J_{sc} [mA cm^{-2}]	FF [%]	PCE [%]
PBT-F:IT-4F	1:0.5	0.83	15.20	42.5	5.33 [5.16]
	1:1	0.83	18.96	45.3	7.11 [7.02]
	1:1.5	0.81	15.78	40.7	5.22 [5.05]

	1:2	0.82	17.20	45.9	6.49 [6.28]
PBT-SF:IT-4F	1:0.5	0.87	12.99	32.5	3.66 [3.21]
	1:1	0.86	17.36	46.2	6.94 [6.78]
	1:1.5	0.86	16.68	49.9	7.18 [7.07]
	1:2	0.86	17.14	48.0	7.11 [7.02]

The values in square brackets are the average PCE obtained from 6 devices.

Table S2 Photovoltaic performance of the PSCs based on **PBT-F**:IT-4F (1:1, w/w) and **PBT-SF**:IT-4F (1:1.5, w/w) blend film processed by different additive under the illumination of AM 1.5 G at 100 mW cm^{-2}.

Active layer	Treatment	V_{oc} [V]	J_{sc} [mA cm^{-2}]	FF [%]	PCE [%]
PBT-F:IT-4F	1% DIO	0.69	15.00	46.1	4.79 [4.52]
PBT-F:IT-4F	1% PN	0.67	18.19	36.1	4.37 [4.05]
PBT-SF:IT-4F	1% DIO	0.81	16.84	44.5	6.04 [5.89]
PBT-SF:IT-4F	1% CN	0.87	17.76	53.1	8.21 [8.02]
PBT-SF:IT-4F	1% DPE	0.84	19.15	40.5	6.50 [6.36]

The values in square brackets are the average PCE obtained from 6 devices. 1,8-diiodooctane (DIO); 1-Phenylnaphthalene (PN); 1-chloronaphthalene (CN); diphenyl ether (DPE). The values in square brackets are the average PCE obtained from 6 devices.

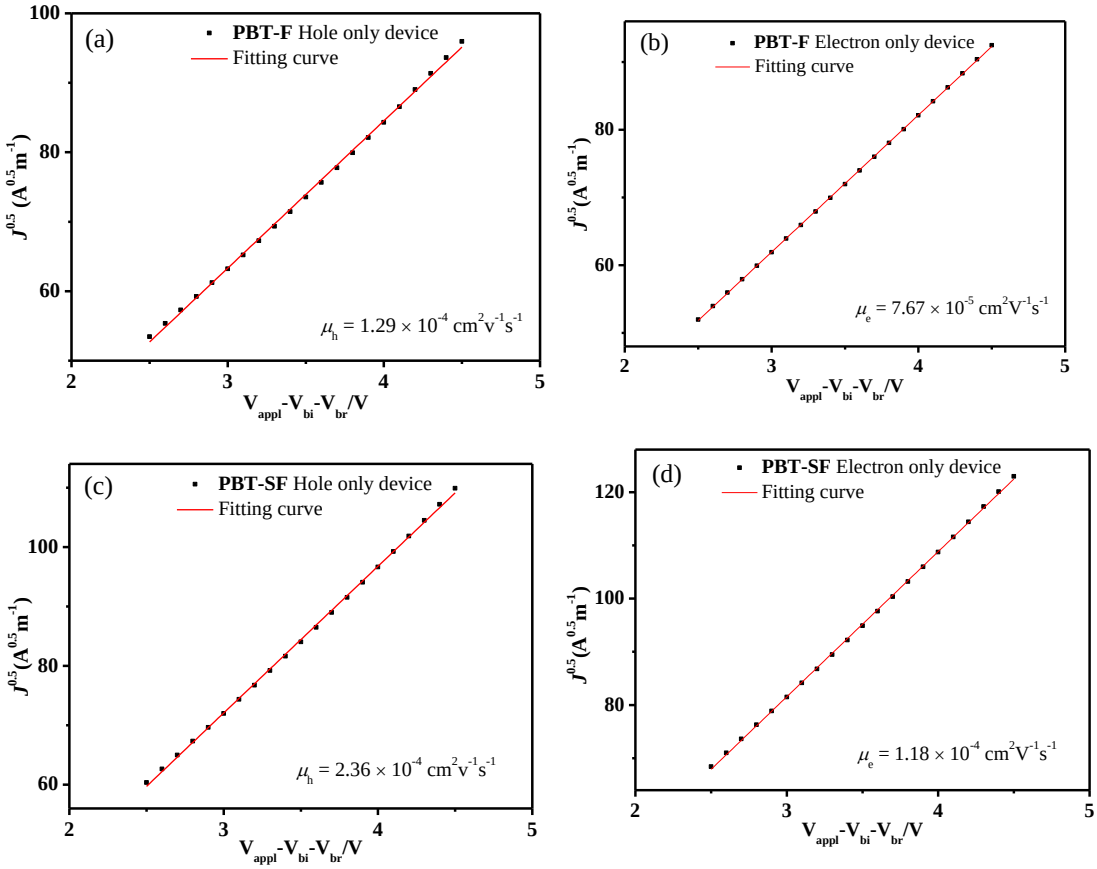


Fig. S5 $J^{0.5}$ vs (V_{app}-V_{bi}-V_{br}) plots (a) hole-only and (b) electron only devices of **PBT-F**:IT-4F (1:1, w/w) blend film; (c) hole-only and (d) electron only devices of **PBT-F**:IT-4F (1:1.5, w/w) blend film.

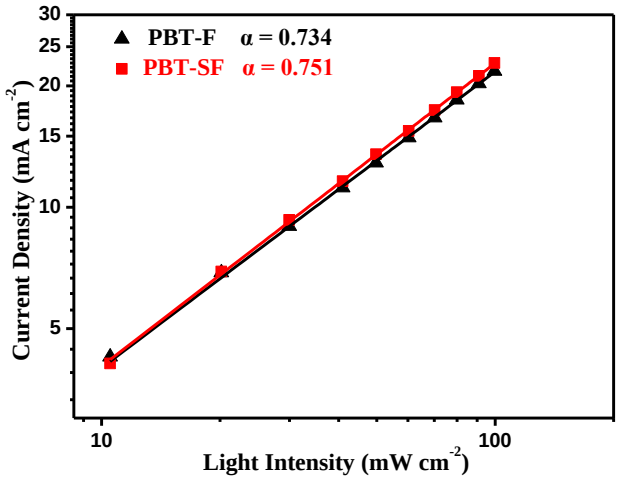


Fig. S6 The dependence of J_{sc} values on light intensity of **PBT-F**:IT-4F (1:1, w/w) and **PBT-SF**:IT-4F (1:1.5, w/w) based devices without any extra-treatment, respectively.

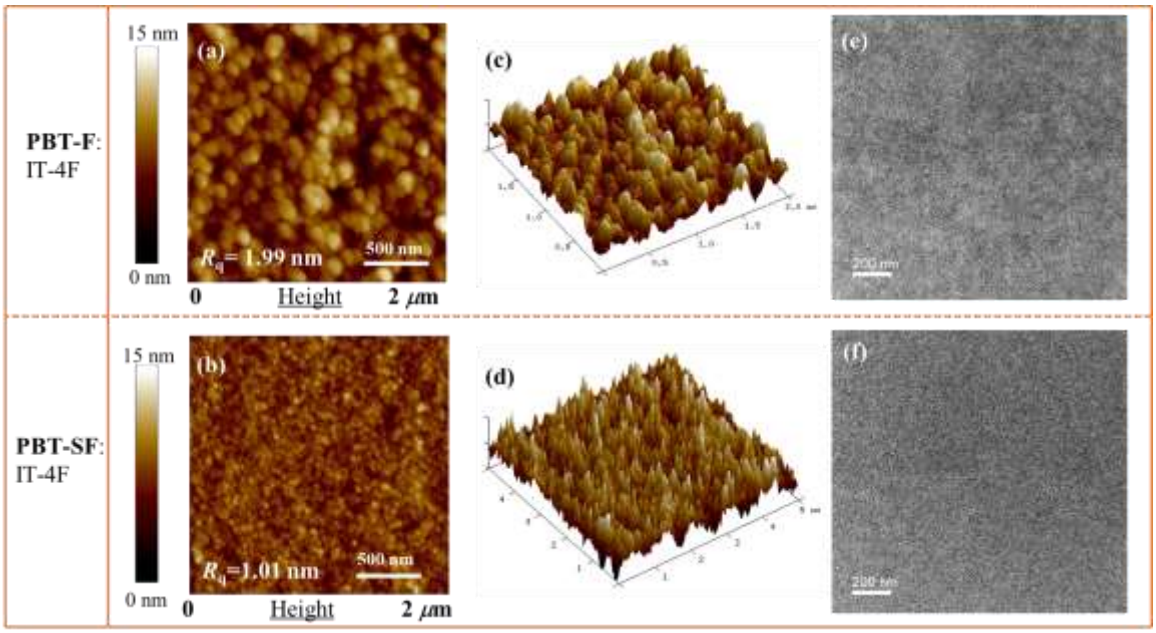


Fig. S7 (a, b) AFM topography, (c, d) AFM 3D topography, and (e, f) TEM images of the **PBT-F**:IT-4F (1:1, w/w) and **PBT-SF**:IT-4F (1:1.5, w/w) as-cast blend film, respectively.

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