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Electronic Supplementary Information

Length Evolution of Fused-Ring Electron Acceptors toward Optimal Blend Morphology in Polymer Solar Cells Incorporating Asymmetric Benzodithiophene Based Donors

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1. Materials and Methods

All reagents and starting materials were obtained commercially as analytical grade and used directly without any purification. Toluene and THF were distilled over sodium/benzophenone and calcium hydride under N_2 prior to use. Synthesis of polymer PBDTsTh-BDD, [1] monomer ThsBDTPh-Sn[2] and ThsBDTPhPh-Sn[2] were the same as our previous work. Acceptor ITIC-4T (ITIC)[3] and ITIC-2T (IC-1IDT-IC)[4] were synthesized as reported in the literatures. ^1H NMR and ^{13}C NMR spectra were taken on a Bruker AVANCE-III 600 Spectrometer. Thermal gravimetric analysis (TGA) measurement was performed on STA-409 at a heating rate of 10 °C min^{-1}. UV-Vis absorption spectrum was measured with a Hitachi U-4100 spectrophotometer. The organic molecule films on quartz used for absorption spectral measurement were prepared by spin-coating their chlorobenzene solutions. Cyclic voltammetry (CV) was performed using a CHI660D electrochemical workstation with a glassy carbon working electrode, a saturated calomel reference electrode (SCE) and a platinum wire counter electrode at a scan rate of 100 mV s^{-1}. Tetrabutylammonium phosphorus hexafluoride (Bu_4NPF_6, 0.1 M) in acetonitrile was used as the supporting electrolyte. Polymer film was prepared by drop-casting onto the glassy carbon working electrode from chlorobenzene solution and dried before measurements. The redox potential of the Fc/Fc$^+$ internal reference is 0.39 V vs. SCE. The highest occupied molecular orbit (HOMO) was determined by calculating the empirical formulas[5] of $E_{\mathrm{HOMO}} = -\mathrm{e}(E_{\mathrm{ox}} + 4.8 - E_{1/2}^{(\mathrm{Fc/Fc+})})$, where E_{ox} was the onset oxidation potential. The lowest unoccupied molecular orbit (LUMO) energy level was calculated from the equation of $E_{\mathrm{LUMO}} = E_{\mathrm{HOMO}} + E_{\mathrm{g}}^{\mathrm{opt}}$, where $E_{\mathrm{g}}^{\mathrm{opt}}$ was the optical band gap. Density functional theory (DFT) calculations were carried out by the Gaussian 09 program suite at the B3LYP/6-31G(d,p) level.[6] Transmission electron microscopy (TEM) images were acquired using a HITACHI H-7650 electron microscope operating at an acceleration voltage of 100 kV.

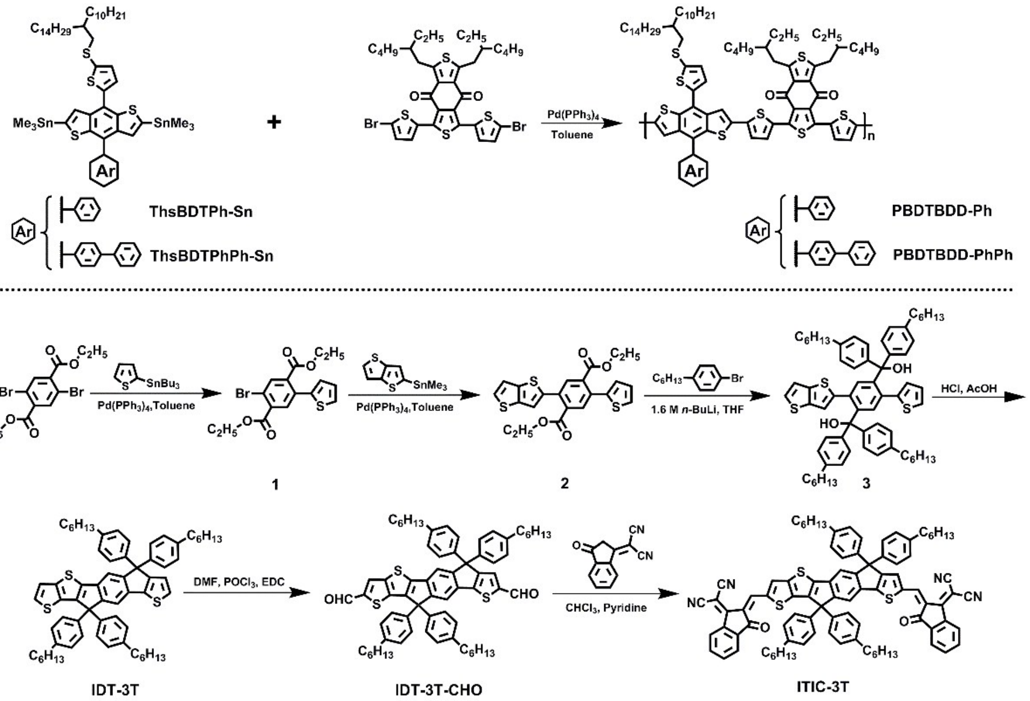
2. Device Fabrication and Testing

Photovoltaic devices were fabricated on pre-patterned indium tin oxide (ITO) coated glass substrates with a layered structure of ITO/PEDOT:PSS/active layer/PFN-Br (5 nm)/Al (100 nm). The ITO coated glass substrates were cleaned sequentially with detergent, de-ionized water, acetone and isopropanol, followed by drying with N_2 flow. And then, oxygen plasma treatment was made for 20 min, then spin-coated with PEDOT:PSS at 5000 rpm, and dried under argon for 20 min at 120 °C. Subsequently, the active layer was spin-coated from different blend weight ratios of donor and acceptor in chlorobenzene solution on the ITO/PEDOT:PSS substrate, then spin-coated with PFN-Br at 2000 rpm. The thickness of the active layer was controlled by changing the spin speed during the spin-coating process and measured using Veeco Dektak 150 surface profiler in our laboratory. Finally, aluminum (100 nm) was thermally evaporated at a vacuum of $\sim 2\times10^{-4}$ Pa on top of PFN-Br. The effective area of the device was measured to be 0.1 cm^2. The current density-voltage (J-V) characteristics were measured with a Keithley 2420 source measurement unit under simulated 100 mW cm^{-2} (AM 1.5 G) irradiation from a Newport solar simulator. Light intensity was calibrated with a standard silicon solar cell. The external quantum efficiencies (EQE) of solar cells were analyzed using a certified Newport incident photon conversion efficiency (IPCE) measurement system. Hole mobility and electron mobility were measured using the space charge limited current (SCLC) model, using a device configuration of ITO/PEDOT:PSS/active layer/Au and ITO/ZnO/active layer/PFN-Br/Al, respectively, and fitting the results to a space charge limited form, where the SCLC is described by:

$$J = (9/8)\varepsilon\mu(V^2/L^3)$$

where ε is the static dielectric constant of the medium and μ is the carrier mobility, V is the voltage drop across the device ($V = V_{\mathrm{appl}} - V_{\mathrm{bi}} - V_{\mathrm{rs}}$, where V_{appl} is the applied voltage to the device, V_{bi} is the built-in voltage due to the difference in work function of the two electrodes, and V_{rs} is the voltage drop due to series resistance across the electrodes), and L is the active layer thickness.

3. Synthesis and Characterization



Scheme S1. Synthetic routes of polymer donors and fullerene-free acceptors.

Synthesis of PBDTBDD-Ph

To a 25 mL flask, compound ThsBDTPh-Sn (135.6 mg, 0.13 mmol), 1,3-bis(5-bromothiophen-2-yl)-5,7-bis(2-ethylhexyl)-4*H*,8*H*-benzo[1,2-*c*:4,5-*c*']dithiophene-4,8-dione (99.7 mg, 0.13 mmol) and $Pd(PPh_3)_4$ (7.5 mg, 0.0065 mmol) were added under nitrogen. After the addition of toluene (5 mL), the mixture was heated to 110 °C and maintained at the same temperature for 6 h. After cooling to room temperature, the mixture was poured into methanol. The precipitates were collected and purified by column chromatography over silica using chlorobenzene as the eluant. Then, the solution was poured into methanol again. The product was collected and dried overnight under vacuum at 40 °C with the yield 59% for PBDTBDD-Ph as dark solid. GPC: M_n=48.6 KDa, PDI=1.98. T_d=341 °C.

Synthesis of PBDTBDD-PhPh

PBDTBDD-PhPh was synthesized as dark solid with a yield of 53% according to the method of PBDTBDD-Ph described above. GPC: M_n=55.8 KDa, PDI=2.12. T_d=335 °C.

Synthesis of diethyl 2-bromo-5-(thiophen-2-yl)terephthalate (1)

To a 100 mL flask, diethyl 2,5-dibromoterephthalate (3.80 g, 10 mmol), tributyl(thiophen-2-yl)stannane (4.10 mg, 11 mmol) and $Pd(PPh_3)_4$ (577.8 mg, 0.5 mmol) were added under nitrogen. After the addition of toluene (50 mL), the mixture was heated to 110 °C and maintained at the same temperature for 24 h. After cooling to room temperature, the mixture was extracted with petroleum ether. The organic phase was dried over Na_2SO_4. After removing the solvent under vacuum, residue was purified by silica column chromatography with petroleum ether/ethyl acetate (20/1, v/v) to give compound 1 as colourless oil (1.38 g, 36%). ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.98 (s, 1H), 7.85 (s, 1H), 7.40-7.38 (m, 1H), 7.07-7.06 (m, 2H), 4.42 (q, *J*=7.1 Hz, 2H), 4.21 (q, *J*=7.2 Hz, 2H), 1.41 (t, *J*=7.2 Hz, 3H), 1.16 (t, *J*=7.2 Hz, 3H).

Synthesis of diethyl 2-(thieno[3,2-b]thiophen-2-yl)-5-(thiophen-2-yl)terephthalate (2)

To a 100 mL flask, compound 1 (1.15g, 3 mmol), trimethyl(thieno[3,2-*b*]thiophen-2-yl)stannane (1.21g, 4 mmol) and $Pd(PPh_3)_4$ (173.3 mg, 0.15 mmol) were added under nitrogen. After the addition of toluene (30 mL), the mixture was heated to 110 °C and maintained at the same temperature for 24 h. After cooling to room temperature, the mixture was extracted with chloroform. The organic phase was dried over Na_2SO_4. After removing the solvent under vacuum, residue was purified by silica column chromatography with petroleum ether/dichloromethane (1/1, v/v) to give compound 2 as light yellow solid (1.01 g, 76%). ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.86 (s, 1H), 7.84 (s, 1H), 7.41-7.39 (m, 2H), 7.29-7.26 (m, 2H), 7.12-7.10 (m, 1H), 7.09-7.08 (m, 1H), 4.25-4.21 (m, 4H), 1.16 (t, *J*=7.1 Hz, 3H), 1.12 (t, *J*=7.1 Hz, 3H). Elemental analysis calcd (%) for $C_{22}H_{18}O_4S_3$: C 59.70, H 4.10, S 21.74, found: C 59.54, H 4.17, S 21.89.

Synthesis of (2-(thieno[3,2-*b*]thiophen-2-yl)-5-(thiophen-2-yl)-1,4-phenylene)bis(bis(4-hexylphenyl)methanol) (3)

To a solution of 1-bromo-4-hexylbenzene (4.34 g, 18 mmol) in THF (20 mL) at -78 °C was added dropwise n-BuLi (11.25 mL, 18 mmol, 1.6 M in hexane), the mixture was kept at -78 °C for 1 h, and a solution of compound 2 (0.89 g, 2 mmol) in THF (20 mL) was then added slowly. The mixture was stirred for 6 h and then poured into water and extracted with chloroform. The organic phase was dried over Na_2SO_4. After removing the solvent under vacuum, the resulting solid was washed with hexane to give compound 3 as offwhite solid (1.32 g, 66%). ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.27 (d, *J*=4.4 Hz, 1H), 7.14 (d, *J*=5.1 Hz, 1H), 7.11-7.08 (m, 17H), 6.80 (d, *J*=2.6 Hz, 2H), 6.72-6.70 (m, 1H), 6.14 (d, *J*=3.5 Hz, 1H), 6.10 (s, 1H), 3.42 (s, 1H), 3.39 (s, 1H), 2.61-2.58 (m, 8H), 1.62-1.57 (m, 8H), 1.32-1.26 (m, 24H), 0.89-0.86 (m, 12H). Elemental analysis calcd (%) for $C_{66}H_{78}O_2S_3$: C 79.31, H 7.87, S 9.62, found: C 79.56, H 7.95, S 9.45.

Synthesis of IDT-3T

Compound 3 (1.0 g, 1 mmol) was dissolved in acetic acid (25 mL) and concentrated HCl (2 mL) was added to the solution. The mixture was stirred at 80 °C for 2 h and then poured into water and extracted with chloroform. The organic phase was dried over Na_2SO_4. After removing the solvent under vacuum, residue was purified by silica column chromatography with petroleum ether to give compound IDT-3T as light yellow solid (0.69 g, 72%). ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.49 (s, 1H), 7.43 (s, 1H), 7.27-7.24 (m, 3H), 7.16 (d, *J*=8.3 Hz, 8H), 7.06 (d, *J*=8.2 Hz, 8H), 6.99 (d, *J*=4.9 Hz, 1H), 2.57-2.54 (m, 8H), 1.60-1.55 (m, 8H), 1.32-1.26 (m, 24H), 0.88-0.85 (m, 12H). Elemental analysis calcd (%) for $C_{66}H_{74}S_3$: C 82.27, H 7.74, S 9.98, found: C 82.46, H 7.65, S 9.75.

Synthesis of IDT-3T-CHO

$POCl_3$ (2.4 mL) was added slowly to the mixture of 1,2-dichloroethane (30 mL) and DMF (2 mL) at 0 °C under nitrogen. Then, a solution of compound IDT-3T (578.1 mg, 0.6 mmol) in 1,2-dichloroethane (30 mL) was added. After stirring at 85 °C for 24 h, the mixture was poured into water and extracted with chloroform. The organic phase was dried over Na_2SO_4. After removing the solvent under vacuum, residue was purified by silica column chromatography with petroleum ether/dichloromethane (2/1, v/v) to give compound IDT-3T-CHO as yellow solid (526.1 mg, 86%). ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 9.89 (s, 1H), 9.82 (s, 1H), 7.94 (s, 1H), 7.65 (d, *J*=6.1 Hz, 2H), 7.53 (s, 1H), 7.16-7.12 (m, 8H), 7.10-7.08 (m, 8H), 2.58-2.54 (m, 8H), 1.61-1.54 (m, 8H), 1.33-1.27 (m, 24H), 0.88-0.85 (m, 12H). Elemental analysis calcd (%) for $C_{68}H_{74}O_2S_3$: C 80.11, H 7.32, S 9.44, found: C 80.32, H 7.45, S 9.21.

Synthesis of ITIC-3T

Compound IDT-3T-CHO (254.9 mg, 0.25 mmol) and 2-(3-oxo-2,3-dihydro-1*H*-inden-1-ylidene) (194.2 mg, 1 mmol) were dissolved in chloroform (60 mL), and then pyridine (0.5 mL) was added to the mixture under nitrogen. After stirring at 80 °C for 12 h, the mixture was poured into water and extracted with chloroform. The organic phase was dried over Na_2SO_4. After removing the solvent under vacuum, residue was purified by silica column chromatography with petroleum ether/dichloromethane (1/1, v/v) to give compound ITIC-3T as dark blue solid (250.4 mg, 73%). ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.89 (s, 1H), 8.87 (s, 1H), 8.68 (d, *J*=7.5 Hz, 2H), 8.21 (s, 1H), 7.93-7.89 (m, 2H), 7.77-7.72 (m, 5H), 7.69 (s, 1H), 7.58 (s, 1H), 7.20 (d, *J*=8.2 Hz, 4H), 7.17-7.13 (m, 8H), 7.11 (d, *J*=8.3 Hz, 4H), 2.59-2.56 (m, 8H), 1.62-1.57 (m, 8H), 1.35-1.27 (m, 24H), 0.88-0.84 (m, 12H). ^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) 188.43, 188.14, 160.38, 160.31, 159.25, 157.73, 156.40, 155.67, 152.50, 148.08, 146.90, 143.86, 142.54, 142.34, 141.15, 140.37, 140.03, 139.96, 139.84, 139.44, 138.88, 138.51, 138.20, 138.13, 136.89, 136.87, 136.76, 135.98, 135.23, 135.17, 134.52, 134.48, 128.91, 128.74, 127.82, 127.73, 125.34, 123.80, 123.77, 122.97, 122.16, 119.72, 118.78, 114.65, 114.61, 114.57, 114.51, 69.58, 69.17, 63.24, 62.99, 35.61, 35.56, 31.71, 31.32, 31.25, 29.15, 29.11, 22.59, 22.58, 14.10, 1.03. MS (MALDI-TOF): cacld for $C_{92}H_{82}N_4O_2S_3$ $[M]^+$: 1370.55944; found: 1370.55876. Elemental analysis calcd (%) for $C_{92}H_{82}N_4O_2S_3$: C 80.55, H 6.02, N 4.08, S 7.01, found: C 80.34, H 6.18, N 4.02, S 7.11. T_d=339 °C.

4. TGA, DFT, UV-Vis and CV Measurements and Basic Properties

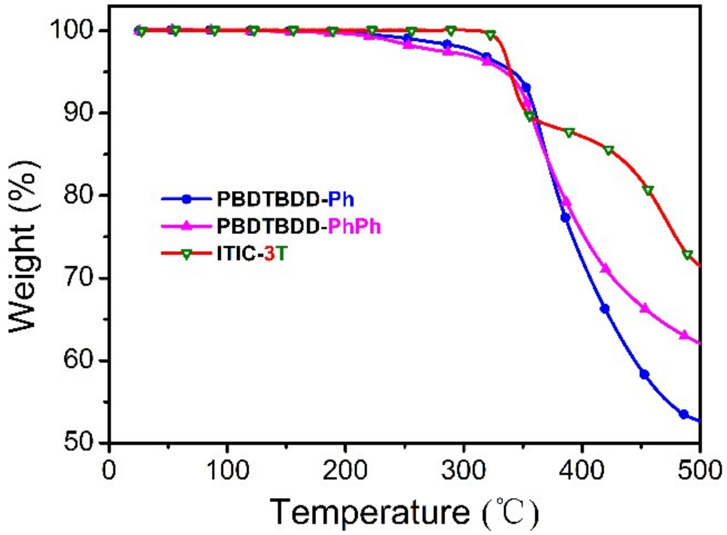


Figure S1 Thermogravimertic analysis (TGA) of the polymers.

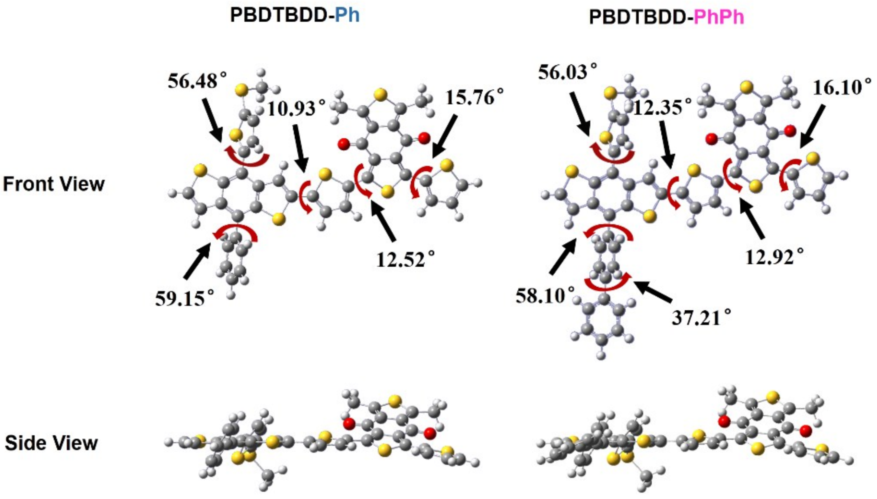


Figure S2 Simulated molecular geometries of the polymers by DFT caculations.

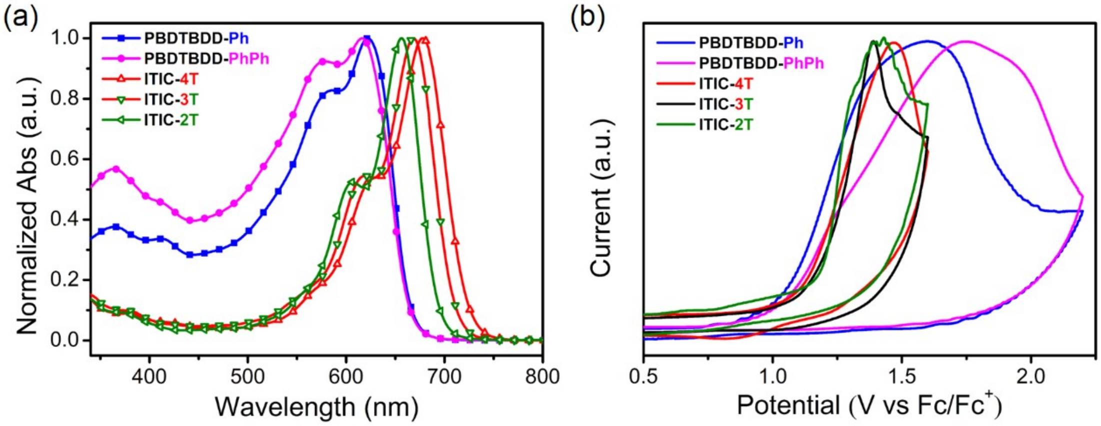


Figure S3 (a) Absorption spectra of donors and acceptors in chlorobenzene solution at room temperature; (b) Electrochemical cyclic voltammetry curves of donors and acceptors.

Table S1 Basic characteristics of the materials

materials	M_n (KDa)	PDI	T_d (°C)	solution		film			HOMO [b] (eV)	LUMO[c] (eV)
				λ_{max} (nm)	λ_{onset} (nm)	λ_{max} (nm)	λ_{onset} (nm)	$E_g^{opt[a]}$ (eV)		
PBDTBDD-Ph	48.6	1.98	341	623	669	628	671	1.85	-5.42	-3.57
PBDTBDD-PhPh	55.8	2.12	335	616	669	622	671	1.85	-5.43	-3.58
ITIC-4T	—	—	—	678	726	711	785	1.58	-5.52	-3.94
ITIC-3T	—	—	339	669	710	706	769	1.61	-5.54	-3.93
ITIC-2T	—	—	—	656	691	684	738	1.68	-5.61	-3.93

[a] Calculated from the absorption onset; [b] Measured by cyclic voltammetry; [c] Calculated from HOMO energy levels and optical band gaps.

5. Detailed Optimized Device Parameters

Table S2 Photovoltaic parameters based on the active layers with different D/A ratios

Polymer/Acceptor	D/A (w/w)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF	PCE[a] (%)
PBDTBDD-Ph/ITIC-4T	1:0.8	0.938	15.48	0.576	8.36 (8.12)
	1:1	0.935	16.94	0.625	9.90 (9.82)
	1:1.5	0.944	16.21	0.537	8.21 (8.06)
PBDTBDD-Ph/ITIC-3T	1:0.8	0.933	17.26	0.600	9.66 (9.42)
	1:1	0.924	17.51	0.681	11.02 (10.86)
	1:1.5	0.929	17.33	0.588	9.47 (9.18)
PBDTBDD-Ph/ITIC-2T	1:0.8	0.878	10.46	0.413	3.79 (3.68)
	1:1	0.920	13.56	0.502	6.26 (6.18)
	1:1.5	0.903	11.93	0.438	4.72 (4.56)
PBDTBDD-PhPh/ITIC-4T	1:0.8	0.921	14.01	0.554	7.15 (6.98)
	1:1	0.936	16.27	0.513	7.81 (7.65)
	1:1.5	0.948	13.12	0.530	6.60 (6.51)
PBDTBDD-PhPh/ITIC-3T	1:0.8	0.894	11.37	0.609	6.19 (6.01)
	1:1	0.934	15.73	0.523	7.68 (7.49)
	1:1.5	0.924	11.93	0.572	6.31 (6.05)
PBDTBDD-PhPh/ITIC-2T	1:0.8	0.883	8.66	0.454	3.47 (3.32)
	1:1	0.929	12.30	0.461	5.27 (5.11)
	1:1.5	0.910	10.57	0.492	4.73 (4.48)

[a] Average PCE in brackets (15 devices).

Table S3 Photovoltaic parameters based on the active layers with different thermal annealing temperature

Polymer/Acceptor	D/A (w/w)	Thermal annealing (°C)[a]	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF	PCE[b] (%)
PBDTsTh-BDD/ITIC-3T	1:1	—	0.945	12.54	0.527	6.25 (6.17)
PBDTsTh-BDD/ITIC-2T	1:1	—	0.962	9.61	0.508	4.70 (4.64)
PBDTBDD-Ph/ITIC-4T	1:1	80	0.931	15.34	0.630	9.00 (8.91)
	1:1	100	0.926	16.94	0.595	9.33 (9.12)
	1:1	120	0.919	16.00	0.624	9.18 (8.98)
PBDTBDD-Ph/ITIC-3T	1:1	80	0.914	17.38	0.632	10.04 (9.93)
	1:1	100	0.908	16.88	0.599	9.18 (9.05)
	1:1	120	0.897	16.57	0.609	9.05 (8.92)
PBDTBDD-Ph/ITIC-2T	1:1	80	0.901	14.00	0.455	5.74 (5.65)
	1:1	100	0.896	13.29	0.448	5.33 (5.24)
	1:1	120	0.886	14.10	0.451	5.63 (5.45)
PBDTBDD-PhPh/ITIC-4T	1:1	80	0.932	14.62	0.537	7.32 (7.25)
	1:1	100	0.924	13.50	0.530	6.60 (6.47)
	1:1	120	0.909	14.20	0.522	6.73 (6.49)
PBDTBDD-PhPh/ITIC-3T	1:1	80	0.920	13.83	0.542	6.89 (6.77)
	1:1	100	0.902	14.38	0.544	7.06 (6.91)
	1:1	120	0.891	14.13	0.554	6.97 (6.75)
PBDTBDD-PhPh/ITIC-2T	1:1	80	0.921	8.58	0.573	4.52 (4.42)
	1:1	100	0.914	8.56	0.512	4.01 (3.92)
	1:1	120	0.900	8.81	0.492	3.90 (3.76)

[a] The blend films were thermal annealed for 10 mins; [b] Average PCE in brackets (15 devices).

Table S4 Photovoltaic parameters based on active layers with different additive (DIO) volume fraction

Polymer/Acceptor	D/A (w/w)	Additive DIO (v%)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF	PCE[a] (%)
PBDTBDD-Ph/ITIC-4T	1:1	0.5	0.918	9.91	0.268	2.44 (2.34)
	1:1	1	0.920	10.12	0.284	2.65 (2.45)
PBDTBDD-Ph/ITIC-3T	1:1	0.5	0.889	10.17	0.449	4.06 (3.95)
	1:1	1	0.856	8.17	0.434	3.03 (2.94)
PBDTBDD-Ph/ITIC-2T	1:1	0.5	0.885	5.62	0.407	2.02 (1.98)
	1:1	1	0.897	5.26	0.460	2.17 (2.10)
PBDTBDD-PhPh/ITIC-4T	1:1	0.5	0.917	6.39	0.345	2.02 (1.89)
	1:1	1	0.921	8.49	0.336	2.63 (2.57)
PBDTBDD-PhPh/ITIC-3T	1:1	0.5	0.903	6.77	0.493	3.01 (2.78)
	1:1	1	0.891	6.64	0.490	2.90 (2.65)
PBDTBDD-PhPh/ITIC-2T	1:1	0.5	0.893	3.60	0.440	1.42 (1.33)
	1:1	1	0.895	3.68	0.453	1.49 (1.37)

[a] Average PCE in brackets (15 devices).

6. Hole Mobility, Electron Mobility and Photoluminescence Measurements

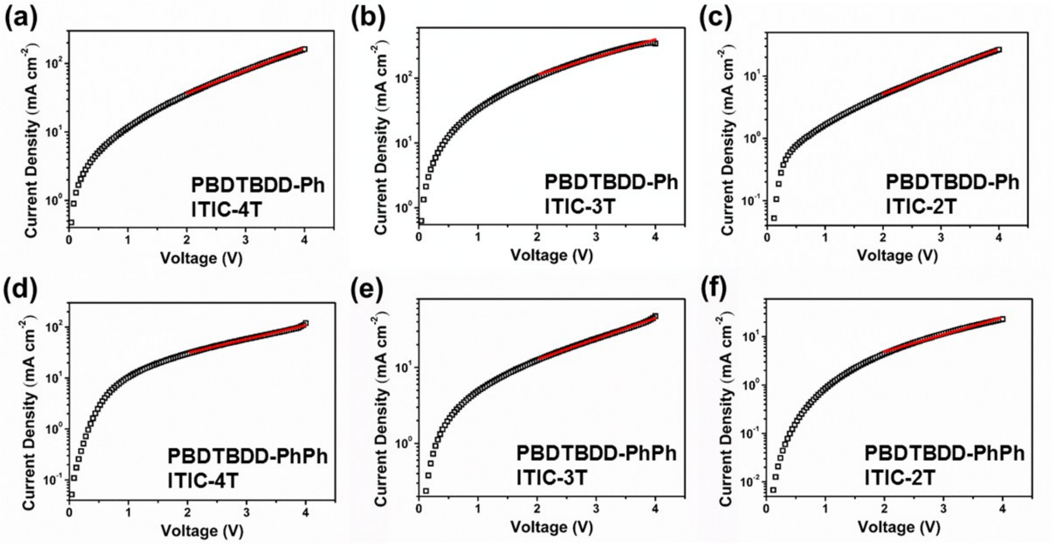


Figure S4. SCLC curves for hole-only based on optimized devices. (a) PBDTBDD-Ph/ITIC-4T, (b) PBDTBDD-Ph/ITIC-3T, (c) PBDTBDD-Ph/ITIC-2T, (d) PBDTBDD-PhPh/ITIC-4T, (e) PBDTBDD-PhPh/ITIC-3T, (f) PBDTBDD-PhPh/ITIC-2T (the symbols are experimental data for transport of hole, and the red lines are fitted according to the space-charge-limited-current model. The thicknesses of the active layers were about 100 nm).

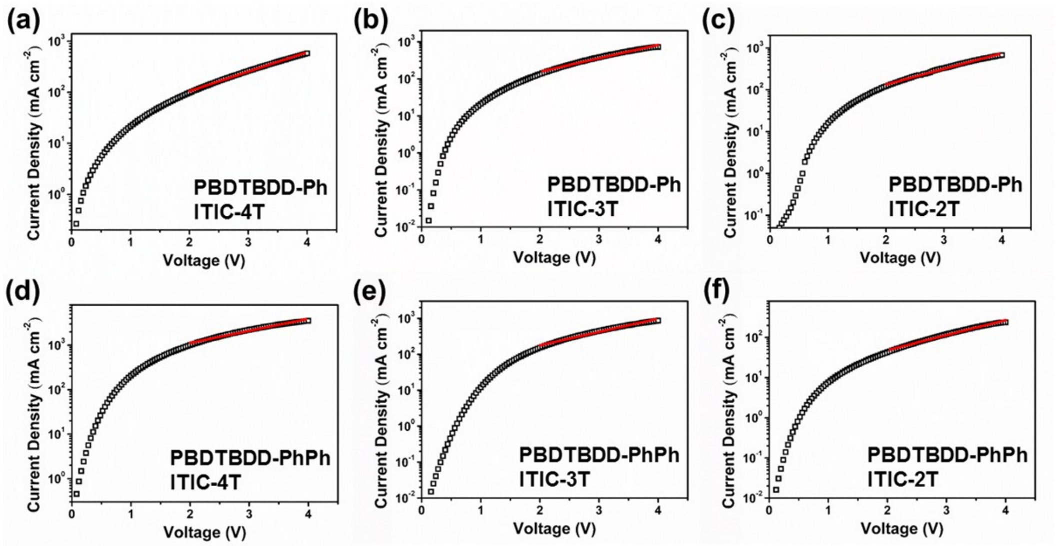


Figure S5. SCLC curves for electron-only based on optimized devices. (a) PBDTBDD-Ph/ITIC-4T, (b) PBDTBDD-Ph/ITIC-3T, (c) PBDTBDD-Ph/ITIC-2T, (d) PBDTBDD-PhPh/ITIC-4T, (e) PBDTBDD-PhPh/ITIC-3T, (f) PBDTBDD-PhPh/ITIC-2T (the symbols are experimental data for transport of electron, and the red lines are fitted according to the space-charge-limited-current model. The thicknesses of the active layers were about 100 nm).

Table S5 Hole and electron mobilities of the active layers

Active layers	μ_h (cm^2 V^{-1} s^{-1})	μ_e (cm^2 V^{-1} s^{-1})	μ_e/μ_h
PBDTBDD-Ph/ITIC-4T	4.04×10^{-5}	1.30×10^{-4}	3.22
PBDTBDD-Ph/ITIC-3T	9.44×10^{-5}	1.61×10^{-4}	1.71
PBDTBDD-Ph/ITIC-2T	4.56×10^{-6}	8.88×10^{-5}	19.47
PBDTBDD-PhPh/ITIC-4T	2.24×10^{-5}	4.17×10^{-4}	18.61
PBDTBDD-PhPh/ITIC-3T	9.22×10^{-6}	1.18×10^{-4}	12.8
PBDTBDD-PhPh/ITIC-2T	3.10×10^{-6}	6.74×10^{-5}	21.74

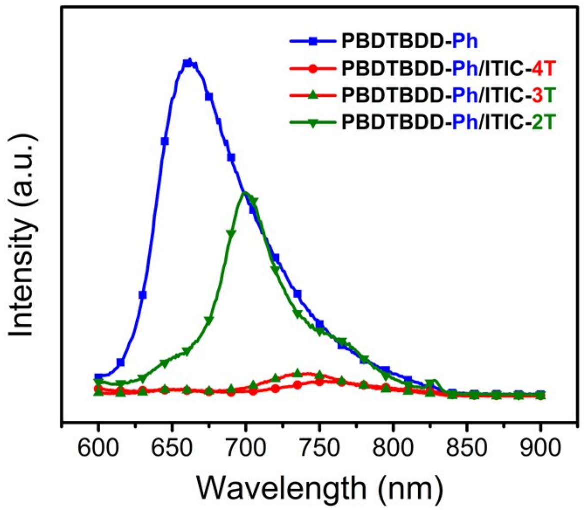


Figure S6. PL spectra of PBDTBDD-Ph and its blend films with ITIC-4T, ITIC-3T and ITIC-2T excited at 550 nm, respectively.

7. NMR Spectra

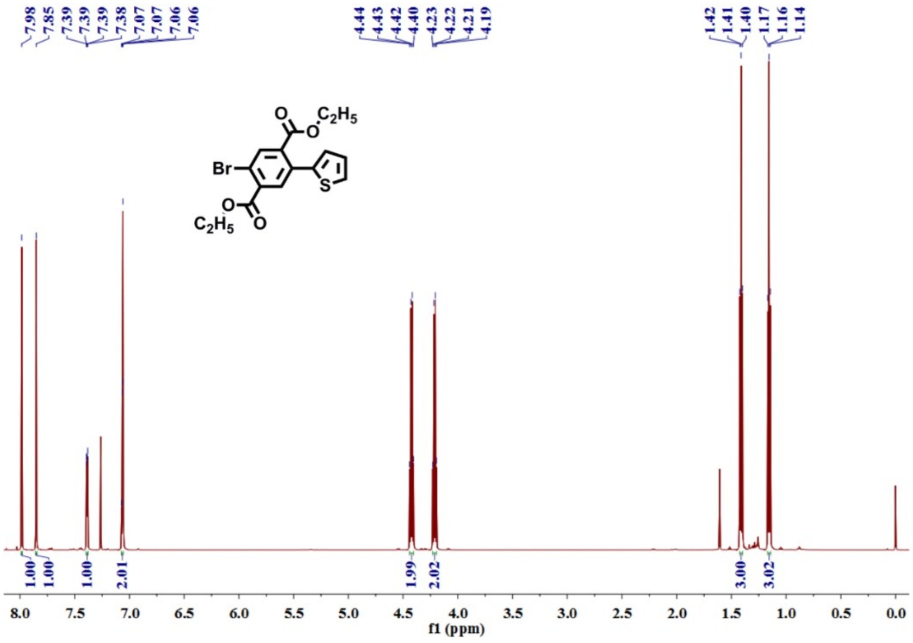


Figure S7 ^{1}H NMR spectrum of compound **1**.

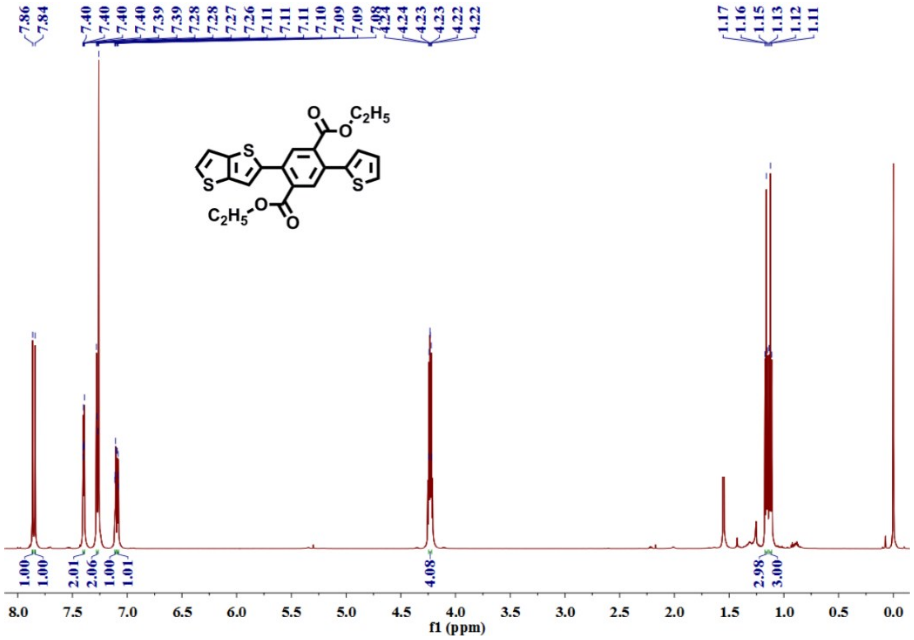


Figure S8 ^{1}H NMR spectrum of compound **2**.

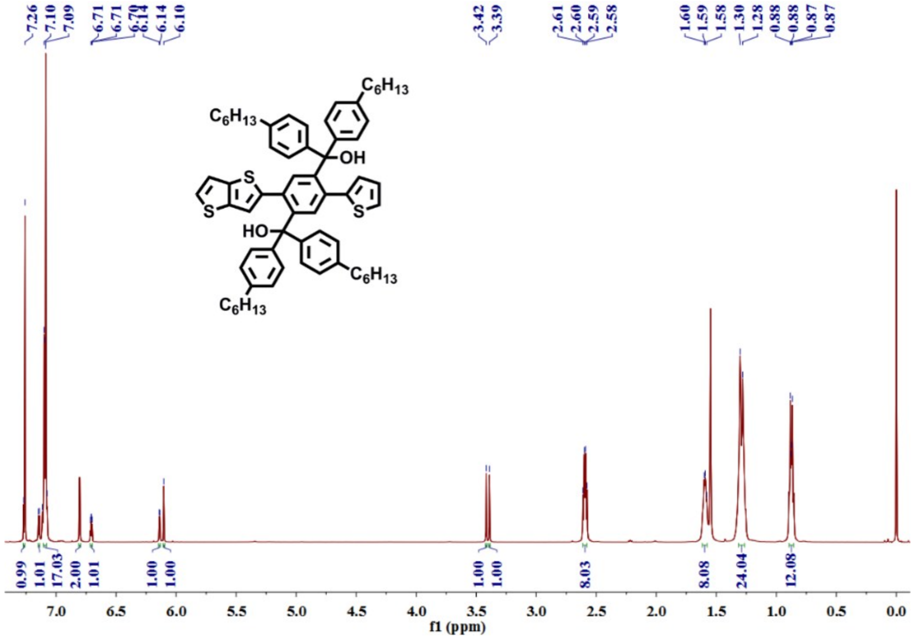


Figure S9 ^{1}H NMR spectrum of compound **3**.

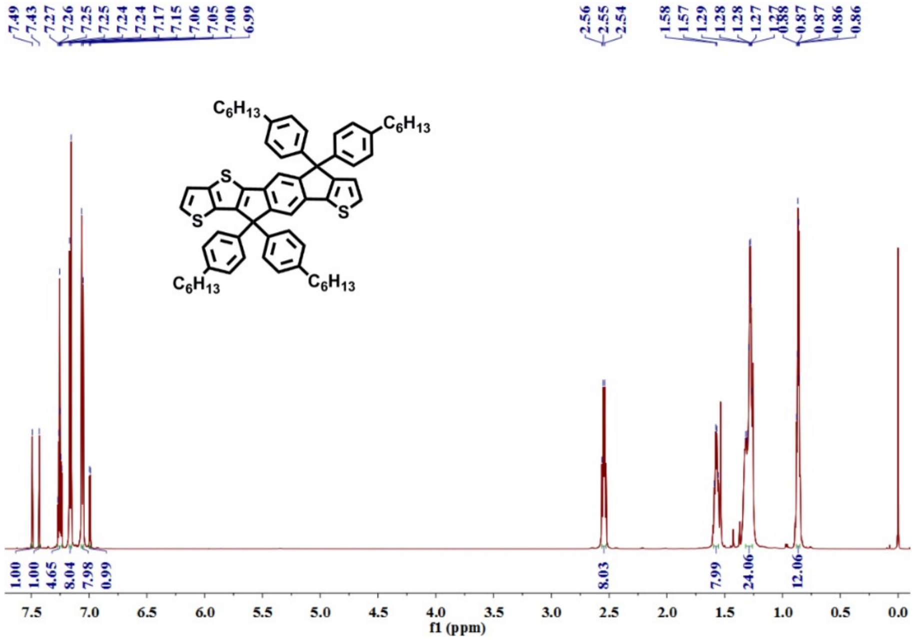


Figure S10 ^{1}H NMR spectrum of compound **IDT-3T**.

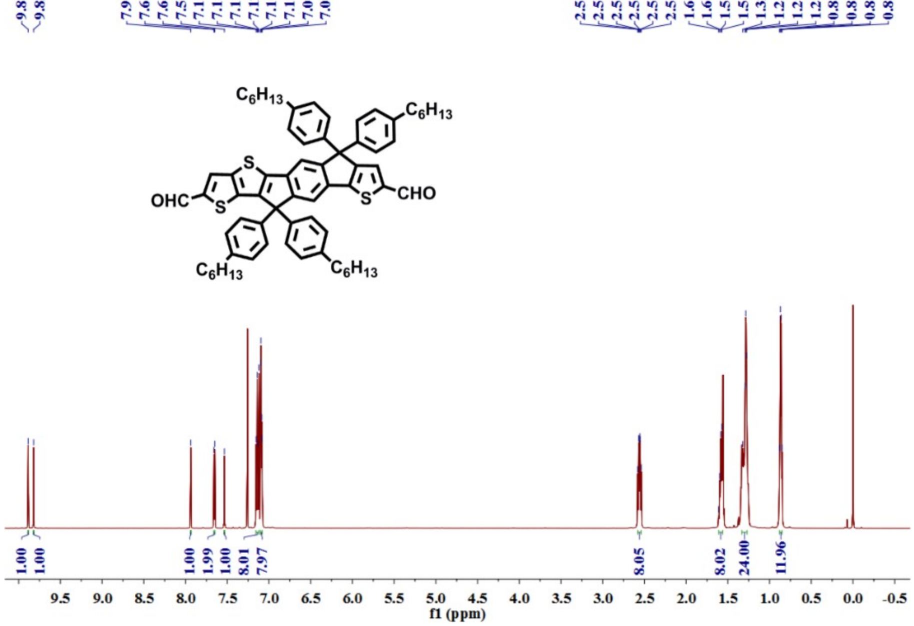


Figure S11 ^{1}H NMR spectrum of compound **IDT-3T-CHO**.

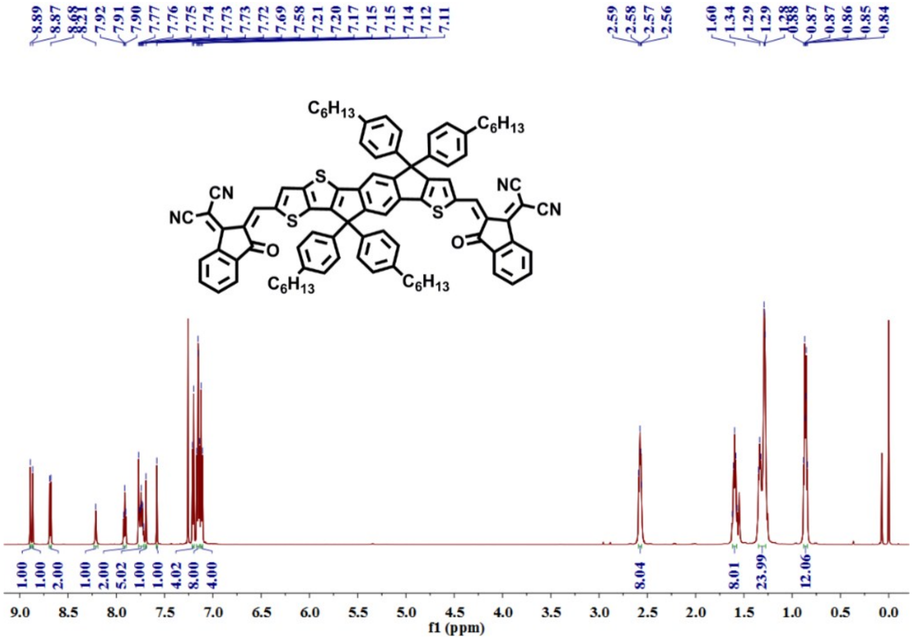


Figure S12 ^{1}H NMR spectrum of compound **ITIC-3T**.

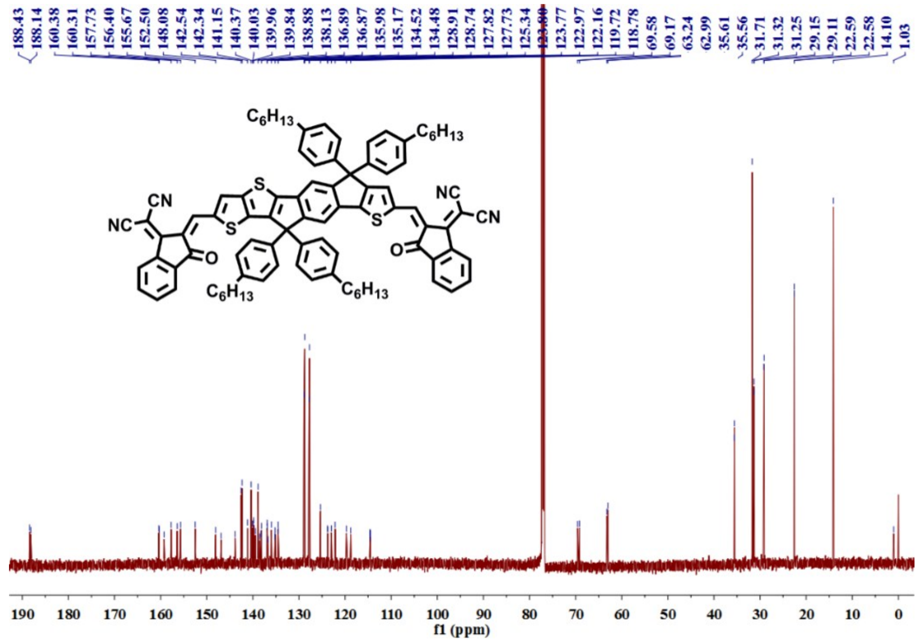


Figure S13 ^{13}C NMR spectrum of compound **ITIC-3T**.

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