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SUPPORTING INFORMATION

Three Pyrido[2,3,4,5-lmn]phenanthridine Derivatives and Their Large Band Gap Copolymers for Organic Solar Cells

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Instruments and measurements

The NMR data were collected on a Bruker AVANCE Digital 300 MHz NMR workstation. Mass spectrometry (MS) data were obtained on a Waters TQD. Matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF) mass spectra were recorded on a Bruker Autoflex III Smartbean. The number-average molecular weights (M_n), weight-average molecular weights (M_w) and polydispersity index (PDI) of copolymers were determined by high-temperature gel permeation chromatography (HT-GPC) using a Waters Alliance GPC 2000 instrument equipped with a refractive index (RI) detector and a set of u-Styragel HT columns of 10^6, 10^5, 10^4, and 10^3 pore size in series. The measurement was performed at 150 ℃ with 1,2,4-trichlorobenzene as the eluent with a flow rate of 0.95 mL/min. Narrow-molecular-weight polystyrene samples were used as standards for calibration. UV-vis absorption spectra were measured using a HP 8453 spectrophotometer. Thermogravimetric analysis (TGA) measurements were performed on a Netzsch TG 209 under N_2. Atomic force microscopy (AFM) measurements were carried out using a Digita Instrumental DI Multimode Nanoscope IIIa in taping mode. External quantum efficiency (EQE) measurements were taken using a monochromator (Newport, Cornerstone 130) joined to the same xenon lamp and a lock-in amplifier (Stanford Research Systems, SR 830) coupled to a light chopper.

Synthesis

Synthesis of monomers:

2,6-Bis(trimethyltin)-4,8-di[(2-butyloctane)oxy]-benzo[1,2-b;3,4-b]dithiophene was prepared according to the reported literature method.[1] All chemicals and reagents were purchased from commercial sources (Aldrich and Alfa Aesar) and used without further purification.

*4,4',6,6'-Tetranitrodiphenic acid (**2**):* Diphenic acid (60.6 g, 0.25 mol) was dissolved in sulfuric acid (400 mL), after that fuming nitric acid (80 mL) was added into the solution. The mixture was heated to 110 ℃ and stirred for 2 h. Then it was cooled and poured into 2 L ice-water. The white precipitate was collected by filtration, washed with water, and dried to get slight yellow powder (86 g, yield 81%). ^{1}H NMR (300 MHz, [$^2H_6$]-DMSO), δ (ppm): 9.12 (s, 2H), 8.95 (s, 2H). ^{13}C NMR (300 MHz, [$^2H_6$]-DMSO), δ (ppm): 164.45, 149.10, 148.00, 136.67, 133.97, 129.17, 122.95.

*2,7-Diamino-4,9-dihydropyrido[2,3,4,5-lmn]phenanthridine-5,10-dione (**3**):* Iron powder (25.0 g, 0.45 mol) was added into 60 mL of 5% aqueous ammonium chloride solution, the mixture was heated to 100 ℃ with vigorous stirring, and a solution of compound **2** (12.7 g, 30 mmol) in 50 ml of 10% ammonium hydroxide was added in 1 h. After stirring the mixture for 30 min, 20 ml of 20% sodium hydroxide solution was added, and the mixture was filtered, and the residue was treated with boiling mixture of N,N-dimethylformamide (DMF) and 25% sodium hydroxide solution (1:1, v/v) several times. The filtrates were combined and acidified to pH 6 with hydrochloric acid, and the precipitate was removed by filtration to give yellow solid (6.2 g, yield 78%). ^{1}H NMR (300 MHz, [$^2H_6$]-DMSO), δ (ppm): 11.42 (s, 2H), 7.13 (s, 2H), 6.78 (s, 2H), 5.72 (s, 4H). ^{13}C NMR (300 MHz, [$^2H_6$]-DMSO), δ (ppm): 161.79, 148.92, 135.55, 124.01, 109.15, 105.58, 103.10.

*2,7-Diiodo-4,9-dihydropyrido[2,3,4,5-lmn]phenanthridine-5,10-dione (**4**):* Compound **3** (2.7 g, 10 mmol) was added into 80 mL of 25% sulfuric acid at 0 ℃, and the resulting suspension was diazotized by adding sodium nitrite (1.4 g, 20 mmol) and stirring for 1 h. Then 30 mL of 30% potassium iodide solution and iodine (0.5 g, 2 mmol) were added into the mixture, warmed to room temperature and stirred overnight. The product was removed by filtration, and the brown solid was washed by water twice and dried in vacuum to give coarse product which could be used directly in the next step without further purification (4.3 g, yield 88%).

*4,9-Di(2-butyloctane)-2,7-diiodopyrido[2,3,4,5-lmn]phenanthridine-5,10-dione (**5a**), 10-(2-butyloctane)oxy-4-(2-butyloctane)-2,7-diiodopyrido[2,3,4,5-lmn]phenanthridin-5-one (**5b**) and 5,10-di(2-butyloctane)oxy-2,7-diiodopyrido[2,3,4,5-lmn]phenanthridine (**5c**):* Compound **4** (4.89 g，10 mmol) and potassium *tert*-butoxide (2.46 g，22 mmol) were added into anhydrous DMF (300 mL) in a two-neck round flask and heated to 100 ℃ under argon protection. After 30 min, 2-butyloctane bromide (7.50 g, 30 mmol) was injected one portion. When the reaction was stirred for 15 h at this temperature, the solution was cooled to room temperature, poured into 500 mL of ice-water and extracted by ethyl ether. The combined organic phase was washed with brine, dried over anhydrous magnesium sulfate, and the organic solvent was removed under vacuum to give a crude product. Isolation and purification of the crude products by column chromatography on silica gel (eluent: hexane:dichloromethane=3:1~1:1) were carried out to give **5a** (1.52 g, yield 18%) as a white solid, **5b** (3.14 g, yield 38%) as a yellow oil and **5c** (0.85 g, yield 10%) as a white solid.

5a. MS (APCI, +MS): M/Z= 825.2; ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.66 (s, 2H), 7.96 (s, 2H), 4.33 (s, 4H), 1.96 (m, 2H), 1.21-1.48 (m, 32H), 0.85-0.91 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 159.65, 136.69, 131.04, 125.94, 125,75, 116.18, 94.87, 46.88, 36.21, 31.78, 31.59, 31.32, 29.62, 28.78, 26.58, 23.03, 22.59, 14.04.

5b. MS (APCI, +MS): M/Z= 825.2; ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.70 (s, 1H), 8.44 (s, 1H), 8.36 (s, 1H), 7.89 (s, 1H), 4.54 (s, 2H), 4.33 (s, 2H), 1.99-2.02 (m, 2H), 1.23-1.54 (m, 32H), 0.89-0.97 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 160.25, 158.68, 142.04, 138.09, 136.99, 133.02, 126.86, 124.70, 124.03, 120.73, 118.41, 117.65, 94.50, 94.27, 70.22, 46.67, 37.54, 36.15, 31.88, 31.78, 31.64, 31.44, 31.36, 29.68, 29.62, 29.18, 28.82, 26.92, 26.62, 23.05, 22.68, 22.59, 14.11, 14.04.

5c. MS (APCI, +MS): M/Z= 825.2; ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.56 (s, 4H), 4.56 (s, 4H), 2.02 (m, 2H), 1.32-1.57 (m, 32H), 0.88-0.98 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 159.23, 141.96, 136.06, 128.62, 120.04, 119.95, 94.08, 70.05, 37.62, 31.91, 31.79, 31.48, 29.71, 29.23, 26.97, 23.07, 22.70, 14.12.

*4,9-Di(2-butyloctane)-2,7-di(thiophen-5-yl)-pyrido[2,3,4,5-lmn]phenanthridine-5,10-dione (**6a**):* 2-(Tributylstannyl)thiophene (1.61 g，4.3 mmol), **5a** (1.65 g，2 mmol) and 60 mg of $Pd(PPh_3)_4$ were stirred at 100 ℃ in toluene (30 mL) under argon protection for 16 h. After being cooled to room temperature, the reaction mixture was poured into 150 mL of water and extracted with dichloromethane. The organic phase was combined and dried over magnesium sulfate. After the solvent was removed, the product was further purified by column chromatography on silica gel to get a yellow solid (1.32 g，90%). MS (APCI, +MS): M/Z= 737.5; ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.59 (s, 2H), 7.81 (s, 2H), 7.56 (d, 2H), 7.42 (d, 2H), 7.17 (m, 2H), 4.51 (s, 4H), 1.99 (m, 2H), 1.22-1.55 (m, 32H), 0.87-0.95 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 161.12, 143.31, 136.21, 135.13, 128.49, 126.19, 125.03, 124.57, 119.06, 116.08, 113.97, 46.72, 36.67, 31.80, 31.56, 29.71, 29.11, 26.91, 23.12, 22.58, 14.05, 14.02.

*10-(2-Butyloctane)oxy-4-(2-butyloctane)-2,7-di(thiophen-5-yl)-pyrido[2,3,4,5-lmn]phenanthridin-5-one (**6b**):* **6b** was synthesized according to the procedure as described above for the synthesis of **6a**, giving a yellow solid in 88% yield. MS (APCI, +MS): M/Z= 737.5; ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.67 (s, 1H), 8.30 (s, 1H), 8.25 (s, 1H), 7.77 (s, 1H), 7.59 (d, 1H), 7.49 (d, 1H), 7.41 (d, 1H), 7.37 (d, 1H), 7.19 (t, 1H), 7.14 (t, 1H), 4.59 (d, 2H), 4.43 (d, 2H), 1.99-2.02 (m, 2H), 1.23-1.55 (m, 32H), 0.86-0.97 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 161.89, 159.95, 144.02, 143.76, 141.77, 136.67, 135.21, 134.76, 128.43, 128.30, 126.06, 125.93, 125.89, 124.37, 124.25, 125.16, 121.66, 120.23, 118.75, 117.98, 114.94, 112.63, 69.86, 46.61, 37.69, 36.61, 31.92, 31.81, 31.62, 30.98, 29.76, 29.24, 29.15, 27.84, 27.01, 23.11, 22.70, 22.58, 17.52, 14.11, 14.07, 13.56.

5,10-Di(2-butyloctane)oxy-2,7-

*di(thiophen-5-yl)-pyrido[2,3,4,5-lmn]phenanthridine (***6c***):* **6c** was synthesized according to the procedure as described above for the synthesis of **6a**, giving a yellow solid in 92% yield. MS (APCI, +MS): M/Z=737.5; ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.48 (s, 2H), 8.41 (s, 2H), 7.58 (d, 2H), 7.41 (d, 2H), 7.19 (t, 2H), 4.65 (d, 4H), 2.06 (m, 2H), 1.33-162 (m, 32H), 0.87-0.98 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 160.56, 144.37, 141.72, 134.78, 128.23, 125.71, 124.38, 124.09, 120.54, 119.60, 117.11, 69.67, 37.67, 31.88, 31.85, 31.55, 29.70, 29.20, 26.96, 23.04, 22.64, 14.06, 14.01.

*4,9-Di(2-butyloctane)-2,7-di(2-bromo-thiophen-5-yl)-pyrido[2,3,4,5-lmn]phenanthridine-5,10-dione (***7a***):* Compound **6a** (0.52 g，0.7 mmol) was added to 150 mL of chloroform in a flask. Then N-bromosuccinimide (NBS) (0.28 mg, 1.6 mmol) was added in one portion and stirred at room temperature for 16 h. Then the reaction mixture was poured into water and extracted with dichloromethane. The organic phase was combined and dried over magnesium sulfate. After the solvent was removed, the bromide product was recrystallized from chloroform to yield yellow product (0.53 g，83%). MALDI-TOF MS: m/z calcd for $C_{46}H_{58}Br_2N_2O_2S_2$, 892.23; found 893.3. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.37 (s, 2H), 7.60 (s, 2H), 7.24 (d, 2H), 7.10 (d, 2H), 4.38 (s, 4H), 1.98 (m, 2H), 1.24-1.48 (m, 32H), 0.81-0.90 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 160.96, 144.50, 136.31, 134.36, 131.36, 125.09, 124.77, 118.64, 116.14, 113.55, 113.30, 46.72, 36.76, 31.85, 31.59, 29.67, 29.20, 27.02, 23.15, 22.61, 14.08.

*10-(2-Butyloctane)oxy-4-(2-butyloctane)-2,7-di(2-bromo-thiophen-5-yl)-pyrido[2,3,4,5-lmn]phenanthridin-5-one (***7b***):* **7b** was synthesized according to the procedure as described above for the synthesis of **7a**, giving a yellow solid in 86% yield. MALDI-TOF MS: m/z calcd for $C_{46}H_{58}Br_2N_2O_2S_2$, 892.23; found 893.2. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.40 (s, 1H), 8.10 (s, 1H), 8.03 (s, 1H), 7.52 (s, 1H), 7.24 (d, 1H), 7.18 (d, 1H), 7.11 (d, 1H), 7.05 (d, 1H), 4.57 (d, 2H), 4.34 (d, 2H), 1.99-2.01 (m, 2H), 1.23-1.54 (m, 32H), 0.83-0.99 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 161.45, 159.74, 145.20, 144.97, 141.66, 136.58, 134.20, 133.83, 131.23, 131.18, 125.28, 124.42, 124.32, 124.02, 120.86, 120.07, 118.55, 117.78, 114.39, 113.03, 112.79, 111.89, 70.06, 46.49, 37.66, 36.64,31.94, 31.85, 31.63, 31.58, 29.80, 29.76, 29.25, 27.04, 23.13, 22.73, 22.61, 14.15, 14.11, 14.06.

5,10-Di(2-butyloctane)oxy-2,7-di(2-bromo-thiophen-5-yl)-pyrido[2,3,4,5-lmn]phenanthridine (7c): **7c** was synthesized according to the procedure as described above for the synthesis of **7a**, giving a yellow solid in 80% yield. MALDI-TOF MS: m/z calcd for $C_{46}H_{58}Br_2N_2O_2S_2$, 892.23; found 893.3. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 8.29 (s, 2H), 8.24 (s, 2H), 7.27 (d, 2H), 7.12 (d, 2H), 4.63 (d, 4H), 2.04 (m, 2H), 1.33-155 (m, 32H), 0.86-0.98 (m, 12H). ^{13}C NMR (300 MHz, $CDCl_3$), δ (ppm): 160.56, 145.73, 141.83, 134.04, 131.18, 124.29, 123.95, 120.64, 119.68, 116.76, 112.62, 69.86, 37.70, 31.93, 31.59, 29.25, 27.02, 23.09, 22.71, 14.11.

Synthesis of polymers

***Pa**:* Compound **7a** (223 mg, 0.25 mmol) and **8** (222 mg, 0.25 mmol) were dissolved in degassed toluene (10 mL), and $Pd(PPh_3)_4$ (9 mg) was added under a stream of argon. Then the mixture was refluxed under argon for 48 h with stirring. After that, the mixture was poured into methanol and the precipitated product was collected by filtration. The crude product was subjected to Soxhlet extractions with methanol, acetone, hexane, and $CHCl_3$ in succession. The polymer was reprecipitated from methanol to yield **Pa** as a red solid (257 mg, yield 80%). GPC: M_w= 76.2 kDa, M_n= 31.7kDa, PDI = 2.4.

***Pb**:* The polymerization procedure for compound **7b** (223 mg, 0.25 mmol) and compound **8** (222 mg, 0.25 mmol) is similar to that of **Pa** which has been described above. **Pb** was obtained as a red solid (212 mg, yield 65%). GPC: M_w= 52.5 kDa, M_n= 24.9 kDa, PDI = 2.1.

***Pc**:* The polymerization procedure for compound **7c** (223 mg, 0.25 mmol) and compound **8** (222 mg, 0.25 mmol) is similar to that of **Pa** which has been described above. **Pc** was obtained as an orange solid (245 mg, yield 76%). GPC: M_w= 45.2 kDa, M_n= 22.6 kDa, PDI = 2.0.

Thermogravimetric analysis (TGA)

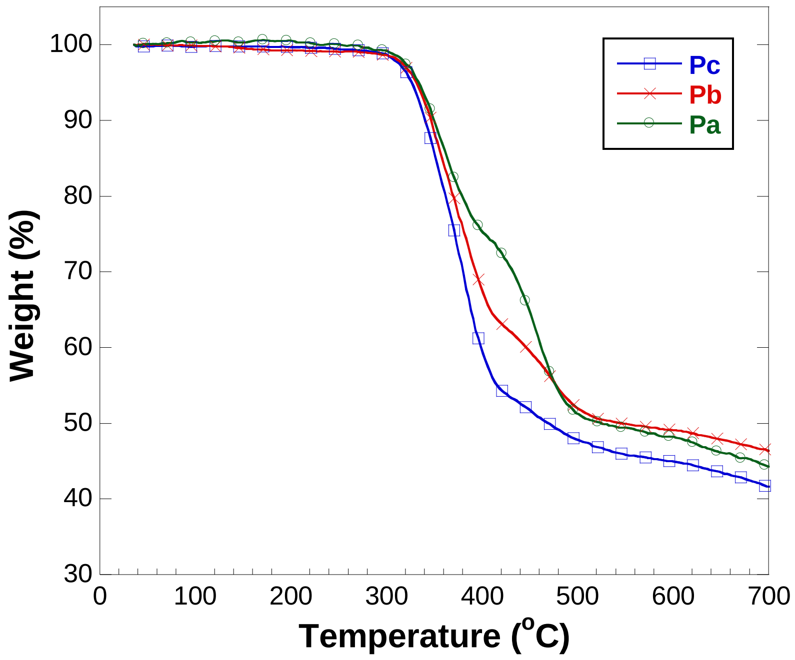

Figure S1. TGA plots of polymers **Pa**, **Pb** and **Pc**.

Density functional theory (DFT) calculation

Density functional theory (DFT) calculations were performed for the calculation of HOMO and LUMO energy levels by using the Gaussian suite of programs (Gaussian 03W).[2] The ground state structures were optimized with B3LYP/6-31G(d) method, and the single-point energies were calculated with B3LYP/6-311+G(d,p) method.

Table S1. Calculated HOMO and LUMO energy levels and energy band gaps (E_g^{cal}) for the repeat units of BDT-DAPPD, BDT-AOAPPO and BDT-DAOPP. The molecular structures were simplified by replacing alkyls with methyl groups.

repeat units	BDT-DAPPD	BDT-AOAPPO	BDT-DAOPP
LUMO (eV)[a]	-2.54	-2.44	-2.28
HOMO (eV)[a]	-5.48	-5.51	-5.42
E_g^{cal} (eV)[a]	2.94	3.07	3.14

[a] Obtained by density functional theory (DFT) calculations (B3LYP/6-31G(d)//B3LYP/6-311G+(d,p), Gaussian 03W).

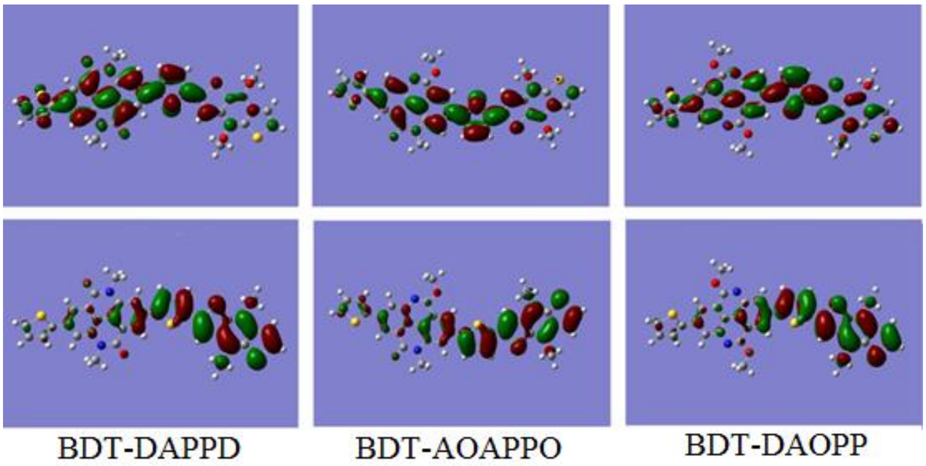

Figure S2. Calculated frontier orbitals of HOMOs (*bottom*) and LUMOs (*top*) for the repeat units of BDT-DAPPD, BDT-AOAPPO and BDT-DAOPP. The molecular structures were simplified by replacing alkyls with methyl groups.

Electrochemical cyclic voltammetry (CV)

Electrochemical cyclic voltammetry measurements were carried out using a CHI800 electrochemical workstation equipped with a graphite working electrode, a saturated calomel electrode as the reference electrode, and a Pt sheet counter electrode. The measurements were done in anhydrous acetonitrile with tetrabutylammonium hexafluorophosphate (0.1 M) as the supporting electrolyte under an argon atmosphere at a scan rate of 50 mV s^{-1}. The potential of the saturated calomel reference electrode was internally calibrated using the ferrocene/ferrocenium redox couple (Fc/Fc^+), which has an absolute energy level of -4.8 eV. The polymer films for electrochemical measurements were coated from their chloroform solutions. HOMO energy levels were calculated by the following equation.

$$\text{HOMO} = -(E_{ox} + 4.8\ \text{eV}) \qquad (1)$$

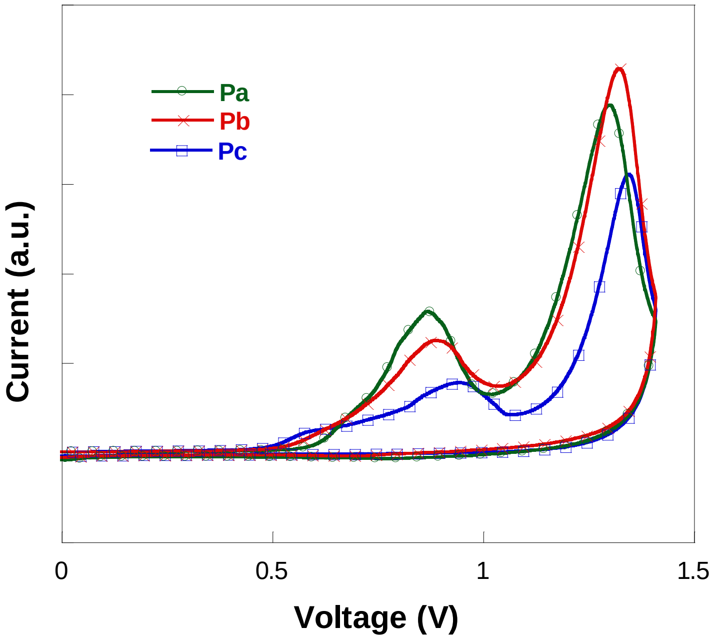

Figure S3. Cyclic voltammograms of polymers **Pa**, **Pb** and **Pc**.

Hole mobility measurement

Space charge limited current (SCLC) studies were performed in a hole-only device structure of ITO/PEDOT:PSS/polymer:$PC_{71}BM$ (100 nm)/MoO_3 (10 nm)/Al. The mobility was determined by fitting the dark current to the model of a single carrier SCLC, which is described by the equation:

$$\boldsymbol{J} = \frac{9}{8}\varepsilon_0\varepsilon_r\mu_h\frac{V^2}{d^3} \qquad (2)$$

where $\boldsymbol{J}$ is the current, μ_h is the zero-field mobility, ε_0 is the permittivity of free space, ε_r is the relative permittivity of the material, d is the thickness of the active layer, and V is the effective voltage. The effective voltage can be obtained by subtracting the built-in voltage (V_{bi}) and the voltage drop (V_s) from the substrate's series resistance from the applied voltage (V_{appl}).

$$V=V_{appl} - V_{bi} - V_s \qquad (3)$$

The hole mobility can be calculated from the slope of the $J^{1/2} \sim V$ curves. The active area is 0.16 cm^2.

Table S2. Hole mobilities of the active layers of polymer:$PC_{71}BM$ (1:1, by weight)

active layer	**Pa**:$PC_{71}BM$	**Pb**:$PC_{71}BM$	**Pc**:$PC_{71}BM$
Thickness (nm)	100	100	100
Mobility ($cm^2\ V^{-1}\ s^{-1}$)	8.3×10^{-5}	1.6×10^{-5}	4.9×10^{-5}

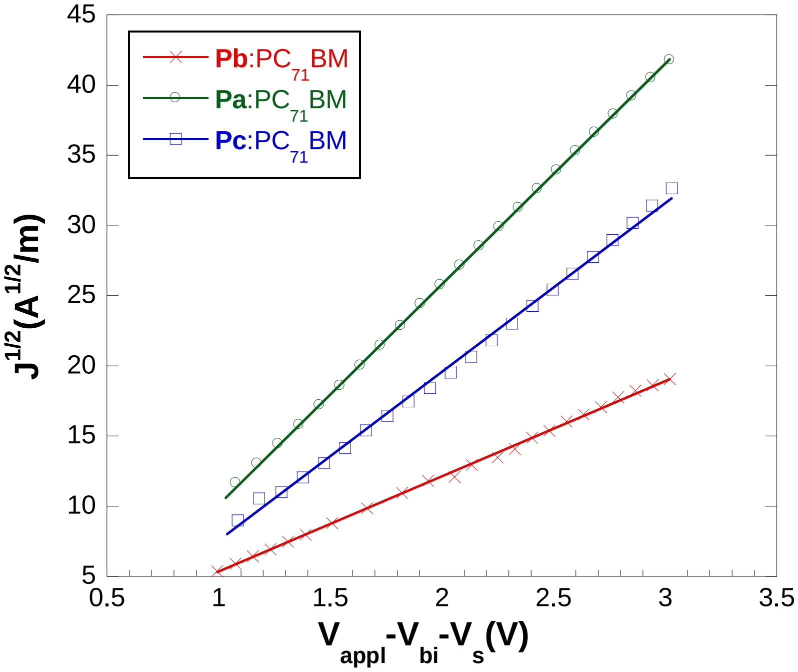

Figure S4. *$J^{1/2}$~V* characteristics of the hole-only devices in a structure of ITO/PEDOT:PSS/polymer:$PC_{71}BM$ (100 nm)/MoO_3 (10 nm)/Al measured at ambient temperature.

Film morphology

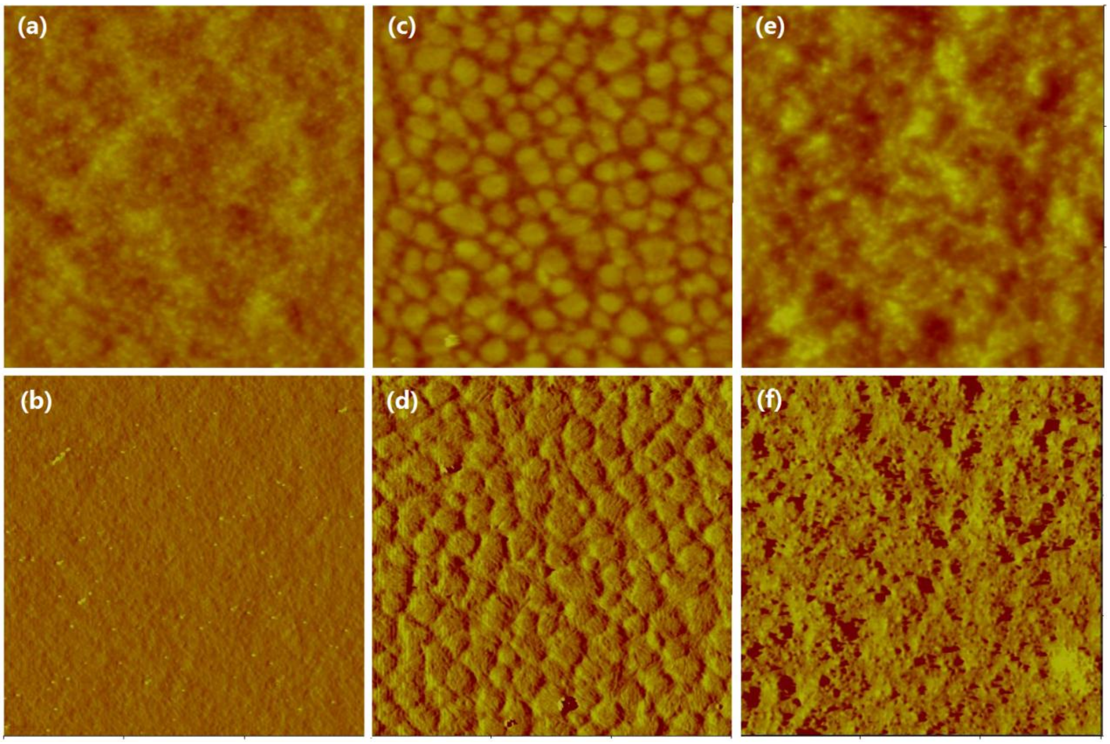

Figure S5. AFM images (size: 3 μm × 3 μm) of spin-coated polymer:PC$_{71}$BM blend films on glass substrates. a) Topographic and b) phase images of **Pa**:PC$_{71}$BM; c) topographic and d) phase images of **Pb**:PC$_{71}$BM; and e) topographic and f) phase images of **Pc**:PC$_{71}$BM.

Fabrication and characterization of PSCs

Patterned indium tin oxide (ITO)-coated glass substrates were used as the anode in the polymer solar cells. The ITO-coated glass substrates were cleaned by sonication in detergent, deionized water, acetone and isopropyl alcohol, and then dried in a nitrogen stream, followed by an oxygen plasma treatment.

For the conventional PSCs, the surface of the ITO substrate was modified by spin-coating a conducting PEDOT:PSS (Clevios P4083) layer with a thickness of 40 nm, followed by baking at 140 ℃ for 10 minutes under ambient conditions. The substrates were then transferred into an argon-filled glove box. The copolymers were blended with $PC_{71}BM$ in a weight ratio of 1:1 in 1,2-dichlorobenzene (*o*-DCB) and then spin-coated onto the PEDOT:PSS layer at 800-1000 rpm as the active layer with a thickness of about 90 nm. Finally, the devices were transferred into the vacuum chamber and then Ca (4 nm) and Al (80 nm) were thermally deposited onto the active layer through a shadow mask with a defined active area of 0.16 cm^2 under high vacuum.

For the inverted PSCs, the cleaned ITO-coated glass substrates were spin-coated with a 10-nm-thin film of cross-linkable PF_3N-OX from its solution in methanol and acetic acid (100:1) (0.5 mg mL^{-1}). Cross-linking process was carried out by heating the half-dried films under 130 °C and fluorescence lamp illumination (no UV lamps required) for 20 min. The bulk heterojunction (BHJ) composite of polymer:$PC_{71}BM$ (1:1, by weight) with a thickness of approximate 90 nm was then spin-coated on the cross-linked PF_3N-OX layer from their 1,2-dichlorobenzene solution. After that, a 10-nm-thin layer of molybdenum oxide (MoO_3) was thermally deposited on top of the polymer:$PC_{71}BM$ active layer through a shadow mask in a vacuum chamber with base pressure of 3×10^{-6} mbar. The active area of the device is 0.16 cm^2 as determined by the shadow mask used during deposition of Al cathode.

Power conversion efficiencies (PCEs) were measured under an AM 1.5 G solar simulator (Oriel model 91192). The power of the sun simulation was calibrated before the testing using a standard silicon solar cell, giving a value of 100 mW cm^{-2} during the test. The current density–voltage (*J*–*V*) characteristics were recorded with a Keithley 236 source meter. The spectral response was measured with a commercial photo modulation spectroscopic setup (Oriel). A calibrated Si photodiode was used to determine the photosensitivity.

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