Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Low Band Gap Disk-shaped Donors for Solution-Processed Bulk-Hetrojunction Solar Cells

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Synthetic procedures of 6-18.

6: A solution of 5-bromo-3-hexylthiophene-2-carbaldehyde (0.18g, 0.66mmol), 3-hexyl-2-thiopheneboronic acid pinacol ester (0.29g, 0.99mmol) and $Pd(PPh_3)_4$ (15mg, 0.02mmol) in toluene (8ml), THF (9.6ml) and 2.0 M K_2CO_3 aqueous solution (5ml) was refluxed for 48 h under nitrogen. After cooling to room temperature, the reaction mixture was poured into water, extracted with CH_2Cl_2. The organic layer was dried over magnesium sulfate and the solvent was evaporated. The residue was purified by column chromatography on silica gel by eluting with CH_2Cl_2 and recycling preparative HPLC to give **6** as yellow oil (0.13g, yield 54 %). ^{1}H-NMR (400.13MHz, $CDCl_3$): δ (ppm) =10.00 (s, 1H, Ar*H*), 7.24 (d, *J*=5.2Hz, 1H, Ar*H*), 7.02 (s, 1H, Ar*H*), 6.94 (d, *J*=5.2Hz, 1H, Ar*H*), 2.93 (t, *J*=7.6Hz, 2H, -CH_2-), 2.80 (t, *J*=7.6Hz, 2H, -CH_2-), 1.75-1.62 (m, 4H, -CH_2-), 1.43-1.27 (m, 12H, -CH_2-), 0.93-0.88 (m, 6H, -CH_3). ^{13}C-NMR ($CDCl_3$, 100.61Hz): δ (ppm) =182.1, 153.7, 145.9, 142.4, 136.8, 131.1, 130.3, 128.9, 125.9, 32.1, 32.0, 31.8, 30.8, 30.0, 29.6, 29.4, 28.9, 23.0, 21.7, 14.5.

7: N-Bromosuccinimide (NBS) (67mg, 0.37mmol) was slowly added to the solution of **6** (0.11g, 0.31mmol) in chloroform (10ml) and acetic acid (10ml). The reaction mixture was refluxed for 24h and poured into water. After extraction with CH_2Cl_2, the organic layer was dried over magnesium sulfate and the solvent was evaporated. The residue was purified by column chromatography on silica gel by eluting with CH_2Cl_2 and recycling preparative HPLC to give **7** as yellow solid (94mg, yield 68%). ^{1}H-NMR (400.13MHz, $CDCl_3$): δ (ppm) =10.00 (s, 1H, -C*H*O), 7.17 (s, 1H, Ar*H*), 7.09 (s, 1H, Ar*H*), 3.12-3.05 (m, 2H, -CH_2-), 2.99-2.90 (m, 2H, -CH_2-), 1.84-1.78 (m, 4H, -CH_2-), 1.51-1.40 (m, 12H, -CH_2-), 1.06-1.01 (m, 6H, -CH_3). ^{13}C-NMR ($CDCl_3$, 100.61Hz): δ (ppm) =182.4, 154.0, 146.2, 142.7, 137.1, 131.4, 130.6, 129.4, 129.2, 126.2, 32.4, 32.3, 32.1, 31.1, 31.0, 29.9, 29.8, 29.2, 23.3, 21.7, 14.7.

Suzuki-Miyaura coupling reaction with pyrene-cores.

8: A solution of 2,7-Bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyrene (32mg, 0.07 mmol), **7** (94mg, 0.21mmol) and $Pd(PPh_3)_4$ (21mg, 0.02mmol) in toluene (25ml), ethanol (8ml) and 2.0 M K_2CO_3 aqueous solution (5ml) was stirred at 120 °C for 48 h under nitrogen. After cooling to room temperature, the reaction mixture was poured into water, extracted with $CHCl_3$. The organic layer was dried over magnesium sulfate and the solvent was evaporated. The residue was purified by column chromatography on silica gel by eluting with $CHCl_3$ and recycling preparative HPLC to give **8** as yellow solid (48mg, yield 74 %). ^{1}H-NMR (400.13MHz, $CDCl_3$): δ (ppm) =10.00 (s, 2H, -C*H*O), 8.09 (s, 4H, Ar*H*), 7.88 (s, 4H, Ar*H*), 7.29 (s, 2H, Ar*H*), 7.02 (s, 2H, Ar*H*), 2.91 (t, *J*=7.9Hz, 4H, -CH_2-), 2.78 (t, *J*=7.9Hz, 4H, -CH_2-), 1.76-1.67 (m, 8H, -CH_2-), 1.48-1.34 (m, 24H, -CH_2-), 0.98-0.93 (m, 12H, -CH_3). ^{13}C-NMR ($CDCl_3$, 100.61Hz): δ (ppm) =181.9, 153.7, 145.7, 144.1, 143.6, 136.5, 131.6, 131.3, 130.3, 128.3, 128.2, 127.4, 124.2, 122.2, 32.2, 32.0, 31.8, 30.8, 30.6, 30.5, 29.8, 29.5, 28.9, 23.1, 14.5. MALDI-TOF-Ms: *m/z*=923.44 (M+H); Calculated for $C_{58}H_{60}O_2S_4$: *m/z*=922.39.

9: Yield 81%. ^{1}H-NMR (400.13MHz, CDCl$_3$): δ (ppm) = 8.49 (d, *J*=9.2Hz, 2H, Ar*H*), 8.19 (s, 2H, Ar*H*), 8.16 (s, 1H, Ar*H*), 8.03 (d, *J*=9.2Hz, 2H, Ar*H*), 7.20 (s, 2H, Ar*H*), 7.03 (s, 2H, Ar*H*), 2.68 (t, *J*=7.9Hz, 4H, -CH_2-), 1.85-1.78 (m, 4H, -CH_2-), 1.56 (s, 9H, -CH_3), 1.54-1.42 (m, 12H, -CH_2-), 0.90 (t, *J*=6.9Hz, 6H, -CH_3). ^{13}C-NMR (CDCl$_3$, 100.61Hz): δ (ppm) =149.9, 144.2, 142.3, 131.7, 130.7, 130.2, 130.0, 129.0, 128.7, 126.0, 125.4, 123.7, 123.0, 121.4, 35.7, 32.4, 32.2, 31.2, 31.0, 29.6, 25.1, 23.2, 14.7. MALDI-TOF-Ms: *m/z*=590.37 (M+H); calculated for $C_{40}H_{46}S_2$: *m/z*=590.30.

11: Yield 66%. ^{1}H-NMR (400.13MHz, CDCl$_3$): δ (ppm) = 8.58 (d, *J*=9.2Hz, 2H, Ar*H*), 8.21 (s, 2H, Ar*H*), 8.09 (d, *J*=9.2Hz, 2H, Ar*H*), 7.22 (s, 1H, Ar*H*), 7.05 (s, 2H, Ar*H*), 6.89 (s, 2H, Ar*H*), 2.86 (t, *J*=8.0Hz, 4H, Ar*H*), 2.61 (t, *J*=7.2Hz, 4H, -CH_2-), 1.89-1.81 (m, 4H, -CH_2-), 1.79-1.73 (m, 4H, -CH_2-), 1.68 (s, 12H, -CH_3), 1.51-1.45 (m, 4H, -CH_2-), 1.38-1.33 (m, 24H, -CH_2-), 0.90 (m, 12H, -CH_3). ^{13}C-NMR (CDCl$_3$, 100.61Hz): δ (ppm) =150.0, 149.3, 144.1, 140.3, 136.2, 132.7, 131.7, 130.3, 129.6, 128.9, 127.7, 126.2, 125.3, 123.7, 120.5, 35.7, 32.4, 32.2, 31.2, 31.0, 30.9, 30.0, 29.8, 29.5, 23.2, 23.1,14.6. MALDI-TOF-Ms: *m/z* = 922.32 (M+H); Calculated for $C_{60}H_{74}S_4$: *m/z*=922.47.

13: Yield 76%. ^{1}H-NMR (400.13MHz, CDCl$_3$): δ (ppm) = 8.54 (s, 4H, Ar*H*), 8.21 (s, 2H, Ar*H*), 7.23 (s, 4H, Ar*H*), 7.09 (s, 4H, Ar*H*), 2.72 (t, *J* = 7.6Hz, 8H, -CH_2-), 1.76-1.69 (m, 8H, -CH_2-), 1.45-1.32 (m, 24H, -CH_2-), 0.91 (t, *J* = 7.2Hz, 12H, -CH_3). ^{13}C-NMR (CDCl$_3$, 100.61Hz): δ (ppm) =144.0, 142.0, 131.3, 130.5, 130.2, 129.2, 126.4, 126.1, 121.5, 32.1, 31.1, 31.0, 29.5, 23.1, 14.5. MALDI-TOF-Ms: *m/z* = 866.51 (M+H); Calculated for $C_{56}H_{66}S_4$: *m/z*=866.40.

15: Yield 80%. ^{1}H-NMR (400.13MHz, CDCl$_3$): δ (ppm) = 8.64 (s, 4H, Ar*H*), 8.26 (s, 2H, Ar*H*), 7.25 (s, 4H, Ar*H*), 7.06 (s, 4H, Ar*H*), 6.93 (s, 4H, Ar*H*), 2.87 (t, *J* = 7.6Hz, 8H, -CH_2-), 2.64 (t, *J* = 7.6Hz, 8H, -CH_2-), 1.79-1.72 (m, 8H, -CH_2-), 1.71-1.63 (m, 8H, -CH_2-), 1.47-1.31 (m, 48H, -CH_2-), 0.92-0.88 (m, 24H, -CH_3). ^{13}C-NMR (CDCl$_3$, 100.61Hz): δ (ppm) =144.1, 140.3, 139.9, 136.1, 132.9, 131.7, 131.0, 130.0, 129.1, 127.8, 126.5, 126.1, 120.5, 32.1, 31.2, 30.9, 30.8, 29.9, 29.8, 29.5, 23.1, 23.0, 14.5. MALDI-TOF-Ms: *m/z*=1530.82 (M+H); Calculated for $C_{96}H_{122}S_8$: *m/z*=1531.74.

17: Yield 64%. ^{1}H-NMR (400.13MHz, CDCl$_3$): δ (ppm) = 8.63 (s, 4H, Ar*H*), 8.25 (s, 2H, Ar*H*), 7.25 (s, 4H, Ar*H*), 7.04 (s, 4H, Ar*H*), 6.93 (s, 4H, Ar*H*), 2.87 (t, *J* = 7.6Hz, 8H), 2.31 (s, 12H, -CH_3), 1.82-1.75 (m, 8H, -CH_2-), 1.79-1.72 (m, 8H, -CH_2-), 1.40-1.34 (m, 16H, -CH_2-), 0.90 (t, *J*=7.2Hz, 24H, -CH_3). ^{13}C-NMR (CDCl$_3$, 100.61Hz): δ (ppm) =140.4, 140.0, 138.5, 136.2, 132.7, 131.7, 131.0, 130.0, 129.1, 128.7, 126.1, 121.2, 32.1, 31.2, 29.9, 29.7, 23.1, 16.2, 14.5. MALDI-TOF-Ms: *m/z*=1250.08 (M+H); Calculated for $C_{76}H_{82}S_8$: *m/z*=1249.98.

Bromination of thiophene terminates.

10: NBS (0.12g, 0.65mmol) was slowly added to the solution of **9** (0.15g, 0.32mmol) in dry THF (20ml) at 0°C. The reaction mixture was stirred for 12h at RT and poured into water. After extraction with CH_2Cl_2, the organic layer was dried over magnesium sulfate and the solvent was evaporated. The residue was purified by column chromatography on silica gel by eluting with CH_2Cl_2 and recycling preparative HPLC to give **10** as yellow solid (0.19g, yield 95%). ^{1}H-NMR (400.13MHz, CDCl$_3$): δ (ppm) = 8.32 (d, *J*=9.2Hz, 2H, Ar*H*), 8.11 (s, 2H, Ar*H*), 7.95 (d, *J*=9.2Hz, 2H, Ar*H*), 7.92 (s, 1H, Ar*H*), 6.95 (s, 2H, -CH_2-), 2.56 (t, *J*=7.9Hz, 4H, -CH_2-), 1.80-1.78 (m, 4H, -CH_2-), 1.64 (s, 9H, -CH_3), 1.52-1.38 (m, 4H, -CH_2-), 0.81 (t, *J*=7.2Hz, 6H, -CH_3). ^{13}C-NMR (CDCl$_3$, 100.61Hz): δ (ppm) =150.1, 143.1, 142.0, 131.5, 130.2, 129.6, 129.2, 129.1, 126.0, 125.6, 124.9, 123.5, 110.1, 35.7, 32.4, 32.3, 30.4, 30.3, 29.6, 23.2, 14.6. MALDI-TOF-Ms: *m/z*=747.95 (M+H); Calculated for $C_{40}H_{44}Br_2S_2$: *m/z*=746.12.

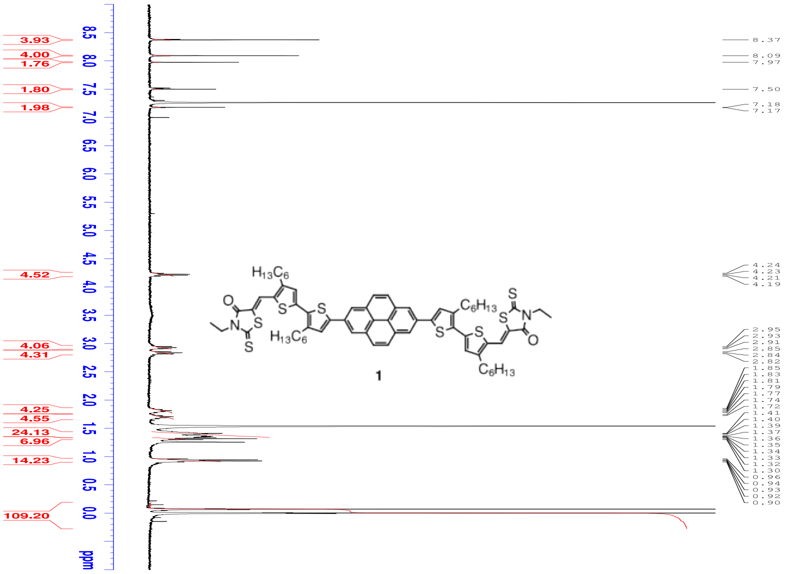
14: Yield 94%. ^{1}H-NMR (400.13MHz, $CDCl_3$): δ (ppm) = 8.49 (s, 4H, Ar*H*), 8.09 (s, 2H, Ar*H*), 7.07 (s, 4H, Ar*H*), 2.68 (t, *J* = 7.2Hz, 8H, -C*H*$_2$-), 1.73-1.65 (m, 8H, -C*H*$_2$-), 1.45-1.33 (m, 24H, -C*H*$_2$-), 0.91 (t, *J* = 7.2Hz, 12H, -C*H*$_3$). ^{13}C-NMR ($CDCl_3$, 100.61Hz): δ (ppm) =143.2, 141.5, 129.8, 129.4, 126.2, 126.1, 110.3, 32.0, 30.2, 30.1, 29.4, 23.0, 14.5. MALDI-TOF-Ms: *m/z*=1182.36 (M+H); Calculated for $C_{56}H_{62}Br_4S_4$: *m/z*=1182.04.

Formylation of thiophene terminates.

12: A solution of **11** (0.19g, 0.21mmol) in dry 1,2-dichloroethane (15ml) was stirred at 0˚C. Vilsmeir-reagent, which was prepared with 1 ml of $POCl_3$ in dry DMF 5 ml, was added. The mixture was refluxed for overnight and quenched 10% aqueous solution of NaOAc after cooling. After extraction with CH_2Cl_2, the organic layer was dried over magnesium sulfate and the solvent was evaporated. The residue was purified by column chromatography on silica gel by eluting with CH_2Cl_2 and recycling preparative HPLC to give **12** as yellow solid (0.15g, Yield 74%). ^{1}H-NMR (400.13MHz, $CDCl_3$): δ (ppm) = 10.05 (s, 2H, Ar*H*), 8.56 (d, *J*=9.2Hz, 2H, Ar*H*), 8.29 (s, 2H, Ar*H*), 8.22 (s, 1H, Ar*H*), 8.14 (d, *J*=9.3Hz, 2H, Ar*H*), 7.30 (s, 2H, Ar*H*), 7.15 (s, 2H, Ar*H*), 2.96 (t, *J*=7.6Hz, 8H, -C*H*$_2$-), 1.85-1.78 (m, 4H, -C*H*$_2$-), 1.77-1.70 (m, 4H, -C*H*$_2$-), 1.64 (s, 9H, -C*H*$_3$), 1.55-1.48 (m, 4H, -C*H*$_2$-), 1.45-1.34 (m, 20H, -C*H*$_2$-), 0.98-0.93 (m, 12H, -C*H*$_3$). ^{13}C-NMR ($CDCl_3$, 100.61Hz): δ (ppm) =182.0, 153.7, 145.6, 143.0, 142.3, 136.9, 132.2, 131.5, 130.0, 129.4, 129.1, 128.8, 126.0, 124.8, 123.5, 35.7, 32.3, 32.0, 31.8, 30.9, 30.4, 29.8, 29.4, 28.9, 25.1, 23.1, 23.0, 21.8, 14.5. MALDI-TOF-Ms: *m/z*=978.42 (M+H); Calculated for $C_{62}H_{74}O_2S_4$: *m/z*=978.46.

16: Yield 76%. ^{1}H-NMR (400.13MHz, $CDCl_3$): δ (ppm) =10.05 (s, 4H, -C*H*O), 8.63 (s, 4H, Ar*H*), 8.27 (s, 2H, Ar*H*), 7.30 (s, 4H, Ar*H*), 7.14 (s, 4H, Ar*H*), 3.00-2.91 (m, 16H, -C*H*$_2$-), 1.82-1.70 (m, 16H, -C*H*$_2$-), 1.50-1.31 (m, 48H, -C*H*$_2$-), 0.90 (m, 24H, -C*H*$_3$). ^{13}C-NMR ($CDCl_3$, 100.61Hz): δ (ppm) =182.1, 153.8, 145.3, 143.0, 141.8, 137.0, 132.5, 131.8, 129.8, 129.4, 129.0, 126.3, 32.1, 32.0, 31.8, 20.9, 30.3, 29.7, 29.4, 29.9, 23.1, 23.0, 14.5. MALDI-TOF-Ms: *m/z*=1642.37 (M+H); Calculated for $C_{160}H_{122}O_4S_8$: *m/z*=1642.71.

18: Yield 49%. ^{1}H-NMR (400.13MHz, $CDCl_3$): δ (ppm) =10.03 (s, 4H, -C*H*O), 8.40 (s, 4H, Ar*H*), 8.14 (s, 2H, Ar*H*), 7.21 (s, 4H, Ar*H*), 7.06 (s, 4H, Ar*H*), 2.90 (t, *J* = 7.6Hz, 8H, -C*H*$_2$-), 2.58 (s, 12H, -C*H*$_3$), 1.81-1.72 (m, 8H, -C*H*$_2$-), 1.52-1.44 (m, 8H, -C*H*$_2$-), 1.39-1.33 (m, 16H, -C*H*$_2$-), 0.90 (t, *J* = 7.2Hz, 12H, -C*H*$_3$). ^{13}C-NMR ($CDCl_3$, 100.61Hz): δ (ppm) =182.1, 148.2, 145.2, 143.0, 141.9, 136.9, 132.4, 131.7, 131.0, 129.7, 129.3, 128.7, 125.9, 32.1, 30.9, 30.4, 29.8, 23.1, 14.6. MALDI-TOF-Ms: *m/z*=1362.25 (M+H); Calculated for $C_{80}H_{82}O_4S_8$: *m/z*=1362.40.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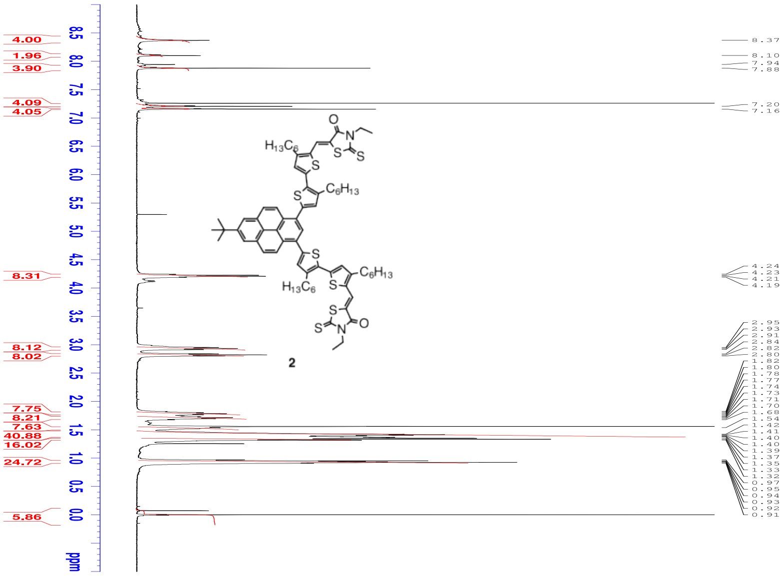
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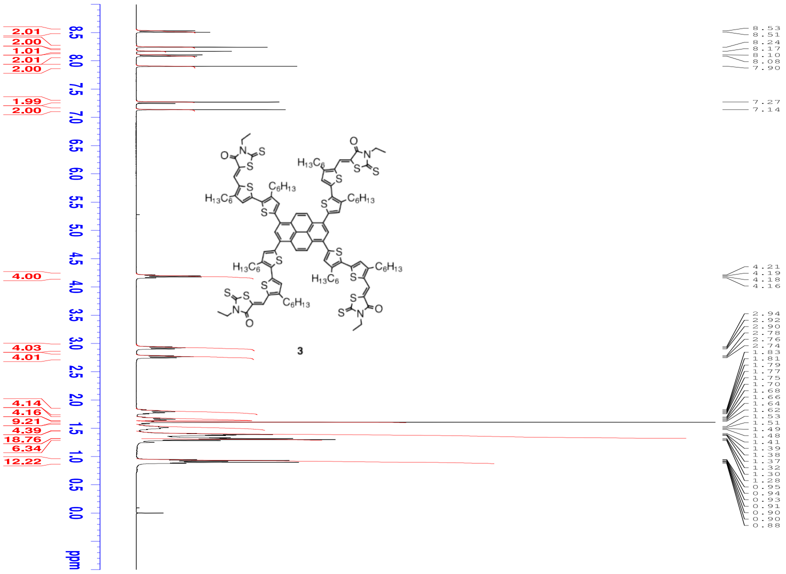

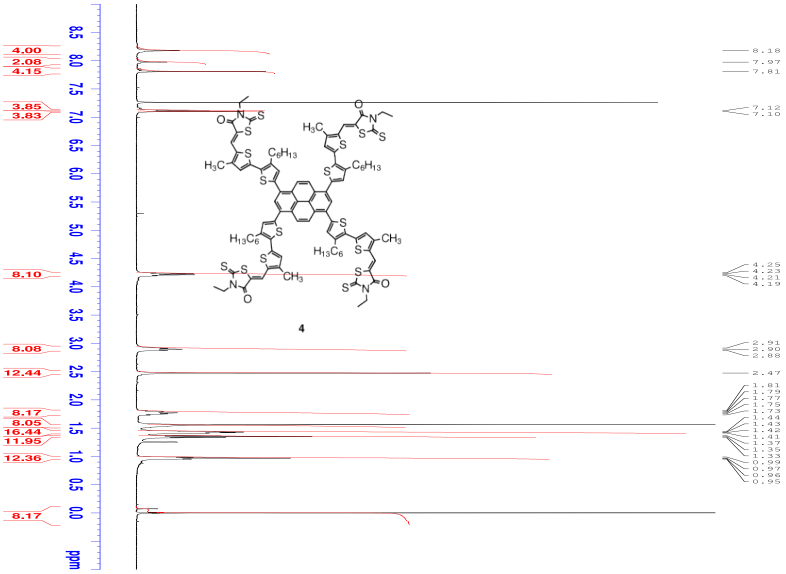

Fig. S1. ^{1}H-NMR spectra of **1-4** in $CDCl_3$.

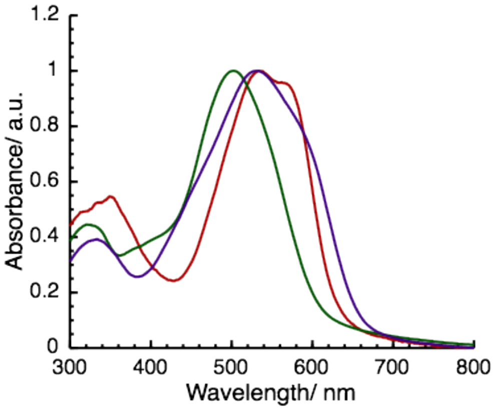

Fig. S2. Absorption spectra of spin-coated thin films of **1**(red), **2**(green) and **4**(purple).

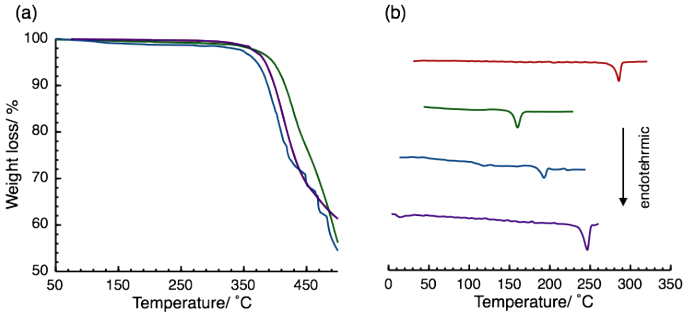

Fig. S3. TGA (a) and DSC (b) profiles for **1** (red), **2** (green), **3**(blue) and **4**(purple) at scan rate of 10˚C/ min.

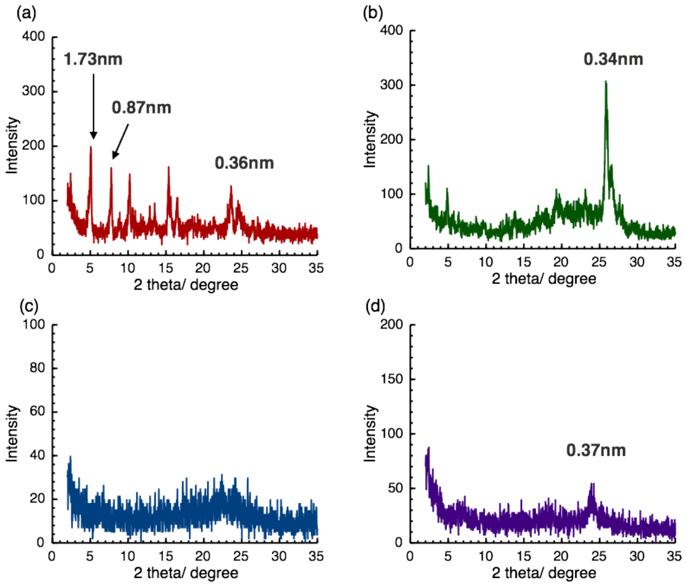

Fig. S4. XRD patterns of **1**(a), **2**(b), **3**(c) and **4**(d) at RT.

Hole-mobility measurement

Hole-mobility of donor materials were carried out with the device structure of ITO/ PEDOT:PSS/ donor material/ Au by taking current-voltage curves in the range of 0-7V. The hole-mobility was calculated using the space charge current limited (SCLC) method using the Mott-Gurney square law[1-4] (Eq. 1),

$$J = \frac{9}{8}\varepsilon_0\varepsilon_r\mu_h\frac{V^2}{L^3} \quad (1)$$

where J is the current density, ε_0 is the permittivity of free space (8.85×10^{-12} F m^{-1}), ε_r is the relative dielectric constant of the transport of medium (assumed to be 3), μ_h is the hole mobility, V is the internal voltage in the device ($V = V_{appl} - V_r - V_{bi}$, where V_{appl} is the applied voltage in the device, V_r is voltage drop due to the contact resistance, V_{bi} is the built-in voltage due to relative work function difference between the two electrodes. The V_{bi} can be determined from the transition between the Ohmic region and SCLC region) and L is the thickness of film.

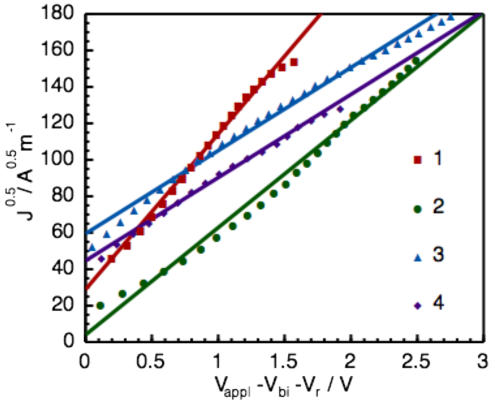

Fig. S5. $J^{0.5}$-V plots for **1** (red), **2** (green), **3** (blue) and **4** (purple) hole-only devices under dark condition. The solid lines are fitted with the data points. Film thickness: **1**, 35nm; **2**, 50nm, **3**, 30nm; **4**, 45nm.

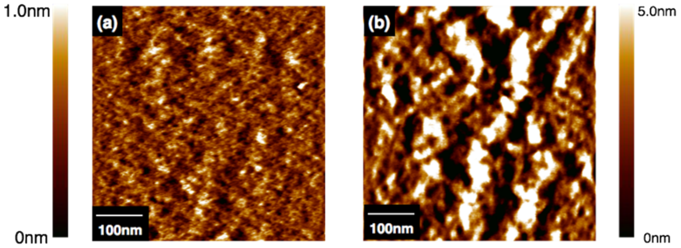

Fig. S6. Tapping-mode AFM height images of a) **4**/$PC_{71}BM$ and b) P3HT/$PC_{61}BM$ blended films.

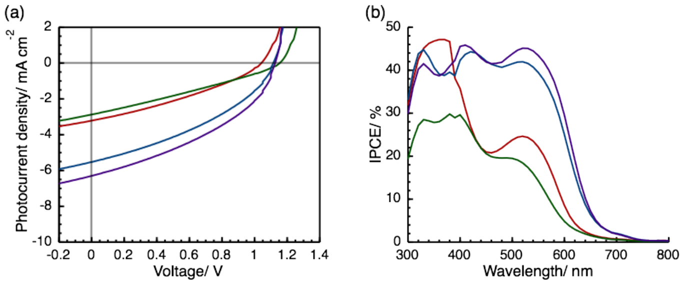

Fig. S7. (a) Photocurrent voltage curve obtained with BHJ solar cells based on **1** (red), **2** (green), **3** (blue) and **4**(purple)/$PC_{61}BM$ blended active layers under a standard global AM 1.5 solar condition. b) Incident photon-to-current conversion efficiency spectrum based on **1** (red), **2** (green), **3** (blue) and **4** (purple)/$PC_{61}BM$ and blended active layers.

Table S1. Summary of device parameters of BHJ solar cells based on mixed active layers composed of **1-4** and $PC_{61}BM$ with different composition.

Active layer (Weight ratio)	thickness /nm	V_{oc} /V	J_{sc} /mA cm^{-2}	*FF*	PCE /%
1/ $PC_{61}BM$ (1:1)	60	0.67	1.66	0.39	0.4
1/ $PC_{61}BM$ (1:2)	65	1.04	3.21	0.33	1.1
1/ $PC_{61}BM$ (1:3)	65	0.92	2.66	0.34	0.8
2/ $PC_{61}BM$ (1:3)	75	0.71	2.53	0.29	0.5
2/ $PC_{61}BM$ (1:4)	70	1.15	2.87	0.29	1.0
2/ $PC_{61}BM$ (1:5)	70	0.83	2.59	0.28	0.6
3/ $PC_{61}BM$ (1:3)	70	0.96	5.58	0.38	2.0
3/ $PC_{61}BM$ (1:4)	70	1.11	5.53	0.38	2.3
3/ $PC_{61}BM$ (1:5)	70	1.01	5.01	0.40	2.0
4/ $PC_{61}BM$ (1:2)	70	1.10	5.50	0.36	2.1
4/ $PC_{61}BM$ (1:3)	70	1.13	6.30	0.39	2.8
4/ $PC_{61}BM$ (1:4)	70	1.10	5.97	0.39	2.5

Discussion about the open circuit voltage

The dark injected current J_{inj} versus applied voltage for **1-4** and P3HT /$PC_{61}BM$ devices was exponentially fitted according to Eq. 2, therefore to determine reverse saturation current density $J_{0,n}$ (Fig. S8). [5]

$$J_{inj} = J_{0,n} exp\left(\frac{qV}{nkT}\right) \quad (2)$$

J_{so} is calculated according to Eq. 3. [6]

$$J_{0,n} = J_{so} exp\left(\frac{-\Delta E_{DA}}{2nkT}\right) \quad (3)$$

For comparison, the V_{oc} values of **1-4** and P3HT/ $PC_{61}BM$ were calculated from Eq. 4, and the calculated V_{oc} values were consistent with the experimental V_{oc} (Table S2).[6]

$$V_{oc} = \frac{nkT}{q}\ln\left(\frac{J_{sc}}{J_{0,n}} + 1\right) \approx \frac{nkT}{q}\ln\left(\frac{J_{SC}}{J_{SO}}\right) + \frac{\Delta E_{DA}}{2q} \quad (4)$$

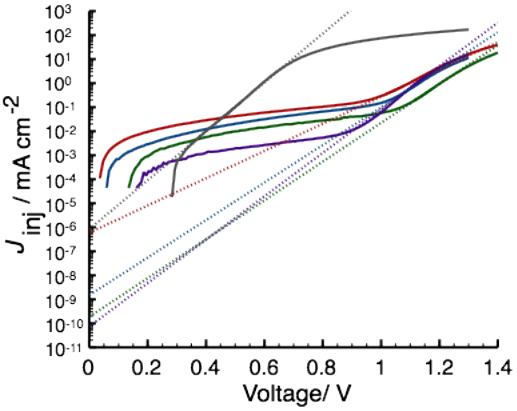

Fig. S8. Dark injected current J_{inj} versus voltage V for **1** (red), **2** (green), **3** (blue) and **4**(purple) and P3HT (black)/PC$_{61}$BM blended active layers. The dotted lines represent exponential fits, allowing determination of $J_{0,n}$.

Table S2. Summary of measured and simulated device parameters of BHJ solar cells based on mixed active layers composed of **1-4** and P3HT/ PC$_{61}$BM.

active layer (weight ratio)	$J_{0,n}$ /mA cm^{-2}	ΔE_{DA}[a]	J_{so} /mA cm^{-2}	$V_{oc,\ cal}$/ V	$V_{oc,\ exp}$/ V
1/ PC$_{61}$BM (1:3)	5.91×10^{-7}	1.43	6.70×10^{-3}	1.19	1.04
2/ PC$_{61}$BM (1:4)	1.85×10^{-10}	1.53	2.81×10^{-4}	1.26	1.15
3/ PC$_{61}$BM (1:4)	1.94×10^{-9}	1.36	3.06×10^{-4}	1.23	1.11
4/ PC$_{61}$BM (1:3)	7.40×10^{-11}	1.33	7.52×10^{-5}	1.21	1.13
P3HT/ PC$_{61}$BM (2:1)	8.28×10^{-7}	1.09	2.93×10^{-1}	0.69	0.65

[a] the energy difference between the HOMO of donor and the LUMO of acceptor materials.

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