

Supporting Information

Poly(pentacyclic Lactam-alt-Diketopyrrolopyrrole) for Field-Effect Transistors and Polymer Solar Cells Processed from Non-Chlorinated Solvents

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1. GPC

Molecular weight was determined with GPC at 140 °C on a PL-GPC 220 system using a PL-GEL 10 μm MIXED-B column and *o*-DCB as the eluent against polystyrene standards. Low concentration of 0.1 mg mL⁻¹ polymer in *o*-DCB was applied to reduce aggregation.

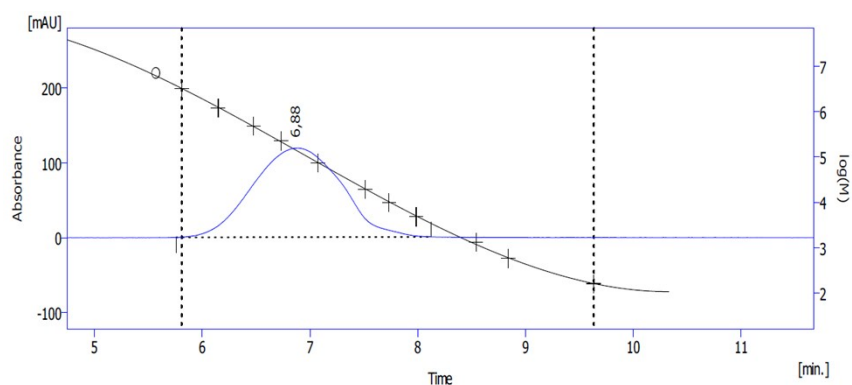


Fig. S1 GPC recorded at 140 °C with *o*-DCB as eluent for PDPP2TPCL. $M_n = 72.8 \text{ kg mol}^{-1}$, $M_w = 239.9 \text{ kg mol}^{-1}$ and PDI = 3.3.

2. BGBC FETs

Table S1 Field effect hole mobilities of the polymer PDPP2TPCL in a BGBC configuration. The polymer thin films were thermal annealed 100 °C or 150 °C for 10 min before measurement. The hole mobilities of devices from the thin films without thermal annealing (25 °C) were also summarized in the table.

| solvent | Annealing temp | μ_h [cm ² V ⁻¹ s ⁻¹] | V_T [V] | I_{on}/I_{off} |
|-------------------|----------------|---|--------------|------------------|
| CHCl ₃ | 25 °C | 0.029 | -10.8 | 7×10^4 |
| CHCl ₃ | 100 °C | 0.31 | -4.9 | 1×10^4 |
| CHCl ₃ | 150 °C | 0.33 | -9.3 | |
| Toluene | 25 °C | 0.024 | -4.1 | 2×10^5 |
| Toluene | 100 °C | 0.24 | -2.3 | 4×10^3 |
| Toluene | 150 °C | 0.27 | -4.8 | 6×10^3 |
| Toluene/DPE (2%) | 25 °C | 0.056 | -2.8 | 1×10^5 |
| Toluene/DPE (2%) | 100 °C | 0.32 | -5.2 | 7×10^4 |
| Toluene/DPE (2%) | 150 °C | 0.35 | -10.1 | 8×10^4 |

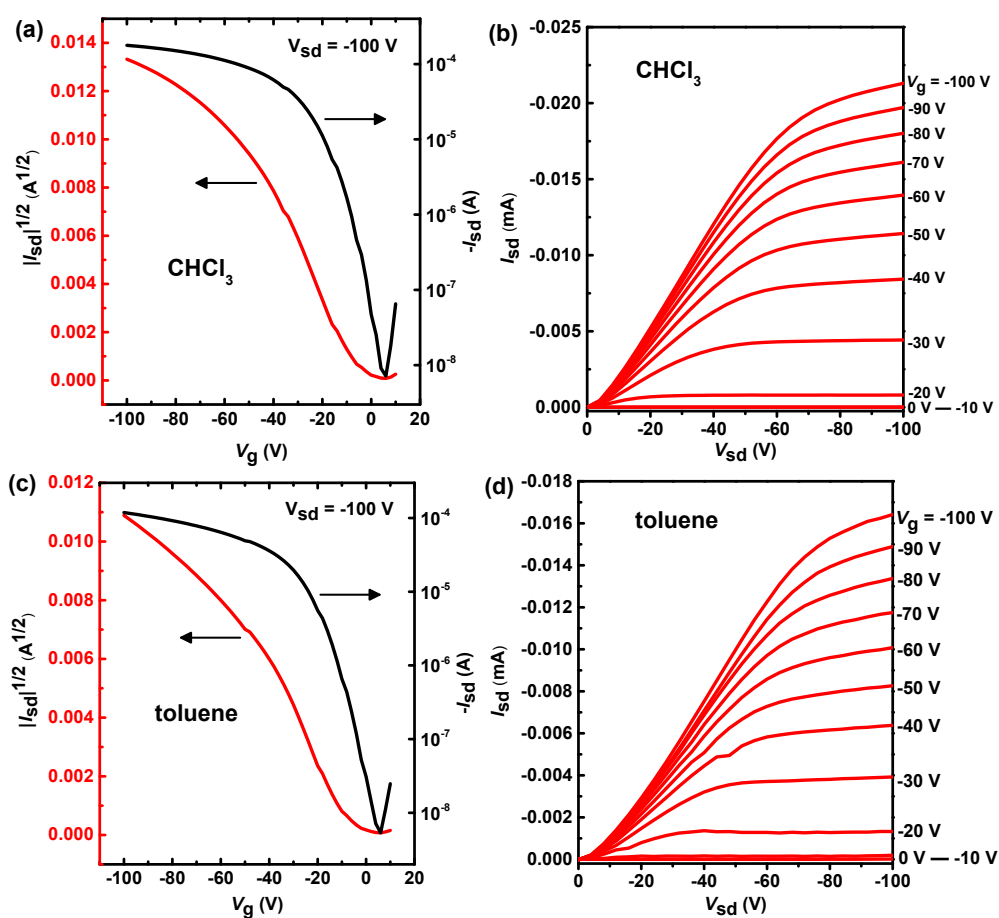


Fig. S2 (a), (c) Transfer and (b), (d) output curves obtained from bottom-contact OFETs devices with PDPP2TPCL thin film annealed at 120 °C for 10 min. The thin films were spin coated from (a), (b) CHCl₃, (c) and (d) toluene solution.

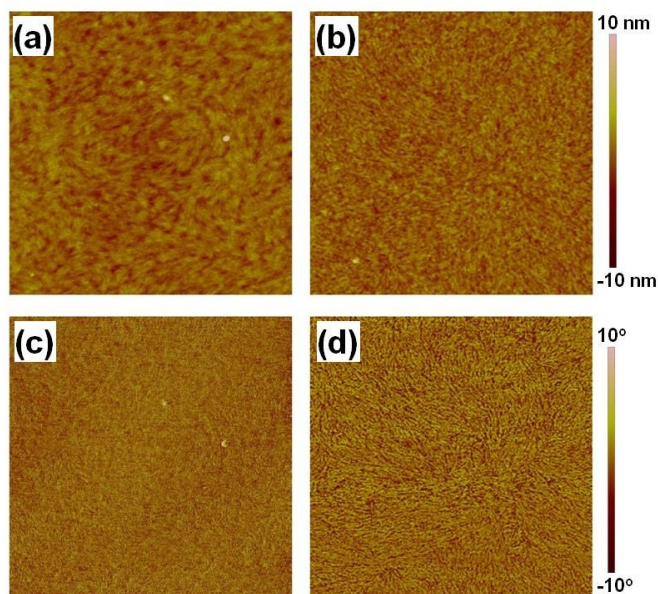


Fig. S3 (a) and (b) AFM height images and (c) and (d) phase images (3×3 μm²) of the PDPP2TPCL thin films spin coated from CHCl₃ or toluene annealed at 120 °C. (a) and (c) from CHCl₃, and (b) and (d) from toluene. The root-mean-square (RMS) roughnesses are 0.87 nm and 0.88 nm for (a) and (b).

3. TGBC FETs

Top-gate/Bottom-contact (TGBC) FET devices were fabricated on bare glass substrates. First, the substrates were subjected to cleaning by using ultrasonication in acetone, deionized water, and ethanol. Next, gold was evaporated to form source/drain electrodes on the surface of glass substrates through a metal shadow mask ($L/W = 20 \mu\text{m}/1400 \mu\text{m}$). Then the substrates were washed with ethanol. In a N₂ glovebox, the polymer PDPP2TPCL dissolved in CHCl₃, toluene or toluene/DPE was spincoated onto the glass substrates, yielding a polymer film with a thickness of ~30 nm. For annealed polymer films, the samples were further annealed at 120 °C for 10 min. Then polymethylmethacrylate (PMMA) ($M_w = 100 \text{ KDa}$) solution in anhydrous *n*-butyl acetate (60 mg mL⁻¹) was spin-coated onto the surface of the polymer films. PMMA thickness is ~700 nm with capacitance of 3.79 nF/cm². The samples were then dried at 80 °C for 30 min in vacuum. The aluminum gate electrodes (thickness ~ 60 nm) were then

evaporated through a shadow mask onto the PMMA gate dielectric. Top-gate FETs were measured in ambient air with relative humidity of 30–50%.

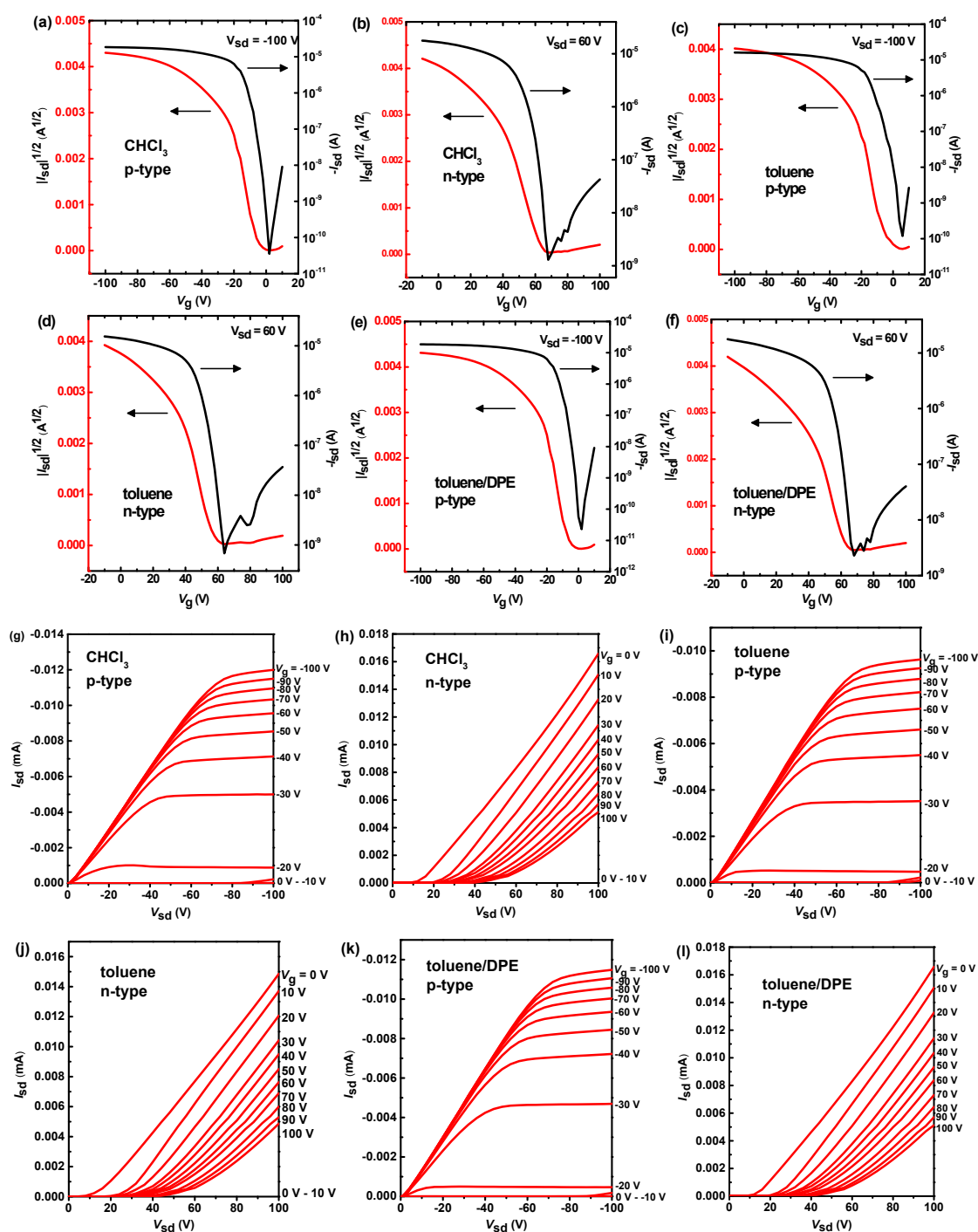


Fig. S4 (a) – (f) Transfer, (g) – (l) output curves obtained from TGBC OFETs devices with PDPP2TPCL thin films annealed at 120 °C, processed from different solvents. Solvents, p-type and n-type are indicated in the figure.

Table S2. Field effect hole mobilities of the polymer PDPP2TPCL in a TGBC configuration. The polymer thin films were thermal annealed at 120 °C for 10 min before measurement.

| solvent | hole mobilities | | | electron mobilities | | |
|-------------------|---|--------------|-------------------|---|--------------|------------------|
| | μ_h [cm ² V ⁻¹ s ⁻¹] | V_T [V] | I_{on}/I_{off} | μ_e [cm ² V ⁻¹ s ⁻¹] | V_T [V] | I_{on}/I_{off} |
| CHCl ₃ | 0.3 | -6.1 | 1×10 ⁶ | 6.9×10 ⁻⁴ | 73.1 | 10 |
| Toluene | 0.24 | -6.1 | 1×10 ⁵ | 8.1×10 ⁻⁴ | 75.2 | 10 |
| Toluene/DPE (2%) | 0.37 | -7.5 | 1×10 ⁶ | 9.9×10 ⁻⁴ | 74.6 | 10 |

4. Polymer solar cells

Table S3 Characteristics of PDPP2TPCL:[60]PCBM (1:3) inverted solar cells spin coated from different solution.

| Solvent | Thickness [nm] | J_{sc}^a [mA cm ⁻²] | V_{oc} [V] | FF | PCE [%] |
|---------------------------------------|-------------------|--------------------------------------|-----------------|------|------------|
| CHCl ₃ | 100 | 1.3 | 0.75 | 0.58 | 0.5 |
| CHCl ₃ /DIO (2.5%) | 100 | 6 | 0.77 | 0.56 | 2.6 |
| CHCl ₃ / <i>o</i> -DCB 10% | 120 | 5.5 | 0.78 | 0.64 | 2.8 |
| CHCl ₃ /DPE (2%) | 100 | 6.7 | 0.77 | 0.66 | 3.4 |
| toluene | 110 | 2 | 0.74 | 0.51 | 0.8 |
| toluene:DPE 2% | 120 | 9.5 | 0.77 | 0.64 | 4.7 |

^a J_{sc} was calculated by integrating the EQE spectrum with the AM1.5G spectrum.

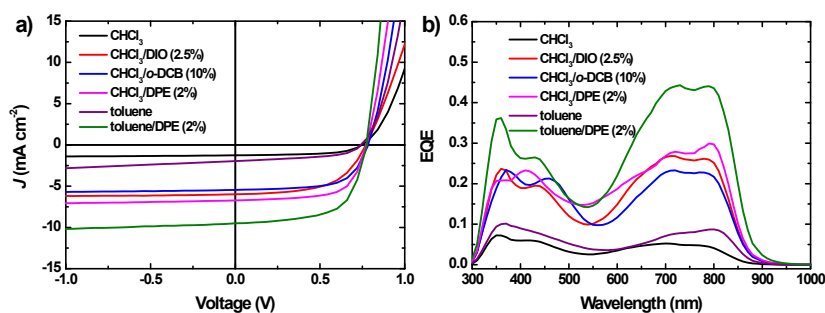


Fig. S5 (a) J - V characteristics under white light illumination and (b) EQE of the PDPP2TPCL:[60]PCBM (1:3) inverted solar cells fabricated from different solution.

Table S4 Characteristics of PDPP2TPCL:[60]PCBM inverted solar cells spin coated from toluene/DPE (2%) with different ratio of donor to acceptor.

| ratio | Thickness [nm] | J_{sc}^a [mA cm ⁻²] | V_{oc} [V] | FF | PCE [%] |
|-------|-------------------|--------------------------------------|-----------------|------|------------|
| 1:1 | 110 | 6.8 | 0.78 | 0.57 | 3 |
| 1:2 | 80 | 10 | 0.78 | 0.57 | 4.5 |

| | | | | | |
|-----|-----|-----|------|------|-----|
| 1:3 | 120 | 9.5 | 0.77 | 0.64 | 4.7 |
| 1:4 | 130 | 9 | 0.76 | 0.62 | 4.2 |

^a J_{sc} was calculated by integrating the EQE spectrum with the AM1.5G spectrum.

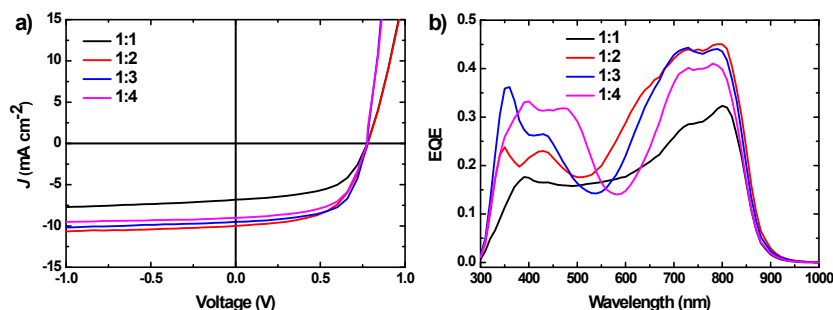


Fig. S6 (a) J - V characteristics under white light illumination and (b) EQE of the PDPP2TPCL:[60]PCBM inverted solar cells fabricated from toluene/DPE (2%) with different ratio of donor to acceptor.

Table S5 Characteristics of PDPP2TPCL:[60]PCBM (1:3) inverted solar cells spin coated from toluene/DPE (2%) with different thickness of active layers.

| Thickness | J_{sc}^a | V_{oc} | FF | PCE |
|-----------|------------------------|----------|------|-----|
| [nm] | [mA cm ⁻²] | [V] | | [%] |
| 100 | 8.6 | 0.77 | 0.61 | 4 |
| 120 | 9.5 | 0.77 | 0.64 | 4.7 |
| 150 | 9.6 | 0.76 | 0.54 | 3.9 |

^a J_{sc} was calculated by integrating the EQE spectrum with the AM1.5G spectrum.

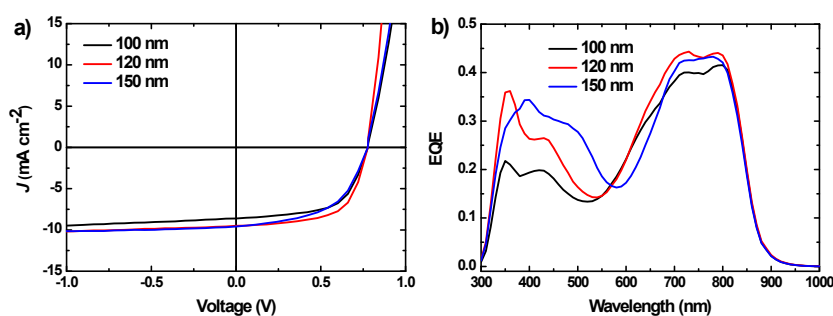


Fig. S7 (a) J - V characteristics under light illumination and (b) EQE of the PDPP2TPCL:[60]PCBM (1:3) solar cells fabricated from toluene/DPE (2%) solution with the different thickness.