

Supporting Information

Efficient charge generation and low open circuit voltage loss enable a PCE of 10.3% in small molecule donor and polymer acceptor organic solar cells

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1. Characterization method

(1) Molecular structure/properties characterization, calculation (NMR, MS spectra, DFT, contact angle).

¹H NMR (400 MHz) and ¹³C NMR (101 MHz) spectra were obtained on a Bruker DMX-400 NMR Spectrometer and using tetramethylsilane as internal standard. MS spectra (MALDI-TOF-MS) were determined on a Micromass GCT-MS spectrometer. The infrared spectrum (IR) was measured using micro-infrared spectrometer (sp-200i) by transmission-mode. The melting point was obtained by differential scanning calorimetry (DSC) Q100 V9.0 Build 275 analyzer under purified nitrogen gas flow with a 10 °C min⁻¹ heating rate. The calculated HOMO and LUMO levels and optimized conformations were optimized by density functional theory (DFT) at the B3LYP/6-31G (d, p) level. All calculations were performed in the gas phase and with Gaussian 09 program.¹⁻³ UV-Vis spectra were obtained with a JASCO-V570 spectrophotometer. Electrochemical cyclic voltammetry was conducted on an electrochemical work station (VMP3 Biologic, France), with a Pt disk coated with a molecular film, a Pt plate, and an Ag⁺/Ag electrode as working, counter, and reference electrodes, respectively, in a 0.1 mol L⁻¹ tetrabutylammonium phosphorus hexafluoride (Bu₄NPF₆) acetonitrile solution. Contact angle (θ) in solutions of small donors, PC₇₁BM, Y6 and PJ1 were measured on ITO/glass substrate by using the pendant drop method with the XG-CAMB3 standard contact angle meter.

(2) Morphology characterization (TEM and GIWAXS)

All films for characterization are prepared under identical optimized conditions of device fabrication in the absence of special emphasis. The TEM images of the blended films were prepared under the best device conditions, the sample on the ITO/PEDOT: PSS substrate was transferred by floating in water. Grazing incidence wide angle x-ray scattering (GIWAXs) measurement was conducted at the beamline of 7.3.3 at the Advanced Light Source (ALS). Samples were prepared on Si/PEDOT: PSS substrates

(3) Device measurements (Solar cell fabrication/measurements, mobility and TPC measurement)

Devices were fabricated with a structure of glass/ITO/PEDOT:PSS/active layer/PFNBr/Ag. The ITO-coated glass substrates were cleaned by the same procedure with inverted devices. The precursor solution of PEDOT:PSS was spin-coated on the ITO at 3,000 r.p.m, then was annealed at 150 °C for 15 minutes. The substrates were transferred into a nitrogen-filled glove box. The mixture of small molecules/PC₇₁BM and additives with total concentration ca. 14.5 mg ml⁻¹ stirred at 50 °C in chloroform for ca. 0.5 hour until they intensively dissolved. Subsequently, the active layer was spin-coated from blend chloroform solutions. Finally, a layer of ~5 nm PFNBr was spin-coated on and then 160 nm Ag layer was evaporated under high vacuum (<1 × 10⁻⁴ Pa).

Device *J-V* characteristics was measured under AM 1.5G (100 mWcm⁻²) using a Newport Thermal Oriel 91159A solar simulator. Light intensity is calibrated with a Newport Oriel PN 91150 V Si-based solar cell. *J-V* characteristics

were recorded using a Keithley 2400 source-measure unit. Typical cells have device areas of approximately 4 mm². EQEs were performed in air with an Oriel Newport system (Model 66902) equipped with a standard Si diode. Monochromatic light was generated from a Newport 300W lamp source.

Mobility measurements of pristine films and blend films were characterized by a hole-only (electron-only) space-charge limited current (SCLC) method with the following diode structures: ITO/PEDOT: PSS/active layer/MoO_x/Ag (Al/active layer/Al) for hole (electron) by taking current–voltage current in the range of 0–5 V and fitting the results to a space–charge-limited form.

Transient photocurrent (TPC) was measured by applying a 488 nm solid state laser (Coherent OBIS CORE 488LS) with a pulse width of ~30 ns. The current traces were recorded using a mixed domain oscilloscope (Tektronix MDO3032) by measuring the voltage drop across a 2 Ω resistor load connected in series with the solar cell.

2. Calculation

(1) Mobility calculation measured from SCLC method

Electron and hole motilities were measured with electron- and hole-only devices by using the SCLC model considering electric-field dependence, as described by

$$J = \frac{9}{8} \epsilon \epsilon_r \mu V^2 \exp\left(0.89 \sqrt{\frac{V}{L}}\right) / L^3$$

where J is the current density, L is the thickness of the active layer, μ is the mobility, ε₀ is the permittivity of free space, ε_r is the relative dielectric constant of the transport medium, V (= V_{app} - V_{bi}) is the internal voltage, where V_{app} is the applied voltage and V_{bi} is the built-in voltage owing to the different work function of two electrodes.

(2) The calculation of surface tension by DCA (dynamic contact angle)

Contact angles were measured with a contact angle meter (GBX DIGIDROP). The solution of each organic material was spin-coated on cleaned ITO substrates. Droplets of water and glycerol were dripped onto the different films.

According to Owens-Wendt method, surface energy could be divided into dispersive and polar components.

$$\gamma = \gamma^d + \gamma^p$$

Furthermore, the dispersive and polar surface energy can be calculated though the formula below based on the contact angles obtained by two solvents.

$$(1 + \cos \theta) \gamma_L = 2 \sqrt{\gamma_S^d \gamma_L^d} + 2 \sqrt{\gamma_S^p \gamma_L^p}$$

where θ is the contact angle of a specific solvent, γ_L is the surface energy of the solvent, γ_S^d and γ_S^p refer to the dispersive and polar surface energy of the solid, respectively, and γ_L^d and γ_L^p refer to the dispersive and polar surface energy of the solvent, respectively.

Thus, the unknown value γ_S^d and γ_S^p can be solved through combining two equations obtained by contact angle measurement of two different solvents.

(3) Calculation of Flory-Huggins interaction parameter(χ) by DCA

Solubility parameter (δ̄) can be calculated from the surface energy,

$$\delta = K \sqrt{\gamma}$$

where γ is the surface energy, K is the proportionality constant (K = 116 × 10³ m^{-1/2}).

And Flory–Huggins interaction parameter (X_{ij}) can be written as a function of two solubility parameter,

$$X_{ij} = \frac{V_0}{RT} (\delta_i - \delta_j)^2$$

where X_{ij} is the Flory–Huggins interaction parameter between the material i and j, V₀ is the geometric mean of

the polymer segment molar volume, R is the gas constant, T is the absolute temperature, and δ_i and δ_j are the solubility parameter of material i and j , respectively.

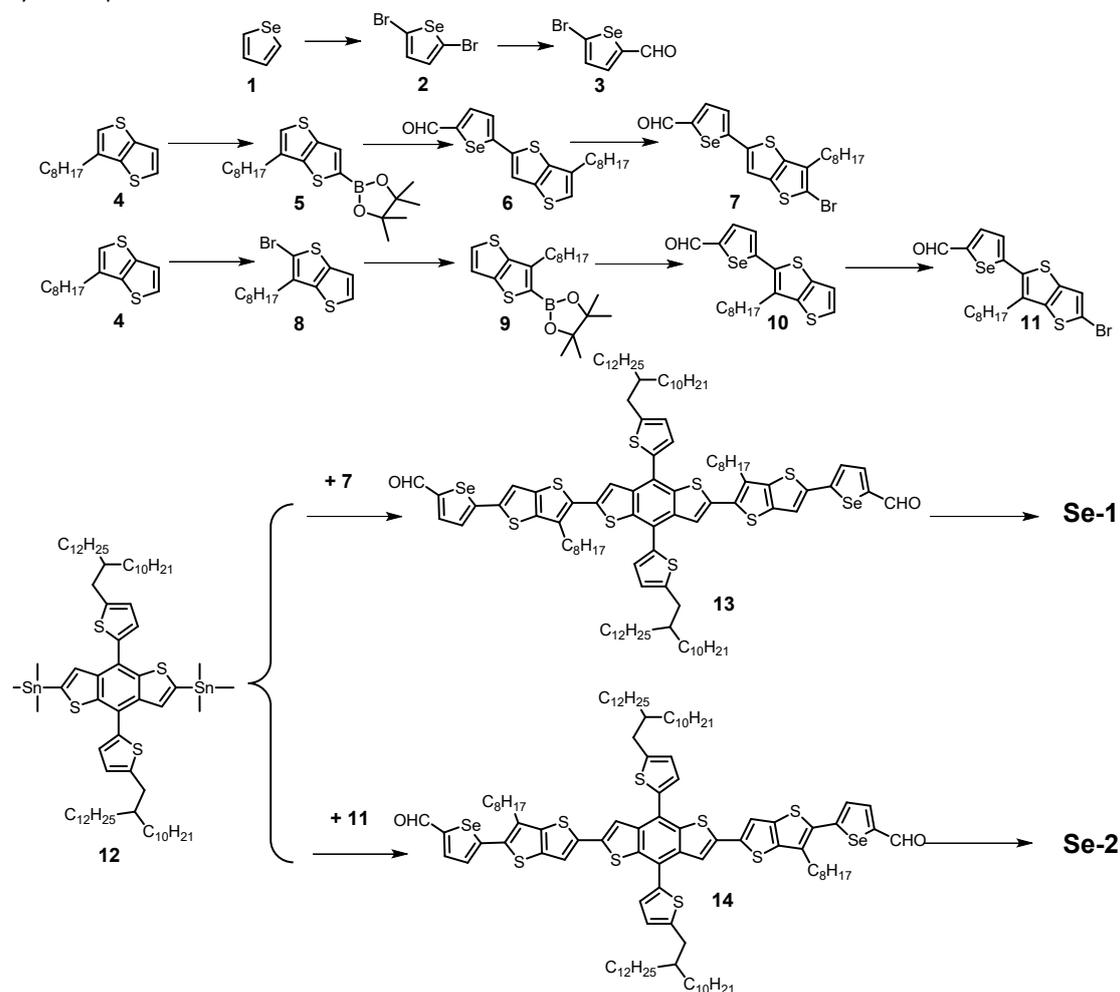
To simplify, we define the parameter $\kappa = K^2V_0/RT$, then the Flory–Huggins interaction parameter can be written as the formula below,

$$\chi_{ij} = \kappa (\sqrt{\gamma_i} - \sqrt{\gamma_j})^2$$

where γ_i and γ_j are the surface energy of material i and j , respectively.

3. Materials and synthesis

All chemicals and solvents were purchased from J&K, Alfa Aesar, Aldrich, Aladdin, Macklin and Beijing Chemical Plant. Toluene was freshly distilled prior to use. Compound **3**, **5**, **9**, **12** were synthesized according to the literatures.^[4-5] Polymer acceptor PJ1 was purchased from Shenzhen Ruixun Optoelectronics Company (China). The detailed synthetic processes of donors were illustrated as follows.



Scheme S1 Synthesis routes of three small molecules

Detailed procedures:

Compound **6**

Under Ar protection, $\text{Pd}(\text{PPh}_3)_4$ was added to the solution of compound **5** (1.91 g, 5 mmol), compound **3** (1g, 4.2 mmol) and NaHCO_3 (1.06g, 12.6 mmol) in the mixture solvent with 10 mL of toluene, 10 mL H_2O and 30 mL THF. Then, Ar gas was bubbled for 20 min; then, the mixture was heated to 85°C and maintained at the temperature for

24 h. After being cooled to ambient temperature, the mixture was extracted by THF, washed by water, saturated NH_4Cl , and water for three times and then dried over MgSO_4 . After evaporation, and the crude product was purified using column chromatography on silica gel with petroleum and dichloromethane (3:1); the product was given as a yellow solid (0.88 g) with a yield of 51%. MS (EI): calcd for $\text{C}_{19}\text{H}_{22}\text{OS}_2\text{Se}$ $[\text{M}]^+$ 410.0, found m/z 411.1. ^1H NMR (400 MHz, CDCl_3) δ 9.75 (s, 1H), 7.91-7.92 (d, 1H), 7.49 (s, 1H), 7.45-7.44(d, 1H), 7.06 (s, 1H), 2.74-2.70 (t, 2H), 1.79-1.71(m, 2H), 1.35-1.28 (m, 10H), 0.90- 0.86 (m, 3H).

Compound 7

In an ice bath, NBS (187 mg, 1.05 mmol) was added in portion to the solution of compound **2** (410 mg, 1 mmol) in a mixed solvent of 30 mL of chloroform and 30 mL of acetic acid. After addition, the mixture was warmed to ambient temperature and left undisturbed overnight. The whole mixture was poured into 50 mL of chloroform: then, the organic layer was washed with water, saturated NaHCO_3 , and water for three times and then dried over MgSO_4 . After concentration, the crude product was purified with column chromatography on silica gel, with petroleum and dichloromethane (2:1) as eluent, and the product was obtained as a yellow solid (300 mg, 61.5%). MS (EI): calcd for $\text{C}_{19}\text{H}_{21}\text{BrOS}_2\text{Se}$ $[\text{M}]^+$ 487.9, found m/z 489.0. ^1H NMR (400 MHz, CDCl_3), ^1H NMR (400 MHz, CDCl_3) ^1H NMR (400 MHz, CDCl_3) δ 9.75 (s, 1H), 7.91-7.90 (d, 1H), 7.45-7.44(d, 1H), 7.40(s, 1H), 2.75-2.71 (t, 2H), 1.73-1.69(m, 2H), 1.35-1.28 (m, 10H), 0.90- 0.86 (m, 3H).

Compound 10

The procedure of synthesis is the same with Compound 6 with a yield of 55%. MS (EI): calcd for $\text{C}_{19}\text{H}_{22}\text{OS}_2\text{Se}$ $[\text{M}]^+$ 410.0, found m/z 411.1. ^1H NMR (400 MHz, CDCl_3) δ 9.78 (s, 1H), 7.95-7.94 (d, 1H), 7.44-7.43(d, 1H), 7.43-7.42(d, 1H), 7.23-7.22(d, 1H), 2.75-2.71 (t, 2H), 1.75-1.69(m, 2H), 1.41-1.27 (m, 10H), 0.90- 0.87 (m, 3H).

Compound 11

The procedure of the synthesis is the same with **compound 7**. The product was given as yellow solid with a yield of 63%. MS (EI): calcd for $\text{C}_{19}\text{H}_{21}\text{BrOS}_2\text{Se}$ $[\text{M}]^+$ 487.9, found m/z 489.0. ^1H NMR (400 MHz, CDCl_3), ^1H NMR (400 MHz, CDCl_3) ^1H NMR (400 MHz, CDCl_3) δ 9.79 (s, 1H), 7.96-7.95 (d, 1H), 7.43-7.42(d, 1H), 7.23(s, 1H), 2.75-2.71 (t, 2H), 1.75-1.69(m, 2H), 1.41-1.27 (m, 10H), 0.90- 0.87 (m, 3H).

Compound 13

Under Ar protection, $\text{Pd}(\text{PPh}_3)_4$ was added to the solution of compound **12** (400 mg, 0.30 mmol) and compound **6** (316.9 mg, 0.65 mmol) in 40 mL of toluene. Then, Ar gas was bubbled for 20 min; then, the mixture was heated to 100 °C and maintained at the temperature overnight. After being cooled to ambient temperature, the mixture was evaporated, and the crude product was purified using column chromatography on silica gel with petroleum and dichloromethane (1:1); the product was given as a red solid (301mg) with a yield of 58.1%. MALDI-TOF MS calcd for $\text{C}_{104}\text{H}_{146}\text{O}_2\text{S}_8\text{Se}_2$ 1857.76 found 1857.9, ^1H NMR (400 MHz, CDCl_3) δ 9.76 (s, 2H), 7.92 (d, 2H), 7.73 (s, 2H), 7.52 - 7.42 (m, 4H), 7.36-7.35 (d, 2H), 6.92-6.91 (d, 2H), 3.10 -2.80 (m, 8H), 1.88 - 1.68 (m, 2H), 1.23-1.54 (m, 92H), 0.87-0.93 (t, 18H).

Compound 14

The procedure of the synthesis is the same with **compound 13**. The product was given as a red solid with a yield of 79.9%. MALDI-TOF MS calcd for $\text{C}_{104}\text{H}_{146}\text{O}_2\text{S}_8\text{Se}_2$ 1857.76 found 1857.5, ^1H NMR (400 MHz, CDCl_3) δ 9.79 (s, 2H), 7.95-7.94 (d, 2H), 7.69 (s, 2H), 7.43-7.42 (d, 2H), 7.38 (s, 2H), 7.36-7.35 (d, 2H), 6.97-6.96 (d, 2H), 2.96-2.93 (m, 6H), 1.81- 1.75 (m, 6H), 1.43 - 1.24 (m, 92H), 0.91 - 0.85 (m, 18H).

Under Ar protection, five drops of piperidine were added into the mixture of compound 6 (187.9 mg, 0.1 mmol) and 4-fluoro-1H-indene-1,3(2H)-dione (164 mg, 1.0 mmol). After being stirred for 24 h at ambient temperature, the mixture was poured into water and extracted using CHCl_3 . The organic layer was washed with brine and water and then dried over MgSO_4 . After being concentrated, the crude product was purified by using column chromatography on silica gel, with a mixture of CHCl_3 and petroleum (1:2) as eluent, and then recrystallized with chloroform and hexane to yield the target compound (87 mg, 45%) as a dark solid. MALDI-TOF MS calcd for $\text{C}_{122}\text{H}_{152}\text{F}_2\text{O}_4\text{S}_8\text{Se}_2$ 2134.8 found 2135.2, ^1H NMR (400 MHz, CDCl_3): 7.82-7.92 (m, 4H), 7.71 (m, 2H), 7.65 (m, 2H), 7.36-7.42 (m, 6H), 6.93(d, 2H), 2.9-2.92 (m, 8H), 1.76-1.85 (m, 6H), 1.22-1.41(m, 104), 0.88-0.91 (t, 6H), 0.83-0.86 (t, 12H). ^{13}C NMR (101 MHz, CDCl_3) δ 189.08, 188.95, 188.55, 187.71, 183.30, 147.91, 147.83, 145.93, 143.50, 143.33, 140.21, 139.79, 139.59, 138.21, 136.77, 135.16, 133.67, 132.44, 127.96, 126.66, 125.49, 123.24, 123.22, 122.42, 122.35, 121.79, 121.66, 119.06, 118.67, 40.14, 34.80, 33.45, 32.01, 31.96, 30.17, 29.83, 29.80, 29.75, 29.72, 29.44, 29.41, 28.88, 26.77, 22.79, 22.72, 14.21, 14.15.

Se-2

The procedure of the synthesis is the same with compound Se-1. The product was given as a dark solid with a yield of 40%. MALDI-TOF MS calcd for $\text{C}_{122}\text{H}_{152}\text{F}_2\text{O}_4\text{S}_8\text{Se}_2$ 2134.8 found 2134.9, ^1H NMR (400 MHz, CDCl_3): 7.73-7.74 (m, 4H), 7.64 (m, 2H), 7.54 (m, 2H), 7.38 (m, 2H), 7.31(m, 2H), 6.97-7.0 (m,4H), 2.98-3.0 (t, 4H), 2.77-2.78 (t, 4H), 1.87(m, 2H), 1.74 (m, 2H), 1.24-1.49(m, 104), 0.83-0.91 (m, 18H). ^{13}C NMR (101 MHz, CDCl_3) δ 188.83, 186.84, 186.63, 184.46, 145.68, 143.44, 142.20, 141.88, 140.37, 140.01, 139.18, 138.81, 138.38, 137.18, 136.37, 135.89, 134.59, 127.84, 125.44, 122.91, 121.46, 121.30, 119.22, 116.80, 40.13, 34.87, 33.55, 31.99, 31.96, 30.27, 30.04, 29.90, 29.86, 29.82, 29.80, 29.74, 29.55, 29.47, 29.43, 28.49, 26.85, 22.78, 22.74, 22.72, 14.24, 14.16.

Supplementary Figures

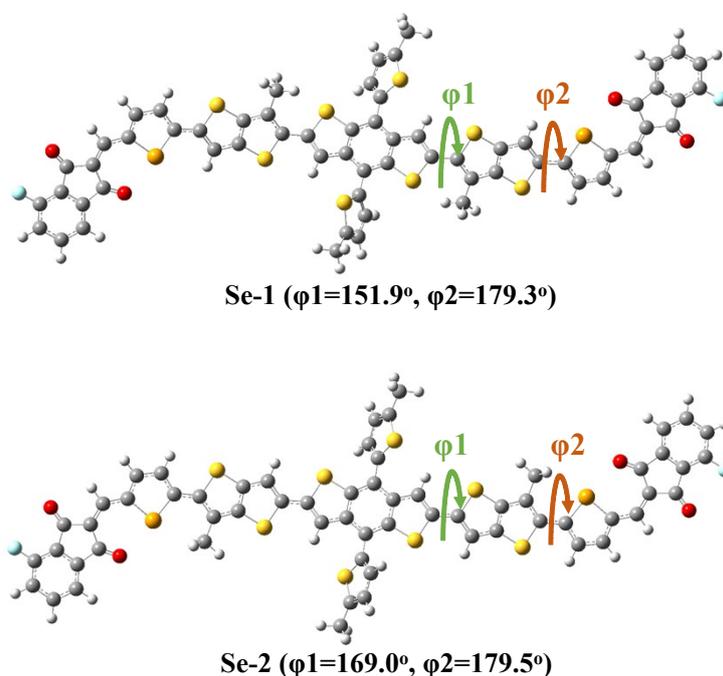


Fig. S1 Optimized structure of the two small molecules calculated by DFT

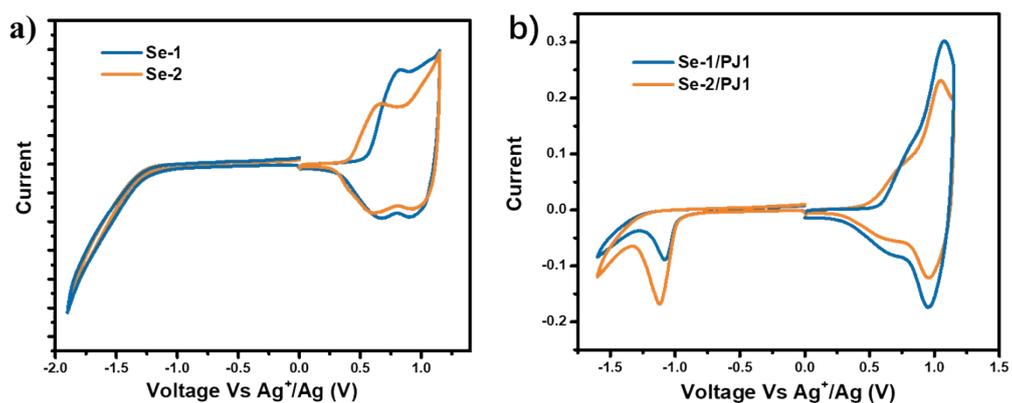


Fig. S2 a) CV curves of the pristine films b) CV curves of the blend films

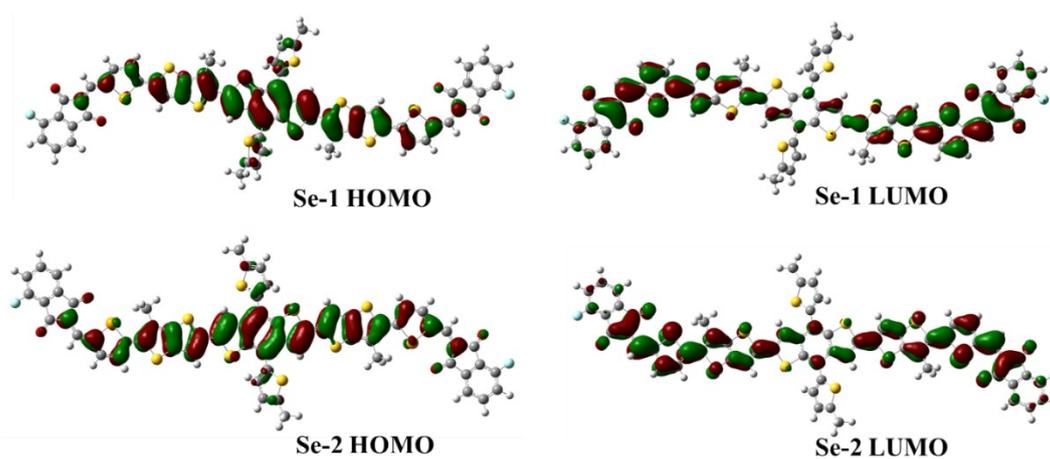


Fig. S3 Calculated HOMO and LUMO orbitals

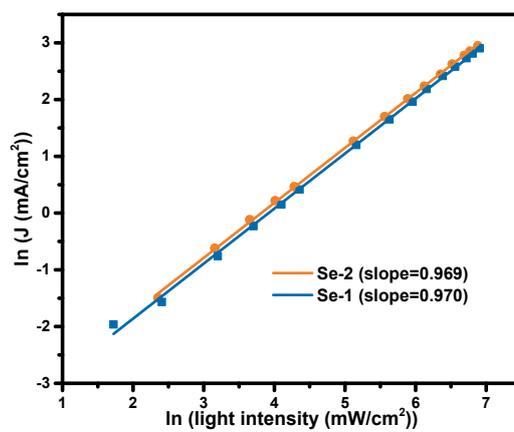


Fig. S4 a) J_{sc} variation with light intensity

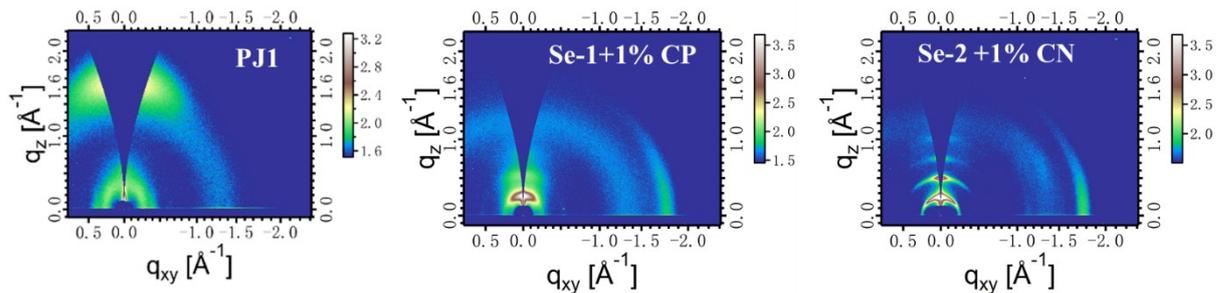


Fig. S5 2-D GIWAXs images for two small molecules with additives and pristine PJ1

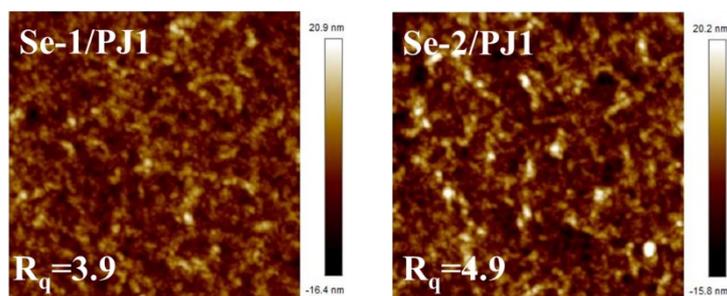


Fig. S6 AFM height images of optimized Se-1/PJ1 and Se-2/PJ1 blend at area of 5 $\mu\text{m} \times 5 \mu\text{m}$

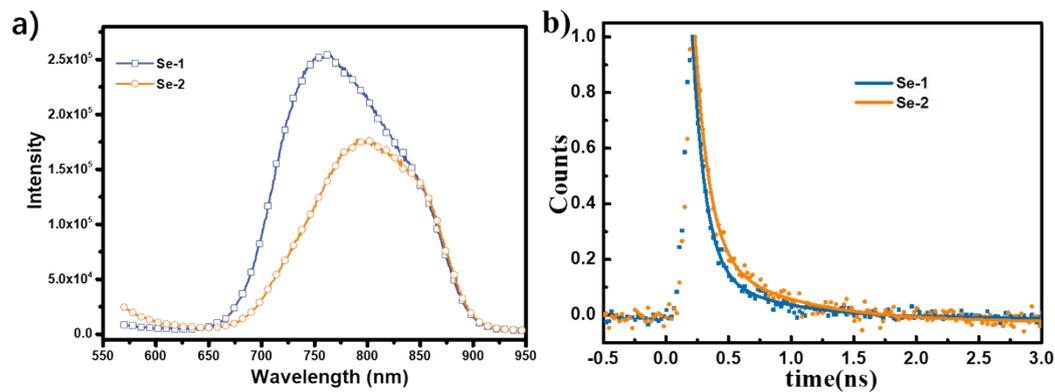


Fig. S7 a) PL spectrum of two small molecules in pristine films; b) TPRL spectrum according to figure a.

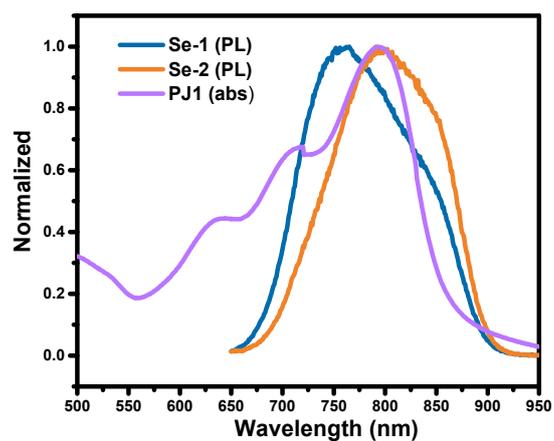


Fig. S8 Normalized PL spectrum of the two small molecules and normalized absorption spectrum of polymer acceptor

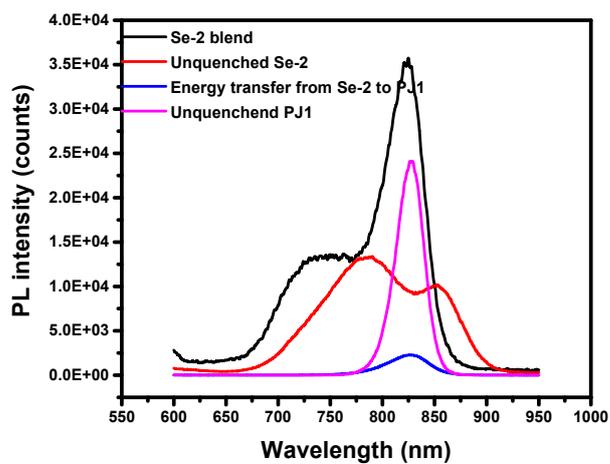
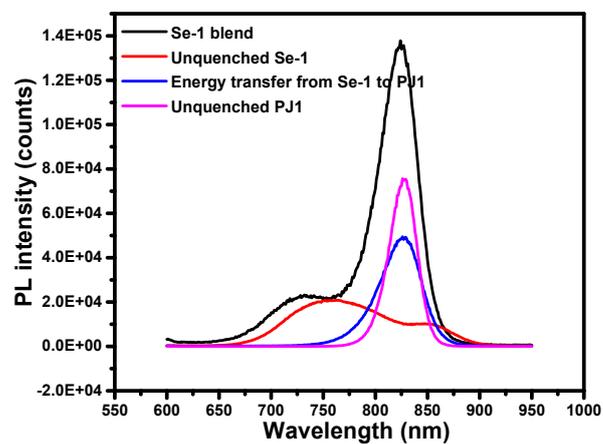


Figure S9 Blend PL spectrum and its corresponding fitted spectrum

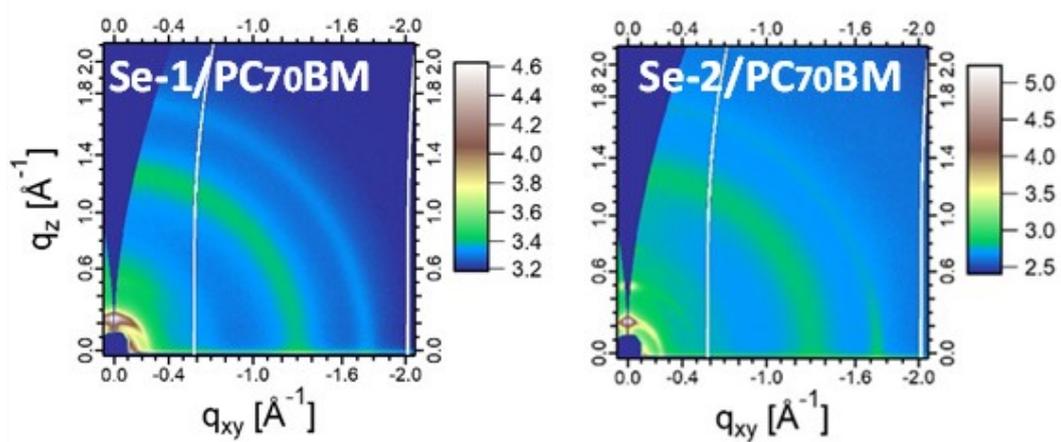


Fig. S10 2-D GIWAXS images for the optimized small molecules blends based on PC₇₀BM as acceptor

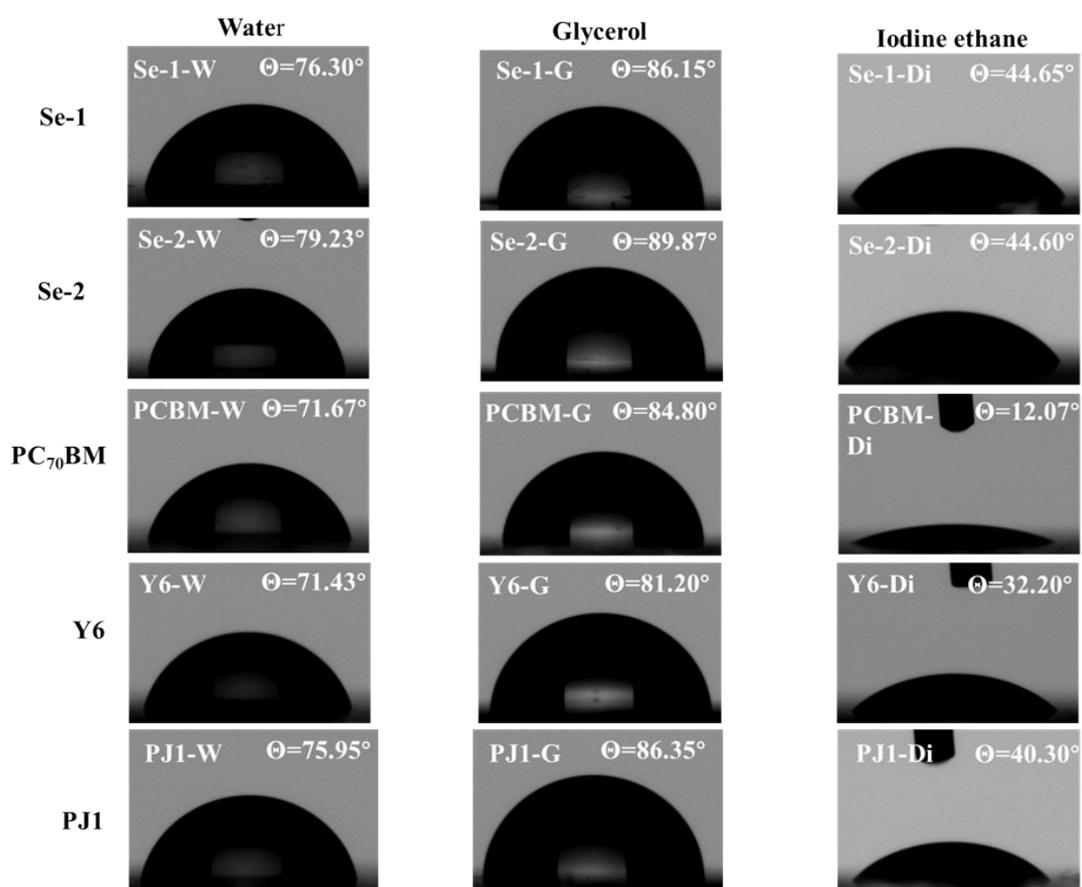


Fig. S11 Contact angle of the donors and acceptors

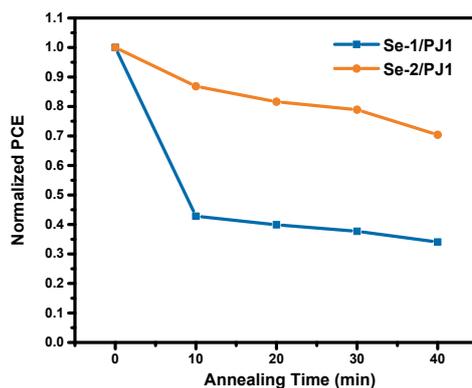


Fig.12 Thermal stability for devices annealing at 150°C

Supplementary Tables

Table S1 Summary of detailed parameters of molecular properties

Materials	Pristine					Blend	
	HOMO _{cv} (eV)	LUMO _{cv} (eV)	HOMO _{cal} (eV)	LUMO _{cal} (eV)	$\epsilon_{\text{film,max}}$ (cm ⁻¹)	HOMO (eV)	LUMO (eV)
Se-1	-5.27	-3.40	-5.10	-2.91	9.00×10^4	-5.30	-3.73
Se-2	-5.11	-3.44	-5.09	-2.92	9.94×10^4	-5.19	-3.73
PJ1	-5.46	-3.78					

Table S2 Detailed device optimization for Se-1/PJ1 blends

ratio	TA (°C)	Concentration (mg/ml)	Additives	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE (%)
1.75:1	None	14	0.4%CN	0.840	14.10	56.84	6.73
1.75:1	None	14	0.4% CP	0.866	16.73	54.97	7.96
1.75:1	None	14	None	0.860	16.12	54.44	7.55
1.75:1	80	14	0.4% CP	0.892	14.52	42.43	5.5
1.75:1	None	14	0.8% CP	0.855	16.89	55.90	8.07
1.75:1	None	14	1.2% CP	0.852	17.12	57.71	8.42
1.5:1	None	14	1% CP	0.846	17.26	60.66	8.85
1.75:1	None	14	1% CP	0.841	18.60	59.90	9.37
2:1	None	14	1% CP	0.840	17.10	61.33	8.81
1.75:1	None	14.5	1% CP	0.838	18.86	59.16	9.35
1.75:1	None	13.5	1% CP	0.843	17.79	60.26	9.04

Table S3 Detailed device optimization for Se-2/PJ1 blends

Ratio	TA (°C)	Concentration (mg/ml)	Additives	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE (%)
1.75:1	None	14	None	0.871	17.69	48.67	7.50
1.75:1	None	14	0.4% CN	0.873	17.87	50.85	7.94
1.75:1	80	14	0.4% CN	0.864	18.37	51.93	8.25
1.75:1	100	14	0.4% CN	0.863	20.05	52.11	9.01
1.75:1	120	14	0.4% CN	0.832	19.41	45.07	7.29
1.5:1	100	14	0.4% CN	0.876	18.21	57.02	8.96
2:1	100	14	0.4% CN	0.860	18.00	57.33	8.94
1.75:1	100	14	0.8% CN	0.878	18.44	56.14	9.09
1.75:1	90	14	0.8% CN	0.876	18.32	55.39	8.89
1.75:1	110	14	0.8% CN	0.878	18.26	56.72	9.05
1.75:1	100	14	1.2% CN	0.878	18.70	58.12	9.53
1.75:1	100	14	1% CN	0.869	18.83	59.07	9.69
1.75:1	100	14.5	1% CN	0.867	19.42	61.24	10.32
1.75:1	100	15	1% CN	0.869	19.36	59.79	10.05

Table S4 Detailed data calculated from 1-D GIWAXS

Materials	OP						IP			
	Donor				PJ1		Donor			
	D	CCL	D	CCL	D	CCL	D	CCL	D	CCL
	(100)	(100)	(010)	(010)	(010)	(010)	(100)	(100)	(010)	(010)
Se-1-S	23.7	125.0	/	/	/	/	27.7	44.2	3.53	40.9
Se-2-S	25.4	199.2	/	/	/	/	25.3	174.8	3.54	48.7
PJ1	/	/	/	/	3.89	19.6	/	/	/	/
Se-1-B	23.4	102.0	/	/	3.79	21.8	24.8	59.68	3.53	30.0
Se-2-B	25.2	146.8	3.55	42.8	3.88	17.3	25.6	158.15	3.52	28.2

Table S5 Lifetime fitted from TPRL spectrum based pristine films

	τ_1 (ps)	error	τ_2 (ps)	error	Averaged (ps)
Se-1	103 (94.8%)	4.2	588 (5.2%)	57.6	128
Se-2	117 (94.3%)	7.2	703 (5.7%)	76.0	150

Table S6 Fitted detailed data from blend PL spectrum

	Δ LUMO (eV)	η ED	η En	Δ HOMO (eV)	η EA
Se-1	0.28	0.699	0.21	0.16	0.563
Se-2	0.3	0.914	0.01	0.27	0.833

Table S7 Optimized device performance based on PC₇₀BM as acceptor with a device

Structure of ITO/ZnO/Active layer/MoOx/Ag

Donors	Condition	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE (%)
Se-1	0.6% CP	0.889	13.37	75.33	8.96
Se-2	0.4% CN	0.791	10.97	59.50	5.16

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